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RETENTION INDICES, RELATIVE RESPONSE FACTORS, AND MASS
SPECTRA OF TRIFLUOROETHYL AND HEPTAFLUOROBUTYL ESTERS
OF CARBOXYLIC ACIDS DETERMINED BY CAPILLARY GC/MS

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ABSTRACT

The GC/MS characteristics of carboxylic acid esters prepared from fluorine-containing alcohols were compared to those of methyl esters. The GC retention of 2,2,2-trifluoroethyl (TFE) esters was less than, and 2,2,3,3,4,4,4-heptafluoro-1-butyl (HFB) esters approximately equivalent to that of methyl esters. The peak shape of both TFE and HFB esters was slightly superior to that of methyl esters. Mass spectra of TFE and HFB aliphatic esters show significantly more intense molecular and key fragment ions than those of methyl esters. Also, owing to their significantly higher molecular weights, TFE or HFB ester molecular ions and most fragment ions of interest occur at significantly higher m/z values than most potential interfering ions.

The GC retention indices, relative GC/MS total ion current response factors, and 70 ev electron impact mass spectra of about 70 TFE and 70 HFB carboxylic acid esters are reported. Results from analysis of a TFE/HFB esterified petroleum carboxylic acid concentrate are discussed in detail.

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INTRODUCTION

Prior work in this laboratory led to the development of a quantitative procedure for combined acylation of hydroxyl groups and esterification of carboxyl groups in petroleum fractions. Initially, this reaction was employed in conjunction with an infrared (IR) method for determination of total OH/COOH content (1,2)*. Derivatization prior to IR analysis improved sensitivity, decreased interferences, and lessened the structural dependence of IR response for the respective groups. Subsequent work showed that trifluoracetylation also provided significant advantages in GC/MS analysis of individual phenolic-type compounds (3). Improved GC resolution and more reliable compound identification via mass spectral matching/interpretation were achieved after trifluoracetylation.

A logical extension of the above work was the evaluation of the GC/MS properties of the carboxylic acid esters produced in the combined acylation/esterification reaction. Alcohols used in the reaction have the general formula: $\text{HOCH}_2(\text{CF}_2)_x\text{CF}_3$. Esterification with fluorinated alcohols has been employed previously in MS analysis of petroleum carboxylic acids (4-8). Several novel carboxylic species were identified, and analytical advantages, such as reduced interference from noncarboxylic types, were noted. However, mass spectra of relatively few (ca. 10) compounds were published in that work. Also, other analytical aspects such as their GC behavior, GC/MS response factors, and GC/MS performance relative to nonfluorinated esters were not addressed. These and other relevant GC/MS characteristics of 2,2,2-trifluoroethyl and 2,2,3,3,4,4,4-heptafluoro-1-butyl esters are the main focus of this report.

Interest in petroleum carboxylic acids arises from the geochemical significance of selected types (e.g., isoprenoid, terpenoid, steroid), their surfactant and lubricating properties, direct commercial use in paints and other products, and their presence in production and refinery waste waters (9). In finished fuels, they are of concern because they increase water solubility and catalyze reactions leading to gum and sediment formation (9,10). As a result, they have been the subject of extensive research over

*Underlined numbers in parentheses refer to references at the end of this report.

the last 100+ years (7,11). Early work was performed via classical methods involving isolation and identification via physical properties; recent work has relied heavily on MS and GC/MS techniques. A typical modern analysis scheme involves extraction or chromatographic isolation of the acids, formation of methyl esters, purification, and analysis via GC/MS and/or high resolution MS (12-18). Because of the widespread practice of analyzing carboxylic acids as their methyl esters, their GC/MS characteristics are compared here with those of the fluorinated alcohol esters.

Direct (without esterification) analysis of carboxylic acids has been reported in conjunction with chemical ionization (19) and fast atom bombardment (20) MS modes. The main problems with this approach stem from the lack of structural information in spectra obtained from these ionization modes and the difficulties in obtaining acceptable gas chromatograms of free carboxylic acids. For example, experience in this laboratory with direct determination of acetic, propionic and C_4 -acids in brines, using capillary columns specifically designed for this purpose, has shown the need for coinjection of oxalic acid to prevent adsorptive losses on GC inlet and other surfaces (21). Also, the upper temperature limits of the available free acid GC columns are typically near 250° C, which limits their application to acids with ca. 14 carbon atoms or less.

The objectives of the work were to: 1) compare the merits of fluorinated vs. nonfluorinated esters in GC/MS analysis of petroleum carboxylic acids and 2) if warranted, acquire a data base sufficient for interpretation of GC/MS results obtained on fluorinated alcohol esters of carboxylic acids. Prior methodology for isolation of carboxylic acid concentrates and preparation of esters was used without modification.

EXPERIMENTAL

Materials

Individual carboxylic acids were obtained commercially (largely from Aldrich Chemical, Milwaukee, WI) and were used without further purification. The carboxylic acid concentrate used in the evaluation of GC/MS characteristics of the esters was isolated via HPLC subfractionation of a whole acid fraction obtained via nonaqueous ion exchange LC. Both separation methods are

described in detail elsewhere (9,22,23). A straight-run 472-649° F distillate (NIPER No. 2415) obtained from a Texas refinery served as the starting material for the separations. Its selection was based on its high-acid neutralization number (0.355 mg KOH/g) and low-sulfur content (0.17 wt %). The yield of the carboxylic acid concentrate was 0.21 wt %. Its IR spectrum and non-aqueous titration assay (9) indicated a carboxylic acid content of nearly 100% and an average molecular weight of 300. Back calculation of the neutralization number for the whole distillate, based on the yield and average molecular weight of the concentrate, gave 0.39 mg KOH/g, which is in reasonable agreement with the result cited above.

Materials used in the esterification and GC/MS steps were specified earlier (1-3,24).

Esterification with Fluoroalcohols

Except where hydroxyl groups were known or suspected to be present, the acylation step of the combined acylation/esterification reaction was typically omitted. The procedure for the complete reaction may be found elsewhere (1,2); the esterification procedure is reproduced below for the reader's convenience.

A known weight of material, typically 5-10 mg, was added to 1 mL of 9:1 (V/V) trifluoroacetic anhydride-2,2,2-trifluoroethanol (or trifluoroacetic anhydride-2,2,3,3,4,4,4-heptafluorobutanol). Esterification was accomplished by heating this mixture in a 5 mL reaction vial to 60° C for ca. 15 minutes. The resulting product was diluted with 4 mL dichloromethane. Excess reagents and trifluoroacetic acid produced as a by-product were removed via extraction with 20 mL of aqueous 0.167 M Na_2HPO_4 - 0.083 M NaH_2PO_4 buffer. The extraction process was repeated to ensure complete removal, and the resulting dichloromethane solution was dried by passing it through a 4-mL cartridge of anhydrous Na_2SO_4 . Quantitative elution from the cartridge was effected by flushing it with an additional 5-10 mL of dichloromethane. The purified product was taken to near dryness under a stream of nitrogen and diluted to obtain nominal concentrations of 5 ng/ μl per component. GC injection volumes were typically 0.2 μl .

Formation of Methyl Esters

Methyl esters were prepared using N,N-dimethylformamide dimethylacetal after the procedure of Thenot et al. (24).

GC/MS

Conditions and instrumentation used for GC/MS were the same as those employed in analysis of trifluoroacetyl esters of phenolic compounds (3). A brief summary is given below:

MS - Kratos MS-80 with DS-55 Data System

Ionization - 70 ev electron impact

Dynamic resolution - 1000

Scan rate - 0.5 sec/decade, 0.4 sec interscan time

Source pressure - 5×10^{-6} torr

Source temperature - 300° C

GC/MS interface - direct (310° C)

GC - Carlo Erba M 4662

Injector - Hewlett-Packard cool on-column

Column - Quadrex 100 m x 0.25 mm ID, 0.5 μ m film thickness, 007 - series
methylsilicone-bonded fused silica

Carrier gas - He, 1 mL/min

Temperature program - 50° C (initial, 2 min hold), 8° C/min to 70° C,
2° C/min to 320° C (10 min hold).

Kratos software was used to average three spectra over each GC peak and further average spectra from corresponding peaks from three or four replicate runs to obtain the reference spectra reported in the appendices. Spectral subtraction routines were also used to correct for background from column bleed and, especially for spectra obtained from petroleum samples, interfering components.

Calculation of Retention Indices and Relative Response Factors

Because of the need for intercomparison of GC retention characteristics of the various types of esters, an independent indexing system was employed. Retention indices (RI) were based on the retention of trifluoroacetyl derivatives of 4-fluorophenol, 1-naphthol, and 9-phenanthrol (RI = 100, 200 and 300, respectively) as shown below:

$$RI = 100 \times \left[1 + \frac{t_{R(x)} - t_{R(4\text{-fluorophenol})}}{t_{R(1\text{-naphthol})} - t_{R(4\text{-fluorophenol})}} \right] \quad (1)$$

$$RI = 100 \times \left[2 + \frac{t_{R(x)} - t_{R(1\text{-naphthol})}}{t_{R(9\text{-phenanthrol})} - t_{R(1\text{-naphthol})}} \right] \quad (2)$$

t_R = retention time (sec)

$t_{R(x)}$ = carboxylic acid ester retention time

Retention indices of carboxylic acid esters eluting before the trifluoroacetyl derivative of 1-naphthol were calculated according to equation 1; those eluting after were calculated using equation 2. Frequently, straight-chain carboxylic acids with indices determined as above were used in turn as internal standards for calculation of indices of other acid esters. These "second generation" indices carried a slightly higher uncertainty than those based directly on the trifluoroacetate derivatives, but were adequate for the purpose. The above RI system is identical to that used in conjunction with GC/MS analysis of trifluoroacetyl derivatives of phenolic compounds (3). This system has the advantages of convenience and improved reproducibility over alternate indexing approaches, including the conventional one based on *n*-paraffins. In particular, a uniform indexing system for both trifluoroacetyl derivatives and carboxylic esters is essential for analysis of samples containing both phenolic and carboxylic types.

Relative GC/MS total ion current (TIC) response factors (RF) were calculated as follows:

$$RF = (A_x/A_s) \cdot (W_s/W_x),$$

where A = area or area percent, and W = weight or weight percent
 x = unknown, and s = standard (n-octanoic acid).

Since the response factors of a given ester series are based on that of the octanoic ester of that series, RF data from different ester series are not directly comparable.

RESULTS AND DISCUSSION

GC Aspects

Figures 1-3 compare GC chromatograms of free acids and methyl, ethyl, 2,2,2-trifluoroethyl (TFE), and 2,2,3,3,4,4,4-heptafluoro-1-butyl (HFB) esters of straight chain carboxylic acids up to eicosanoic acid (C₂₀).

The adsorptive properties of free acids are quite evident from the excessively wide peaks observed and their decreasing height with increasing carbon number (acids $\geq C_{16}$ faded into the baseline). As mentioned in the Introduction, adequate resolution of free carboxylic acids requires use of special GC columns and techniques.

All types of esters exhibited acceptable chromatographic behavior. However, methyl and ethyl ester peaks showed perceptible tailing, which was absent in the chromatograms of TFE and HFB esters. For a given straight chain acid, variation among retention times of different types of esters was relatively small -- typically less than or equal to the difference in retention of the next higher or lower carbon number acid. For acids with carbon numbers ≥ 16 , retention among types of esters increased in the following order TFE < HFB ~ methyl < ethyl. This trend in apparent volatility differs markedly from the order of molecular weights for each ester group: methyl (31), ethyl (45), TFE (99) and HFB (199).

Comparative data for the different esters indicate that the retention effect of a -CF₃ group is slightly negative (decreases retention); a -CF₂- group exerts a zero to very slightly positive influence; while a methylene group increases retention to approximately the same degree regardless of

FIGURE 1. - TIC chromatograms of free acids versus TFE esters for a synthetic blend of straight chain alkanolic acids (C₁₆-C₂₀ acids were not detected in (A)). Peaks A-C in (B) are trifluoroacetyl esters of 4-fluorophenol, 1-naphthol and 9-phenanthrol, respectively.

FIGURE 2. - TIC chromatograms of methyl, ethyl and TFE esters of straight chain alkanic acids. Note the greater volatility and lack of peak tailing for TFE esters. Peaks A-C as in figure 1.

FIGURE 3. - TIC chromatograms of TFE versus HFB esters of straight chain alkanolic acids. Peaks A-C as in figure 1.

whether it is introduced into the carboxyl or alcohol portion of the ester molecule. The negligible effect on GC retention of CF_2 groups in the alcoholic portion of the ester group allows the optimization of fluorinated ester structure to be based largely on MS characteristics.

Table 1 summarizes GC retention indices calculated (see Experimental) for TFE and HFB esters of straight chain and a variety of other types of carboxylic acids. In most cases, the tabulated results represent averages of at least four independent determinations obtained from GC/MS analysis of blends containing 10-20 esterified components. However, data obtained from analysis of the petroleum fraction (see Experimental) reflect single or duplicate determinations. As evident from the standard deviations shown, indices for either type of ester were typically reproducible within one part per thousand. In general, reproducibility was slightly better for TFE than for HFB esters.

Differences in retention between TFE and HFB esters of branched chain, cyclic and aromatic acids were similar to those of straight chain acids noted earlier. Although relatively small throughout, the retention difference ($\Delta\text{RI} = \text{RI}_{\text{HFB}} - \text{RI}_{\text{TFE}}$) clearly diminishes with the increasing molecular weight of the parent acid. Figure 4 shows the relationship between ΔRI and parent acid carbon number. In general, the impact of any structural feature on GC retention decreases with increasing carbon number. This holds true for HFB versus TFE esters as well as for the addition of methylene groups within any of the ester series. The diminishing impact of methylene groups is clearly evident in the progressively closer spacing of consecutive straight chain ester homologs with increasing carbon number in figures 1-3.

For a given carbon number, retention of branched chain acid esters decreases with the number of branches and the proximity of the branch to the ester group. For example 2-, 3-, and 4-methylpentanoic acid esters elute in that order, and 2,3-dimethylbutyric acid esters elute before the corresponding 2-methylpentanoic acid ester. The effect of phenyl substituents on alkanolic acid esters is analogous to that of chain branching, but larger in magnitude. For example, 2-, 3-, and 4-phenylbutyric acid esters elute over a wide retention range. Equivalent alkyl-substituted aromatic acids elute in the order $\text{o} < \text{m} < \text{p}$. 1-Naphthoic acid esters elute before the corresponding 2-naphthoic acid ester.

TABLE 1. - GC retention indices and relative TIC response of fluoroalcohol esters

Parent Acid			2,2,2-Trifluoroethyl Ester				2,2,3,3,4,4,4-Heptafluorobutyl Ester			
Z-Series	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	MW	GC Retention Index ¹	Relative TIC Response ²	
0(0 ₂)	88	Butyric Acid	C ₄ H ₈ O ₂	170	76.05±0.20	0.72±0.23	270	83.37±0.04	0.77±0.05	
0(0 ₂)	102	Trimethylacetic Acid	C ₅ H ₁₀ O ₂	184	74.86±0.08	0.47±0.21	284	81.95±0.18	0.56±0.12	
0(0 ₂)	102	2-Methylbutyric Acid	C ₅ H ₁₀ O ₂	184	82.72±0.03	0.78±0.05	284	91.71±0.02	0.96±0.05	
0(0 ₂)	102	Pentanoic Acid	C ₅ H ₁₀ O ₂	184	89.85±0.12	0.73±0.08	284	103.49±0.07	0.84±0.04	
0(0 ₂)	116	2,2-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	198	89.02±0.05	0.84±0.04	298	99.48±0.02	0.92±0.02	
0(0 ₂)	116	2,3-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	198	93.91±0.11	0.47±0.03	298	104.76±0.03	0.55±0.04	
0(0 ₂)	116	2-Ethylbutyric Acid	C ₆ H ₁₂ O ₂	198	95.56±0.08	0.60	298	107.11±0.47	0.83±0.02	
0(0 ₂)	116	3,3-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	198	89.97±0.08	0.63±0.06	298	100.24±0.10	0.85±0.08	
0(0 ₂)	116	2-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	96.55±0.06	0.95±0.06	298	107.82±0.03	0.98±0.05	
0(0 ₂)	116	3-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	100.15±0.21	0.80±0.09	298	111.70±0.03	0.77±0.12	
0(0 ₂)	116	4-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	100.69±0.03	0.81±0.03	298	112.62±0.04	0.94±0.14	
0(0 ₂)	116	Hexanoic Acid	C ₆ H ₁₂ O ₂	198	107.40±0.04	0.82±0.08	298	122.17±0.04	0.90±0.05	
0(0 ₂)	130	2-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	212	114.50±0.06	0.97±0.05	312	127.25±0.02	0.97±0.04	
0(0 ₂)	130	5-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	212	119.79±0.08	0.67±0.03	312	133.21±0.04	0.72±0.05	
0(0 ₂)	130	Heptanoic Acid	C ₇ H ₁₄ O ₂	212	127.38±0.04	0.92±0.05	312	142.22±0.05	0.95±0.03	
0(0 ₂)	144	Octanoic Acid	C ₈ H ₁₆ O ₂	226	145.31±0.07	1.000	326	162.36±0.04	1.000	
0(0 ₂)	158	Nonanoic Acid	C ₉ H ₁₈ O ₂	240	169.00±0.02	1.02±0.04	340	181.87±0.03	1.02±0.04	
0(0 ₂)	172	Decanoic Acid	C ₁₀ H ₂₀ O ₂	254	188.90±0.03	1.17±0.08	354	200.50±0.05	1.06±0.09	
0(0 ₂)	186	Undecanoic Acid	C ₁₁ H ₂₂ O ₂	268	208.14±0.04	1.09±0.12	368	219.14±0.04	1.01±0.08	
0(0 ₂)	200	Dodecanoic Acid	C ₁₂ H ₂₄ O ₂	282	227.41±0.04	1.24±0.10	382	237.03±0.04	1.14±0.09	
0(0 ₂)	214	Tridecanoic Acid	C ₁₃ H ₂₆ O ₂	296	245.12±0.08	1.25±0.11	396	253.94±0.04	1.13±0.10	
0(0 ₂)	228	2,6,10-Trimethylundecanoic Acid ³	C ₁₄ H ₂₈ O ₂	310	233.64±0.05	-	410	241.87	-	
0(0 ₂)	228	Tetradecanoic Acid	C ₁₄ H ₂₈ O ₂	310	262.22±0.09	1.33±0.11	410	270.12±0.06	1.21±0.11	
0(0 ₂)	242	3,7,11-Trimethyltridecanoic Acid ³	C ₁₅ H ₃₀ O ₂	324	252.53±0.03	-	424	259.91	-	
0(0 ₂)	242	Pentadecanoic Acid ³	C ₁₅ H ₃₀ O ₂	324	278.48±0.02	-	424	285.56	-	
0(0 ₂)	256	4,8,12-Trimethyltridecanoic Acid ³	C ₁₆ H ₃₂ O ₂	338	270.20±0.05	-	438	276.85	-	
0(0 ₂)	256	Hexadecanoic Acid	C ₁₆ H ₃₂ O ₂	338	293.94±0.06	1.29±0.11	438	300.29±0.07	1.19±0.09	
0(0 ₂)	270	5,9,13-Trimethyltetradecanoic Acid ³	C ₁₇ H ₃₄ O ₂	352	285.50±0.05	-	452	291.72	-	
0(0 ₂)	270	Heptadecanoic Acid	C ₁₇ H ₃₄ O ₂	352	308.81±0.14	1.57±0.28	452	314.42±0.07	1.24±0.13	
0(0 ₂)	284	Octadecanoic Acid	C ₁₈ H ₃₆ O ₂	366	323.02±0.15	1.51±0.13	466	328.06±0.08	1.32±0.15	
0(0 ₂)	298	2,6,10,14-Tetraethylpentadecanoic Acid ³	C ₁₉ H ₃₈ O ₂	380	303.89±0.14	-	480	308.37	-	

TABLE 1. - GC retention indices and relative TIC response of fluoroalcohol esters (Continued)

Parent Acid			2,2,2-Trifluoroethyl Ester				2,2,3,3,4,4,4-Heptafluorobutyl Ester			
Z-Series	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	MW	GC Retention Index ¹	Relative TIC Response ²	Relative TIC Response ²
0(0 ₂)	298	Nonadecanoic Acid	C ₁₉ H ₃₈ O ₂	380	336.61±0.15	1.51±0.14	480	341.06±0.07	1.31±0.19	
0(0 ₂)	312	3,7,11,15-Tetramethyl-hexadecanoic Acid ³	C ₂₀ H ₄₀ O ₂	394	319.32±0.05	-	494	323.32	-	
0(0 ₂)	312	Eicosanoic Acid	C ₂₀ H ₄₀ O ₂	394	349.68±0.19	1.55±0.15	494	353.63±0.12	1.35±0.21	
0(0 ₂)	326	Heicosanoic Acid ³	C ₂₁ H ₄₂ O ₂	408	362.34±0.03	-	508	365.73	-	
-2(0 ₂)	114	Cyclopentanecarboxylic Acid	C ₆ H ₁₀ O ₂	196	114.31±0.03	0.69±0.04	296	128.39±0.10	0.83±0.03	
-2(0 ₂)	128	Cyclohexanecarboxylic Acid	C ₇ H ₁₂ O ₂	210	134.59±0.05	0.96±0.01	310	149.59±0.02	0.95±0.05	
-2(0 ₂)	142	1-Methyl-1-cyclohexanecarboxylic Acid	C ₈ H ₁₄ O ₂	224	137.20±0.03	0.90±0.06	324	151.90±0.06	0.95±0.02	
-2(0 ₂)	156	3-Cyclohexylpropionic Acid	C ₉ H ₁₆ O ₂	238	178.69±0.04	1.07±0.07	338	191.49±0.04	1.05±0.04	
-2(0 ₂)	282	9-Octadecanoic Acid	C ₁₈ H ₃₄ O ₂	364	319.60±0.03	0.82±0.06	464	324.53±0.01	0.75±0.06	
-8(0 ₂)	122	Benzoic Acid	C ₇ H ₆ O ₂	204	139.16±0.06	0.58±0.02	304	154.76±0.11	0.52±0.04	
-8(0 ₂)	136	2-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	159.04±0.05	0.79±0.02	318	173.31±0.02	0.86±0.08	
-8(0 ₂)	136	3-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	161.64±0.06	0.76±0.02	318	175.81±0.08	0.75±0.03	
-8(0 ₂)	136	4-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	164.75±0.03	0.82±0.03	318	179.62±0.02	0.85±0.04	
-8(0 ₂)	136	Phenylacetic Acid	C ₈ H ₈ O ₂	218	155.80±0.02	0.90±0.04	318	169.40±0.03	0.97±0.05	
-8(0 ₂)	150	2,3-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	186.22±0.03	0.75±0.03	332	198.72±0.05	0.78±0.01	
-8(0 ₂)	150	2,6-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	171.99±0.02	0.82±0.02	332	183.23±0.01	0.86±0.12	
-8(0 ₂)	150	2-Ethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	173.09±0.04	0.81±0.05	332	185.83±0.04	0.77±0.03	
-8(0 ₂)	150	4-Methylphenylacetic Acid	C ₉ H ₁₀ O ₂	232	177.09±0.02	0.83±0.05	332	188.76±0.03	0.83±0.06	
-8(0 ₂)	164	2-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	177.97±0.06	0.91±0.06	346	188.76±0.03	0.92±0.05	
-8(0 ₂)	164	3-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	186.31±0.02	1.01±0.08	346	197.82±0.06	0.91±0.02	
-8(0 ₂)	164	4-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	200.83±0.04	0.99±0.02	346	212.38±0.09	1.02±0.02	
-8(0 ₂)	164	2,4,6-Trimethylbenzoic Acid	C ₁₀ H ₁₂ O ₂	246	194.59±0.06	0.85±0.06	346	204.28±0.05	0.89±0.19	
-8(0 ₂)	178	5-Phenylpentanoic Acid	C ₁₁ H ₁₄ O ₂	260	221.81±0.03	0.87±0.07	360	232.12±0.04	0.86±0.10	
-8(0 ₂)	220	4-Heptylbenzoic Acid	C ₁₄ H ₂₀ O ₂	302	276.94±0.05	0.79±0.10	402	285.01±0.05	0.75±0.15	
-10(0 ₂)	218	Cyclohexylphenylacetic Acid	C ₁₄ H ₁₈ O ₂	300	256.39±0.02	1.08±0.15	400	262.18±0.07	1.04±0.29	
-14(0 ₂)	172	1-Naphthoic Acid	C ₁₁ H ₈ O ₂	254	243.93±0.01	0.78±0.08	354	253.57±0.04	0.87±0.25	
-14(0 ₂)	172	2-Naphthoic Acid	C ₁₁ H ₈ O ₂	254	246.80±0.06	0.89±0.04	354	256.58±0.19	0.69±0.16	
-14(0 ₂)	186	1-Naphthylacetic Acid	C ₁₂ H ₁₀ O ₂	268	254.11±0.03	0.72±0.07	368	260.74±0.05	0.73±0.12	

TABLE 1. - GC retention indices and relative TIC response of fluoroalcohol esters (Continued)

Parent Acid				2,2,2-Trifluoroethyl Ester			2,2,3,3,4,4,4-Heptafluorobutyl Ester		
Z-Series	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	MW	GC Retention Index ¹	Relative TIC Response ²
-16(O ₂)	198	Biphenyl-2-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	280	249.98±0.03	0.89±0.13	380	255.75±0.04	0.90±0.23
-16(O ₂)	198	Biphenyl-4-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	280	280.78±0.07	0.83±0.05	380	289.68±0.17	0.66±0.14
-16(O ₂)	226	2,2,-Diphenylpropionic Acid	C ₁₅ H ₁₄ O ₂	308	266.54±0.08	0.75±0.14	408	271.80±0.06	0.49±0.05
-16(O ₂)	240	1,2,3,4-Tetrahydro-4-phenanthreneacetic Acid	C ₁₆ H ₁₆ O ₂	322	327.98±0.05	0.51	422	332.73±0.04	0.54
-18(O ₂)	210	1-Fluorene-carboxylic Acid	C ₁₄ H ₁₀ O ₂	292	307.62±0.05	0.78±0.09	392	314.09±0.03	0.59±0.08
-20(O ₂)	222	Anthracene-9-Carboxylic Acid	C ₁₅ H ₁₀ O ₂	304	327.82±0.01	0.75±0.02	404	329.19±0.04	0.51±0.08
-20(O ₂)	222	9-Phenanthroic Acid	C ₁₅ H ₁₀ O ₂	304	335.04±0.06	0.44	404	339.05±0.00	0.40
-8(O ₃)	138	2-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	316	169.98±0.19	0.64±0.17	416	181.19±0.33	0.56±0.03
-8(O ₃)	138	4-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	316	171.99±0.16	0.48	416	185.23±0.23	0.80±0.06
-18(O ₃)	226	9-Xanthanecarboxylic Acid	C ₁₄ H ₁₀ O ₃	308	282.57±0.03	0.38±0.03	408	286.12±0.09	0.26±0.13
-2(O ₄)	88	Malonic Acid	C ₃ H ₄ O ₄	268	101.16±0.16	0.75±0.04	-	-	-
-2(O ₄)	132	Dimethylmalonic Acid	C ₅ H ₈ O ₄	296	105.09±0.08	0.02±0.01	-	-	-
-2(O ₄)	118	Succinic Acid	C ₄ H ₆ O ₄	282	123.38±0.07	-	-	-	-

¹ Based on assigned indices of 100, 200 and 300 for trifluoroacetyl esters of 4-fluorophenol, 1-naphthol, and 9-phenanthrol, respectively. Uncertainties shown are standard deviations.

² Response of octanoic acid esters was assumed = 1.00. TIC = total ion current. Uncertainties shown are standard deviations.

³ From analysis of petroleum fractions. Other data from pure compounds.

Dash - Not available.

Figure 4. Difference in retention of HFB versus TFE esters (ΔRI) as a function of carboxylic acid carbon number ($C_{no.}$)

For branched chain aliphatic acids, a convenient means for expressing retention, besides retention index, is commonly referred to as "equivalent chain length" (ECL). ECL is calculated via linear interpolation of retention times or indices of bracketing straight chain alkanolic acids, with carbon numbers n and $n + 1$:

$$ECL = \frac{RI_x - RI_n}{RI_{n+1} - RI_n} + n = \frac{Rt_x - Rt_n}{Rt_{n+1} - Rt_n} + n \quad (3)$$

RI = retention index

Rt = retention time

n = carbon number of the straight chain alkanolic acid immediately preceding that of the branched acid ester, x . n does not include carbons in the alcohol portion of the ester group.

The main advantage of ECL is that it quantitatively describes elution of a given compound in relation to that of straight chain acids, which are usually present in samples containing appreciable quantities of branched chain acids. As with other retention parameters, ECL is dependent on GC experimental conditions, including the type of column used.

Table 2 shows ECL data calculated for isoprenoid acid esters identified in the petroleum carboxylic acid concentrate. The narrow range in ECL's for a given acid over all ester types indicates relatively consistent spacing of isoprenoid versus straight chain ester GC peaks in each case. As shown in figure 5, the general pattern of resolved GC peaks within the carboxylic acid concentrate is indeed similar for each ester type. However, minor differences in relative retention of less abundant components may be discerned from close inspection of the figure. Variations in relative intensities of peaks over each chromatogram reflect the dependence of TIC response on ester type.

Chain branching significantly reduces retention relative to that of the straight chain acid ester of equivalent carbon number. This effect is equally reflected by both RI and ECL data (tables 1 and 2), but is more easily visualized using the ECL parameter. For example, the isoprenoid acids with three methyl branches (carbon numbers 14-17, table 2) exhibit ECL's from 1.5-1.7 units lower than the corresponding straight chain homologs. ECL's of those

FIGURE 5. - TIC chromatograms of the petroleum carboxylic acid concentrate as methyl, HFB, and IFE esters. Peaks corresponding to isoprenoid (IPREN) and straight chain alkanolic acids are designated by carbon number (carbons in ester groups not included). Note the large hump of unresolved components in each case.

TABLE 2. - Equivalent chain lengths (ECL) of isoprenoid acid esters

Acid		Ester		
Name	Carbon Number	Methyl	TFE	HFB
2,6,10-Trimethylundecanoic acid	14	12.41 (12.19) ¹	12.35	12.29
3,7,11-Trimethyldodecanoic acid	15	13.45 (13.26)	13.43	13.37
4,8,12-Trimethyltridecanoic acid	16	14.54 (14.35)	14.49	14.44
5,9,13-Trimethyltetradecanoic acid	17	15.47 (15.28)	15.46	15.42
2,6,10,14-Tetramethylpentadecanoic acid	19	16.72 (16.41)	16.67	16.57
3,7,11,15-Tetramethylhexadecanoic acid	20	17.88 (17.50)	17.74	17.65

¹ Data obtained on an Apiezon L GC column by Douglas et al. (13).

with four methyl branches range from 2.2 to 2.4 below that of the corresponding straight chain homologs. ECL's of HFB esters with one methyl branch typically ranged from 0.76 (2-methyl), 0.66 (3-methyl), 0.57 (5-methyl), 0.35 (9- or 10-methyl) to 0.27 (11-13 methyl) lower than the corresponding straight chain homologs. Those with two methyl branches ranged from 0.9 to 1.3 ECL units below the corresponding straight chain homologs. Thus, the degree of branching in alkanolic esters of a given carbon number can be reliably assigned from ECL data, and the position of monomethyl branched esters can also be estimated. Alkanolic acids with ethyl- or longer chain branches were not detected in the carboxylic acid concentrate.

MS Aspects

Although their fragmentation patterns and mechanisms are generally identical, significant differences in relative intensities and mass to charge ratios (m/z) of corresponding fragment ions make interpretation and manipulation of spectra for fluorinated alcohol esters considerably easier and more informative from those of nonfluorinated esters.

Figures 6 and 7 compare mass spectra obtained from synthetic blends of straight chain acid esters (figure 2) with those from the carboxylic acid concentrate from the middle distillate (figure 5). Close matches were obtained between spectra from the acid concentrate versus pure compounds in all cases; however, the level of interfering ions (from the "hump" of unresolved components, see figure 5) in the acid concentrate spectra was significant. Although the level of interfering ions is essentially the same in TFE and methyl ester spectra, the TFE spectra are more definitive for two reasons: 1) the mass (m/z) of the molecular ion and the more diagnostic fragment ions extends well beyond the bulk of the interfering ions and 2) their relative intensities are also much greater than those of the interfering ions. The first point was further exaggerated in corresponding spectra for HFB esters, since each CF_2 group increases nominal mass by 50. The second point is quite significant because it results in improved detection limits, more reliable library matching of spectra, and more definitive selected ion plots.

Since both tridecanoic and heptadecanoic acids were prominent components of the carboxylic acid concentrate (figure 5), spectra of all types of esters were of sufficient clarity to enable their identification. However, even at their present concentrations, the intensity of diagnostic fragments (see fragmentation diagrams, figures 6 and 7) is generally only twice that of the interfering ions in methyl ester spectra, while typically an order of magnitude greater in the TFE ester spectra. Conservatively, for these compounds and all others examined, the level of a given compound required for reliable identification in actual petroleum samples was 10 times greater for methyl than for TFE or HFB esters.

Computer searching of prominent component spectra in the above sample turned up the correct library match for methyl esters in only about one in three cases. In most of the instances where incorrect matches were obtained, the computer apparently focused on interfering ions and/or was unable to locate characteristic fragments or the molecular ion needed to obtain the correct match. Spectra of TFE and HFB esters were not available in the commercial spectral library; those shown in the appendices have subsequently been entered as a special NIPER sublibrary.

FIGURE 6. - Mass spectra of methyl tridecanoate (A, C) and 2,2,2-trifluoroethyl tridecanoate (B, D). See origin of fragments shown in corresponding diagrams. The upper spectra (A, B) represent the pure components; the lower spectra (C, D) were obtained from analyses of the carboxylic acid concentrate.

FIGURE 7. - Mass spectra of methyl heptadecanoate (A, C) and 2,2,2-trifluoroethyl heptadecanoate (B, D). See origin of fragments shown in corresponding diagrams. The upper spectra (A, B) represent the pure components; the lower spectra (C, D) were obtained from analyses of the carboxylic acid concentrate.

Figure 8 compares selected ion current (SIC) chromatograms corresponding to McLafferty rearrangement (α -cleavage with δ -hydrogen transfer) ions for methyl (m/z 74), TFE (m/z 142), and HFB (m/z 242) esters. Even though the m/z 74 ion is typically the base peak in spectra for methyl esters of straight- and non- α -branched chain alkanolic acids (figures 6 and 7), a substantial hump of interfering ions is evident in that SIC chromatogram. The SIC chromatograms corresponding to TFE and HFB esters do not show a significant level of interference.

Given the level of interference observed in the m/z 74 methyl ester SIC chromatogram, it should come as no surprise that many SIC chromatograms of relatively weak methyl ester ions exhibited no discernable peaks. Figure 9 compares SIC chromatograms corresponding to methyl and TFE molecular ions for C_{13} and C_{17} alkanolic acids. The greater degree of information obtainable from the TFE ester plots is obvious from this and many other analogous comparisons.

The relatively strong molecular ions produced in spectra of TFE and HFB esters constitutes a significant advantage from the standpoint of mass spectral library matching and SIC plots. Figure 10 compares relative molecular ion intensity as a function of carbon number for straight chain alkanolic acids and four types of esters. Molecular ion intensity for esters generally increases in the order: methyl < ethyl < TFE ~ HFB. The increase in molecular ion intensity with carbon number, observed for all types of esters, parallels that of TIC response (table 1).

To further test the merits of TFE/HFB esters in analysis of the carboxylic acid concentrate, a variety of additional SIC chromatograms were generated and examined. Figures 11 (A-F) reproduce SIC chromatograms of HFB esters selected to illustrate the various methyl-branched alkanolic acids identified. Peaks corresponding to straight chain esters are also labeled on the figures to provide points of reference.

Table 3 shows fragmentation pathways and summarizes diagnostic fragment ions for methyl substitution at various positions on alkyl chains. As indicated in the table, fragments corresponding to cleavage at the point of methyl substitution are typically the most intense and most useful in determining the position of chain branching.

FIGURE 8. - SIC chromatograms corresponding to McLafferty rearrangement ions (see indicated m/z) for methyl, HFB and TFE esters of alkanolic acids in the petroleum concentrate. Straight chain acids are designated by carbon number. Note the greater level of interference for methyl compared to HFB or TFE ester plots.

FIGURE 9. - SIC chromatograms corresponding to molecular ions for methyl (A, B) and TFE (C, D) C_{13} (A, C) and C_{17} (B, D) alkanolic acids. Note the superior signal to noise for TFE esters. Straight chain acids are designated by carbon number.

FIGURE 10. - Molecular ion intensity (percent of base peak) as a function of carbon number for free acids and for TFE, HFB, ethyl, and methyl esters (TFEE, HFBE, EE, and ME, respectively).

FIGURE 11.A,B - SIC chromatograms of characteristic ions for various HFB alkanoids in the petroleum carboxylic acid concentrate. Straight chain and isoprenoid acids are designated by carbon number. Branched chain acids are designated by the position of the methyl group, or (where space permits) position plus the carbon number of the linear portion of the molecule. See text.

FIGURE 11.C,D - SIC chromatograms of characteristic ions for various HFB alkanolic acids in the petroleum carboxylic acid concentrate. Straight chain and isoprenoid acids are designated by carbon number. Branched chain acids are designated by the position of the methyl group, or (where space permits) position plus the carbon number of the linear portion of the molecule. See text.

FIGURE 11.E,F. - SIC chromatograms of characteristic ions for various HFB alkanolic acids in the petroleum carboxylic acid concentrate. Straight chain and isoprenoid acids are designated by carbon number. Branched chain acids are designated by the position of the methyl group, or (where space permits) position plus the carbon number of the linear portion of the molecule. See text.

TABLE 3. - Characteristic fragment ions for methyl-branched alkanolic acid esters¹

Substitution	Partial Fragmentation Scheme	Typical Order of Fragment Ion Intensities (m/z)	Most Characteristic Fragment Ion (m/z)
2-Methyl	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_\gamma\text{CH}_2\text{CH}(\text{CH}_3)\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow +\gamma\text{H } m/z \text{ 156} \\ \nearrow m/z \text{ 127} \\ \searrow m/z \text{ 189} \end{array} \end{array} $	156 >> 189 ~ 127	156
2,2-Dimethyl	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_{\gamma-1}\text{CH}_2\text{C}(\text{CH}_3)_2\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow +\gamma\text{H } m/z \text{ 170} \\ \nearrow m/z \text{ 127} \\ \searrow m/z \text{ 183} \end{array} \end{array} $	170 > 127 > 183	170
2,X-Dimethyl (X > 3)	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_{\gamma-1}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow m/z \text{ 189} \\ \nearrow m/z \text{ 127} \\ \searrow +\gamma\text{H } m/z \text{ 156} \end{array} \end{array} $	156 >> 189 > 127	156
3-Methyl	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_{\gamma-1}\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow m/z \text{ 189} \\ \nearrow +\gamma\text{H } m/z \text{ 142} \\ \searrow m/z \text{ 169} \end{array} \end{array} $	142 > 169	169
4-Methyl	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_{\gamma-2}\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow m/z \text{ 155} \\ \nearrow +\gamma\text{H } m/z \text{ 156} \\ \nearrow +\gamma\text{H } m/z \text{ 142} \\ \searrow m/z \text{ 183} \end{array} \end{array} $	155 > 142 > 156 > 183	155
5-Methyl	$ \begin{array}{c} \text{CH}_3(\text{CH}_2)_{\gamma-3}\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{COCH}_2\text{CF}_3 \\ \begin{array}{l} \nearrow m/z \text{ 189} \\ \nearrow +\gamma\text{H } m/z \text{ 142} \\ \nearrow m/z \text{ 155} \\ \searrow m/z \text{ 197} \end{array} \end{array} $	142 > 189 > 155 > 197	197

¹ TFE values shown; add 100 to all m/z of fragments for HFB esters.

Figures 11A and 11B compare SIC chromatograms of ions characteristic of alkanolic esters with (11B) and without (11A) 2-methyl branches. Since straight chain esters fall into the "without" category and are present at higher concentrations than any of the branched chain esters, they predominate in figure 11A. The two isoprenoid esters with 2-methyl substitution (see table 1) predominate in figure 11 B, but peaks corresponding to homologs with a single branch at the 2-position and two branches (one at the 2-position) are also apparent.

Figures 11C and 11D show SIC chromatograms of ions characteristics of alkanolic esters with 3-methyl substitution (11D) and without substitution at either the 2- or 3-positions (11C). Again, because of their relatively high concentration, the straight chain esters predominate in 11C. However, esters with single branches tentatively assigned to positions 9-12 are also apparent in the figure, along with the isoprenoid ester corresponding to 4,8,12-trimethyltridecanoic acid. The single-branched 3-methylalkanoic and isoprenoid esters with 3-methyl branches (see table 1) predominate in figure 11D. Minor peaks corresponding to esters with 2- and 10-methyl substituents are also present (indicated as "2" and "10" in the figure).

Elucidation of the precise location of methyl substituents occurring at carbons displaced by 4 or more from the carbonyl carbon becomes progressively more difficult because of the decreasing influence of the ester group on fragmentation. Thus, the assignments given for single-branched esters at positions 10 and 12 in figure 11F and 9-12 elsewhere are subject to much greater uncertainty than those for (2-5)-methyl esters. Partial justification for the given structural assignments is shown in figure 11E, which shows the relatively intense fragments observed at m/z 367. As noted in the figure, this ion corresponds to cleavage before and after the methyl-substituted carbon in the case of 12- and 10-methylalkanoic acid, respectively. However, other types of branched chain esters can also give rise to this fragment ion.

ECL (see GC discussion) data were also used in arriving at assignments of locations of methyl substituents far away from the ester group. However, some guesswork is involved in predicting this parameter for unknown isomers. Because ECL's of 2-methyl and terminal-methyl monosubstituted alkanolic acids are relatively consistent -- $X.24$ and $X.8$, respectively, where X = the number of linear chain carbons plus the carbonyl carbon -- the decimal portion of ECL

decreases slightly with increasing carbon number for substitution at any given position. For example, ECL's of 3-methyl- C_{12} , $-C_{14}$, and $-C_{16}$ HFB esters are 12.36, 14.34, and 16.33, respectively. Thus, some extrapolation would be required to predict the precise ECL's of higher 3-methyl homologs. Conceptually, this gradual decrease in ECL decimal with carbon number may be rationalized from either the need to "squeeze in" progressively more methyl isomers within the set retention boundaries of 2-methyl and terminal-methyl isomers, or from the shift in relative distance from the carbonyl versus terminal carbons for a given position with increasing chain length. It also follows that the difference between ECL's of consecutive eluting methyl isomers decreases with increasing carbon number as well as with increasing distance from the carbonyl carbon.

Aside from the difficulties in determining precise locations of branching far removed from the carbonyl carbon, the selected ion plots in figures 11A-F successfully detected and unequivocally identified all straight chain and the vast majority of branched chain alkanolic acids present, with minimal interference from other species. The consistent appearance of selected branched chain isomers at each carbon number demonstrated here has not, to the authors' knowledge, been reported previously. In all probability, this reflects the distinct MS advantages of fluorinated versus methyl esters in GC/MS analysis of carboxylic acids in petroleum or other complex sample types.

Figure 12 shows SIC chromatograms corresponding to molecular ions of benzoic acid (TFE ester) homologs containing up to three carbons in alkyl substituents. As indicated by the TIC chromatogram included in the figure, these species are all present at very low concentrations in the carboxylic acid concentrate. Examination of selected spectra and SIC chromatograms corresponding to characteristic fragments for this series revealed the presence of benzoic acid, all three methylbenzoic acid isomers (phenylacetic acid was not detected), most or all possible dimethylbenzoic acid isomers (other $C_9H_9O_2CH_2CF_3$ species including ethylbenzoic, methylphenylacetic, and phenylpropanoic acids were not detected), plus trimethyl- and perhaps other types of C_3 -benzoic acid isomers. Corresponding SIC chromatograms from analysis of methyl esters (not shown) were less well defined; for example, only the *p*-methylbenzoic acid isomer was evident in the SIC plot for m/z 150 ($C_8H_7O_2CH_3$).

FIGURE 12. - TIC chromatogram (top) versus SIC plots for TFE esters of benzoic (A), methylbenzoic (B), dimethylbenzoic (C) and C₃-benzoic acids (D). Note the low abundance of these compounds in the carboxylic acid concentrate and the absence of other potential isomers (e.g. phenylalkanoic acids).

Substitution of the ester group directly onto an aromatic nucleus is readily differentiated from substitution on an aliphatic side chain by MS fragmentation patterns. For example, figure 13 compares spectra of TFE methylbenzoic acid isomers with that of TFE phenylacetic acid. The most intense fragment (m/z 119) for the TFE methylbenzoic acids corresponds to loss of $-OCH_2CF_3$, which is typical whenever the ester group is attached to an aromatic ring. The tropylium ion (m/z 91) dominates the spectrum of TFE phenylacetic acid. Comparison of SIC chromatograms for m/z 119 and m/z 91 with that for m/z 218 in figure 12 unequivocally identified those components as 2-, 3-, and 4-methylbenzoic acid esters, respectively.

Alkanoic acids with phenyl groups attached to carbon chains generally fragment at benzylic positions, as shown in figure 14. For example, m/z 119 ($H_3C-CH_2CH-C_6H_5^+$) and 105 ($H_3C-CH-C_6H_5^+$) are prominent ions for HFB esters of 2-phenylbutyric acid and 3-phenylbutyric acid, respectively. The 3- and 4-phenyl isomers exhibit additional ions corresponding to hydrogen elimination in conjunction with benzylic cleavage (m/z 118 and 104, respectively). Thus, the position of the phenyl group on the carbon chain largely dictates fragmentation pathways for phenyl-substituted alkanoic acid esters.

Because of the limited commercial availability of cycloalkanoic acids, relatively few spectra of TFE and HFB esters for this acid type were obtained. Based on the available data (see appendices), their fragmentation is analogous to that of acyclic saturated esters in some respects, while analogous to aromatic or phenyl-substituted acids in others. For compounds where the saturated ring is separated from the carbonyl carbon by one or more methylene groups, acyclic alkanoic ester-type fragments corresponding to α -, β -, etc., cleavage with respect to the carbonyl carbon (see table 3) are observed. In cases where the carbonyl carbon is directly attached to a saturated ring, this type of fragmentation still occurs among methylene groups within the ring, but the fragment $CH_2CH_2COOR^+$ (m/z 155 (TFE), m/z 255 (HFB)) is typically by far the most intense. If the ring carbon attached to the carbonyl group is also alkyl substituted (e.g., 1-methyl-1-cyclohexanecarboxylic acid esters), the 1-alkyl group is included in the above fragment with a corresponding increase in its m/z .

FIGURE 13. Mass spectra of TFE esters of acids corresponding to the formula $C_8H_8O_2$. Note the prominence of the m/z 119 fragment in the methylbenzoic acid ester spectra versus its low abundance in that of the phenylacetic acid ester.

FIGURE 14. - Mass spectra of HFB esters of 2-, 3-, and 4-phenylbutyric acids.

Cycloalkyl fragments (e.g., $C_4H_7^+$, $C_5H_9^+$, $C_6H_{11}^+$, $C_7H_{13}^+$; m/z 55, 69, 83, and 97, respectively) typically dominate the lower m/z spectral region of cycloalkyl acid esters. One dominant fragment typically corresponds to the cycloalkyl group present, or to the cycloalkyl group plus one methylene group. A second dominant fragment usually occurs at m/z 55. The overall appearance of the low m/z end of the spectrum of cycloalkyl esters is more reminiscent of aromatic or phenyl-substituted esters than that of acyclic compounds, which show a progressive series of fragments that decrease in intensity with increasing m/z .

DiTFE esters of aliphatic dicarboxylic acids (Appendix A) typically exhibit weak molecular ions, relatively intense fragments corresponding to $CH_2CF_3^+$ (m/z 83) and loss of $-OCH_2CF_3$ (M-99), and moderately intense fragments within the series $(CH_2)_xCOOCH_2CF_3^+$ ($x = 0$, m/z 127; $x = 1$, m/z 141; etc.). The available examples of compounds containing both trifluoroacetyl and TFE or HFB ester groups indicate that fragmentation involving the TFE/HFB group (e.g., M- OCH_2CF_3 /M- $OCH_2(CF_2)_2CF_3$) predominates over fragmentation around the trifluoroacetyl moiety.

Comparison of the relative MS merits of TFE versus HFB esters failed to show a clear-cut superiority for either. The higher m/z for HFB esters decreases the probability of interference but increases the mass range required per scan, which results in increased scan times and more stringent instrument calibration and performance requirements. For these reasons, use of even higher molecular weight fluoroalcohols for GC/MS analysis poses more potential problems than advantages. In cases where hydroxyl groups are coderivatized with trifluoroacetyl groups, TFE esters are less desirable because the empirical formulas of TFE and trifluoroacetyl esters overlap (e.g., $C_9H_7O_2F_3$ could represent TFE benzoate or benzyl trifluoroacetate). Even though TFE versus trifluoroacetyl species can be readily differentiated via fragmentation patterns, the need to examine each spectrum in order to make this assignment significantly increases the task of data interpretation.

Although spectra of TFE and HFB esters are generally analogous, those of TFE esters are often more sensitive to subtle differences in structure, and also reflect major differences more clearly in some cases. For example, figure 15 compares SIC chromatograms of McLafferty fragments from 2-methyl-substituted alkanolic acid TFE versus HFB esters (figure 15B is the same as

FIGURE 15. - Comparison of SIC chromatograms corresponding to McLafferty ions for TFE versus HFB 2-methylalkanoic acids (peaks for straight chain acids, denoted by carbon number, represent ^{13}C -isotopes of fragments resulting from β -chain cleavage). Note the greater intensity of peaks corresponding to 2-methyl and 2,X-dimethyl homologs, compared to straight chain esters, in A.

figure 11B). The heights of 2-methyl- and especially 2,X-dimethyl-branched esters relative to straight chain ester peaks are significantly greater for TFE than for HFB esters. Thus, 2-methyl branching is more clearly differentiated in TFE spectra. Figure 16 shows spectra of HFB esters of 2-, 3-, and 4-methylbenzoic acids. Comparison of these spectra with those of the corresponding TFE esters in figure 13 shows a greater difference between spectra for 3- versus 4-methylbenzoic acids as TFE rather than HFB esters. In particular, the intensities of both molecular and tropylium (m/z 91) ions differ more for the TFE ester isomers, although this difference is still marginal for differentiation based solely on mass spectra. In general, differentiation of m - versus p-alkyl substitution from spectra of any type of benzoic acid ester is quite difficult.

Limitations

From an MS viewpoint, esters of the four types of acids examined -- straight and branched chain alkanoic, cycloalkanoic, phenyl- and other aryl-substituted alkanoic, and aromatic -- may be grouped into two categories: those whose most intense and/or characteristic fragments contain the ester group, and those giving rise to mainly hydrocarbon fragments. The straight and branched chain alkanoic esters clearly belong to the first group, while the behavior of cycloalkanoic acid esters crosses over into both categories. Aromatic and aryl-substituted alkanoic esters largely fall into the second category.

Use of fluorinated esters provides the greatest benefit for acids falling into the first category since the mass and intensities of both molecular ions and characteristic fragments are affected. Only the molecular ions of acids falling into the second category show significant change. However, as found during the analysis of benzoic acid homologs in the carboxylic acid concentrate (figure 12), the simple effect of shifting the molecular ion to higher m/z is of significant analytical value.

Analysis of the "hump" of unresolved compounds in the carboxylic acid concentrate appeared to be beyond the capabilities of present methodology. Numerous attempts were made at resolving the components via SIC plots; figure 17 shows four representative results for HFB esters. The hypothetical structures shown in the figure are included merely to show an example compound with

FIGURE 16. - Mass spectra of HFB esters of 2-, 3-, and 4-methylbenzoic acids. Note that spectra of 3- and 4-methylbenzoic acid esters are nearly identical.

FIGURE 17. - SIC chromatograms for "molecular ions" of HFB esters of cyclic carboxylic acids. Structures indicated are hypothetical.

a molecular weight consistent with each m/z . Obviously, the complexity evident in each plot is orders of magnitude greater than those for corresponding chromatograms of acyclic alkanolic acid molecular ions (figure 9). Whether any or all of the signal evident in figure 17 represents molecular ions of cyclic acid esters is unknown, they are typically represented in the literature to be the main carboxylic type in petroleum (7,11,19).

Past efforts at identification of specific cyclic-saturated carboxylic acids in petroleum have involved tremendous amounts of work per compound, even with the availability of GC/MS (8,15,17,25,26). If figure 17 accurately represents their complexity, the difficulties in their isolation and identification can be appreciated. Use of fluorinated alcohol esters might ultimately prove to be advantageous in analysis of these compounds, but only after extensive prefractionation.

A few SIC chromatograms of cyclic acid esters did show a relatively small number of distinct peaks; e.g., (TFE) m/z 306, 266, 280, 334, and 191. The m/z 191 ion is characteristic of terpenoid compounds (7,15,17,18). Since analysis of the carboxylic acid concentrate was not a primary objective, identification of these peaks was not pursued.

CONCLUSIONS

For GC/MS applications, fluorinated alcohol esters of carboxylic acids offer significant advantages over use of methyl esters or direct analysis of free acids. The two main advantages are the 1) higher molecular weight, and 2) greater intensity of molecular ions and, for aliphatic acids, key fragment ions. Both of these factors enhance detection and identification of carboxylic acids in complex matrices such as petroleum. Fluorinated esters exhibit excellent GC characteristics on nonpolar columns, and their GC elution times are only minimally affected by the number of CF_2 groups in the ester functionality. Because of the latter, alcohols covering a wide molecular weight range are suitable for GC/MS work.

Although it represents a significant amount of effort, the data base provided here comprises only a portion of what is needed to effectively interpret GC/MS results for either TFE or HFB esters of petroleum fractions. Data for saturated cyclic acid esters are particularly sparse. One possible approach for partial fulfillment of this need would be to obtain reference

data directly from oil shale and petroleum samples known to be rich in certain types of carboxylic acids. This is basically the approach used here to obtain data for isoprenoid acid esters, which were easily identified from existing data for isoprenoid methyl esters (13). This approach is fundamentally sound because of the analogous fragmentation pathways for methyl and fluorinated alcohol esters.

The observed markedly dissimilar distributions for acyclic versus cyclic alkanolic acids in the petroleum sample employed for ester performance evaluation indicates a different source or formation process for the two acid types. The repetitive, well-defined, isomeric distribution for acyclic acids suggests a minimal degree of structural alteration from that of the source material. The distribution of the cyclic acids, if accurately portrayed by the present data, is reminiscent of that typically obtained via a degradation process such as oxidation of hydrocarbons.

The effect of structure on GC/MS TIC response of esters is significant. For accurate quantitation, response factors correcting for the observed increase in response with higher alkylation and decreased response with greater aromaticity would be required.

REFERENCES

1. Yu, S.K.-T., and J. B. Green. Infrared-Chemical Derivatization Method for Determination of Total Hydroxyls and Carboxyls in Petroleum and Syncrudes, Topical Rpt. NIPER-363, 1988, 33 pp.
2. Yu, S.K.-T., and J. B. Green. Anal. Chem., v. 61, 1989, p. 1260.
3. Yu, S. K.-T., R. P. Vrana, and J. B. Green. Retention Indices, Relative Response Factors, and Mass Spectra of Trifluoroacetate Esters of Phenolic Compounds Determined by Capillary GC/MS. Topical Rpt. NIPER-396, 1989, 306 pp.
4. Teeter, R. M. Anal. Chem., v. 39, 1967, p. 1742.
5. Seifert, W. K. and R. M. Teeter. Anal. Chem., v. 41, 1969, p. 786.
6. Teeter, R. M. and W. K. Seifert. Am. Chem. Soc., Div. Petrol. Prepr., v. 16, No. 1, 1971, p. A7.
7. Seifert, W. K. Progress in the Chemistry of Organic Natural Products, W. Herz, H. Grisebach and G. W. Kirby (Eds.), Springer-Verlag, New York, 1975, v. 32, pp. 1-49.
8. Seifert, W. K., E. J. Gallegos, and R. M. Teeter. J. Am. Chem. Soc., v. 94, 1972, p. 5880.
9. Green, J. B., S. K.-T. Yu, J. A. Green, D. A. Doughty, J. W. Vogh, R. D. Grigsby, R. P. Vrana, J. S. Thomson, and L. Carbognani. Analysis of Heavy Oils: Method Development and Application to Cerro Negro Heavy Petroleum. Detailed Separation and Analysis of Acidic Compounds (Chapter 3). Topical Rpt. NIPER-322, 1989, 158 pp.
10. Hazlett, R., and G. Kelso. Proc. 2nd Int. Conf. on Long-Term Storage Stabilities of Liquid Fuels, v. 2, L. L. Stavinoha (Ed.), Southwest Research Inst., San Antonio, TX, 1986, p. 541.
11. Lochte, H. L., and E. R. Littman. The Petroleum Acids and Bases, Chemical Pub. Co., NY, 1955.
12. Haug, P., H. K. Schnoes, and A. L. Burlingame. Chem. Geol., v. 7, 1971, p. 213.
13. Douglas, A. G., M. Blumer, G. Eglington, and K. Douraghi-Zadeh. Tetrahedron, v. 27, 1971, p. 1071.
14. Shen, J. Anal. Chem., v. 53, 1981, p. 475.
15. Cyr, T. D., and O. P. Strausz. J. Chem. Soc. Chem. Commun., 1983, p. 1028.
16. Chong, S. L. and J. F. McKay. Fuel, v. 63, 1984, p. 303.

17. Schmitter, J. M., P. Arpino and G. Guiochon. J. Chromatogr., v. 167, 1978, p. 149.
18. Green, J. B., B. K. Stierwalt, J. S. Thomson and C. A. Treese. Anal. Chem., v. 57, 1985, p. 2207.
19. Dzidic, I., A. C. Somerville, J. C. Raia and H. V. Hart. Anal. Chem., v. 60, 1988, p. 1318.
20. Gallegos, E. J. J. Chromatogr. Sci., v. 25, 1987, p. 296.
21. Woodward, P. W., J. B. Green, J. S. Thomson, C. D. Pearson, R. Bryant, K. Chase, S. K.-T. Yu, and J. Y. Shay. Strategic Petroleum Reserve Quarterly Report, October-December 1989, NIPER Rpt. No. B06807-23, 1989, pp. 34-36.
22. Green, J. B., R. J. Hoff, P. W. Woodward, and L. L. Stevens. FUEL, v. 63, 1984, p. 1290.
23. Green, J. B. J. Chromatogr., v. 358, 1986, p. 53.
24. Thenot, J. P., E. C. Hornig, M. Stafford, and M. G. Horning. Anal. Lett., v. 5, 1972, p. 217.
25. Cason, J., and K.-L. Liaw. J. Org. Chem. v. 30, 1965, p. 1763.
26. Cason, J., and A. I. A. Khodair. J. Org. Chem., v. 31, 1966, p. 3618.

APPENDIX A

MASS SPECTRA OF 2,2,2-TRIFLUOROETHYL ESTERS

TABLE A1. - Directory for spectra of 2,2,2-trifluoroethyl esters

Z-Series	Parent Acid			Trifluoroethyl Ester			Page No.
	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	
O(O ₂)	88	Butyric Acid	C ₄ H ₈ O ₂	170	76.05±0.20	0.72±0.23	A-4
O(O ₂)	102	Trimethylacetic Acid	C ₅ H ₁₀ O ₂	184	74.86±0.08	0.47±0.21	A-7
O(O ₂)	102	2-Methylbutyric Acid	C ₅ H ₁₀ O ₂	184	82.72±0.03	0.78±0.05	A-9
O(O ₂)	102	Pentanoic Acid	C ₅ H ₁₀ O ₂	184	89.85±0.12	0.73±0.08	A-11
O(O ₂)	116	2,2-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	198	89.02±0.05	0.84±0.04	A-14
O(O ₂)	116	3,3-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	198	89.97±0.08	0.63±0.06	A-16
O(O ₂)	116	2-Ethylbutyric acid	C ₆ H ₁₂ O ₂	198	95.56±0.08	0.60	A-18
O(O ₂)	116	2-Methylisopentanoic Acid	C ₆ H ₁₂ O ₂	198	93.91±0.11	0.47±0.03	A-20
O(O ₂)	116	2-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	96.55±0.06	0.95±0.06	A-23
O(O ₂)	116	3-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	100.15±0.21	0.80±0.09	A-25
O(O ₂)	116	4-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	198	100.69±0.03	0.81±0.03	A-27
O(O ₂)	116	Hexanoic Acid	C ₆ H ₁₂ O ₂	198	107.40±0.04	0.82±0.08	A-29
O(O ₂)	130	2-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	212	114.50±0.06	0.97±0.05	A-32
O(O ₂)	130	5-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	212	119.79±0.08	0.67±0.03	A-35
O(O ₂)	130	Heptanoic Acid	C ₇ H ₁₄ O ₂	212	127.38±0.04	0.92±0.05	A-38
O(O ₂)	144	Octanoic Acid	C ₈ H ₁₆ O ₂	226	148.31±0.07	1.000	A-41
O(O ₂)	158	Nonanoic Acid	C ₉ H ₁₈ O ₂	240	169.00±0.02	1.02±0.04	A-44
O(O ₂)	172	Decanoic Acid	C ₁₀ H ₂₀ O ₂	254	188.90±0.03	1.17±0.08	A-47
O(O ₂)	186	Undecanoic Acid	C ₁₁ H ₂₂ O ₂	268	208.14±0.04	1.09±0.12	A-50
O(O ₂)	200	Dodecanoic Acid	C ₁₂ H ₂₄ O ₂	282	227.41±0.04	1.24±0.10	A-53
O(O ₂)	214	Tridecanoic Acid	C ₁₃ H ₂₆ O ₂	296	245.12±0.08	1.25±0.11	A-56
O(O ₂)	228	2,6,10-Trimethylundecanoic Acid ³	C ₁₄ H ₂₈ O ₂	310	233.64±0.05	-	A-59
O(O ₂)	228	Tetradecanoic Acid	C ₁₄ H ₂₈ O ₂	310	262.22±0.09	1.33±0.11	A-61
O(O ₂)	242	3,7,11-Trimethyltridecanoic Acid ³	C ₁₅ H ₃₀ O ₂	324	252.53±0.03	-	A-64
O(O ₂)	242	Pentadecanoic Acid ⁵	C ₁₅ H ₃₀ O ₂	324	278.48±0.02	-	A-67
O(O ₂)	256	4,8,12-Trimethyltridecanoic Acid ³	C ₁₆ H ₃₂ O ₂	338	270.20±0.05	-	A-69
O(O ₂)	256	Hexadecanoic Acid	C ₁₆ H ₃₂ O ₂	338	293.94±0.06	1.29±0.11	A-72
O(O ₂)	270	5,9,13-Trimethyltetradecanoic Acid ³	C ₁₇ H ₃₄ O ₂	352	285.50±0.05	-	A-75
O(O ₂)	270	Heptadecanoic Acid	C ₁₇ H ₃₄ O ₂	352	308.81±0.14	1.57±0.28	A-78
O(O ₂)	284	Octadecanoic Acid	C ₁₈ H ₃₆ O ₂	366	323.02±0.15	1.51±0.13	A-81
O(O ₂)	298	2,6,10,14-tetramethylpentadecanoic Acid ³	C ₁₉ H ₃₈ O ₂	380	303.89±0.14	-	A-84
O(O ₂)	298	Nonadecanoic Acid	C ₁₉ H ₃₈ O ₂	380	336.61±0.15	1.51±0.14	A-87
O(O ₂)	312	3,7,11,15-tetramethylhexadecanoic Acid ³	C ₂₀ H ₄₀ O ₂	394	319.32±0.05	-	A-90
O(O ₂)	312	Eicosanoic Acid	C ₂₀ H ₄₀ O ₂	394	349.68±0.19	1.55±0.15	A-94
O(O ₂)	326	Heineicosanoic Acid ⁵	C ₂₁ H ₄₂ O ₂	408	362.34±0.03	-	A-98
-2(O ₂)	114	Cyclopentanecarboxylic Acid	C ₆ H ₁₀ O ₂	196	114.31±0.03	0.69±0.04	A-101
-2(O ₂)	128	Cyclohexanecarboxylic Acid	C ₇ H ₁₂ O ₂	210	134.59±0.05	0.96±0.01	A-103
-2(O ₂)	142	1-Methyl-1-cyclohexanecarboxylic Acid	C ₈ H ₁₄ O ₂	224	137.20±0.03	0.90±0.06	A-105
-2(O ₂)	156	3-Cyclohexylpropionic Acid	C ₉ H ₁₆ O ₂	238	178.69±0.04	1.07±0.07	A-107
-2(O ₂)	282	9-Octadecenoic Acid	C ₁₈ H ₃₄ O ₂	364	319.60±0.03	0.82±0.06	A-110

TABLE A1. - Directory for spectra of 2,2,2-trifluoroethyl esters (contd)

Z-Series	Parent Acid			Trifluoroethyl Ester			Page No.
	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	
-8(O ₂)	122	Benzoic Acid	C ₇ H ₆ O ₂	204	139.16±0.06	0.58±0.02	A-113
-8(O ₂)	136	2-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	159.04±0.05	0.79±0.02	A-115
-8(O ₂)	136	3-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	161.64±0.06	0.76±0.02	A-117
-8(O ₂)	136	4-Methylbenzoic Acid	C ₈ H ₈ O ₂	218	164.75±0.03	0.82±0.03	A-119
-8(O ₂)	136	Phenylacetic Acid	C ₈ H ₈ O ₂	218	155.80±0.02	0.90±0.04	A-121
-8(O ₂)	150	2,3-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	186.22±0.03	0.75±0.03	A-123
-8(O ₂)	150	2,6-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	171.99±0.02	0.82±0.02	A-125
-8(O ₂)	150	2-Ethylbenzoic Acid	C ₉ H ₁₀ O ₂	232	173.09±0.04	0.81±0.05	A-127
-8(O ₂)	150	4-Methylphenylacetic Acid	C ₉ H ₁₀ O ₂	232	177.09±0.02	0.83±0.05	A-129
-8(O ₂)	164	2-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	177.97±0.06	0.91±0.06	A-131
-8(O ₂)	164	3-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	186.31±0.02	1.01±0.08	A-134
-8(O ₂)	164	4-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	246	200.83±0.04	0.99±0.02	A-136
-8(O ₂)	164	2,4,6-Trimethylbenzoic Acid	C ₁₀ H ₁₂ O ₂	246	194.59±0.06	0.85±0.06	A-138
-8(O ₂)	178	5-Phenylpentanoic Acid	C ₁₁ H ₁₄ O ₂	260	221.81±0.03	0.87±0.07	A-141
-8(O ₂)	220	4-Heptylbenzoic Acid	C ₁₄ H ₂₀ O ₂	302	276.94±0.05	0.79±0.10	A-144
-10(O ₂)	218	Cyclohexylphenylacetic Acid	C ₁₄ H ₁₈ O ₂	300	256.39±0.02	1.08±0.15	A-147
-14(O ₂)	172	1-Naphthoic Acid	C ₁₁ H ₈ O ₂	254	243.93±0.01	0.78±0.08	A-150
-14(O ₂)	172	2-Naphthoic Acid	C ₁₁ H ₈ O ₂	254	246.80±0.06	0.89±0.04	A-152
-14(O ₂)	186	1-Naphthylacetic Acid	C ₁₂ H ₁₀ O ₂	268	254.11±0.03	0.72±0.07	A-154
-16(O ₂)	198	Biphenyl-2-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	280	249.98±0.03	0.89±0.13	A-156
-16(O ₂)	198	Biphenyl-4-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	280	280.78±0.07	0.83±0.05	A-159
-16(O ₂)	226	2,2,-Diphenylpropionic Acid	C ₁₅ H ₁₄ O ₂	308	266.54±0.08	0.75±0.14	A-161
-16(O ₂)	240	1,2,3,4-Tetrahydro-4-phenanthreneacetic Acid	C ₁₆ H ₁₆ O ₂	322	327.98±0.05	0.51	A-164
-18(O ₂)	210	1-Fluorene-carboxylic Acid	C ₁₄ H ₁₀ O ₂	292	307.62±0.05	0.78±0.09	A-167
-20(O ₂)	222	Anthracene-9-Carboxylic Acid	C ₁₅ H ₁₀ O ₂	304	327.82±0.01	0.75±0.02	A-170
-20(O ₂)	222	9-Phenanthroic Acid	C ₁₅ H ₁₀ O ₂	304	335.04±0.06	0.44	A-173
-8(O ₃)	138	2-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	316	169.98±0.19	0.64±0.17	A-176
-8(O ₃)	138	4-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	316	171.99±0.16	0.48	A-179
-18(O ₃)	226	9-Xanthanecarboxylic Acid	C ₁₄ H ₁₀ O ₃	308	282.57±0.03	0.38±0.03	A-182
-2(O ₄)	88	Malonic Acid	C ₃ H ₄ O ₄	268	101.16±0.16	0.75±0.04	A-184
-2(O ₄)	132	Dimethylmalonic Acid	C ₅ H ₈ O ₄	296	105.09±0.08	0.02±0.01	A-187
-2(O ₄)	118	Succinic Acid	C ₄ H ₆ O ₄	282	123.38±0.07	-	A-190

¹ Based on assigned indices of 100, 200 and 300 for trifluoroacetyl esters of 4-fluorophenol, 1-naphthol, and 9-phenanthrol, respectively. Uncertainties shown are standard deviations.

² Response of octanoic acid esters was assumed = 1.00. TIC = total ion current. Uncertainties shown are standard deviations.

³ From analysis of petroleum fractions. Other data from pure compounds.

Dash - Not available.

1ALPA.1 [TIC-177844224, 100X-40962048] EI

Butyric acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_2\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	504.00	959	90272.	0.2	0.2	0.0508*	56	167.00	207	40329.	0.1	0.1	0.0227*
2	492.00	959	159112.	0.4	0.4	0.0895*	57	165.00	351	31607.	0.1	0.1	0.0178*
3	483.00	959	173360.	0.4	0.4	0.0975*	58	163.00	103	35889.	0.1	0.1	0.0202*
4	482.00	143	11890.	0.0	0.0	0.0067*	59	161.00	119	8884.	0.0	0.0	0.0050*
5	430.00	959	203500.	0.5	0.5	0.1144*	60	160.00	239	21307.	0.1	0.1	0.0120*
6	421.00	959	156804.	0.4	0.4	0.0882*	61	159.00	287	30224.	0.1	0.1	0.0170*
7	407.00	959	115940.	0.3	0.3	0.0652*	62	157.00	35	41939.	0.1	0.1	0.0236*
8	370.00	831	73272.	0.2	0.2	0.0412*	63	156.00	29	199208.	0.5	0.5	0.1120*
9	357.00	959	83168.	0.2	0.2	0.0468*	64	155.00	59	4083008.	10.0	10.0	2.2958*
10	354.00	959	115268.	0.3	0.3	0.0648*	65	154.00	59	11117.	0.0	0.0	0.0063*
11	340.00	831	74048.	0.2	0.2	0.0416*	66	153.00	21	13309.	0.0	0.0	0.0075*
12	325.00	703	52691.	0.1	0.1	0.0296*	67	152.00	29	39825.	0.1	0.1	0.0222*
13	324.00	351	27581.	0.1	0.1	0.0155*	68	151.00	25	425248.	1.0	1.0	0.2391*
14	314.00	287	21153.	0.1	0.1	0.0119*	69	150.00	29	28731.	0.1	0.1	0.0162*
15	311.00	207	15163.	0.0	0.0	0.0085*	70	149.00	35	83032.	0.2	0.2	0.0467*
16	302.00	479	38752.	0.1	0.1	0.0218*	71	148.00	143	25964.	0.1	0.1	0.0146*
17	301.00	479	34941.	0.1	0.1	0.0196*	72	147.00	175	13312.	0.0	0.0	0.0075*
18	300.00	959	139384.	0.3	0.3	0.0784*	73	145.00	175	43830.	0.1	0.1	0.0246*
19	288.00	479	38952.	0.1	0.1	0.0219*	74	144.00	25	96920.	0.2	0.2	0.0545*
20	283.00	703	52113.	0.1	0.1	0.0293*	75	143.00	35	913136.	2.2	2.2	0.5134*
21	281.00	8	7246.	0.0	0.0	0.0041*	76	142.00	71	20890624.	51.0	51.0	*11.74*
22	275.00	415	33808.	0.1	0.1	0.0190*	77	141.00	25	76344.	0.2	0.2	0.0429*
23	267.00	175	13235.	0.0	0.0	0.0074*	78	140.00	35	41451.	0.1	0.1	0.0233*
24	266.00	831	65568.	0.2	0.2	0.0369*	79	139.00	43	3703.	0.0	0.0	0.0021*
25	265.00	703	47721.	0.1	0.1	0.0268*	80	138.00	119	20115.	0.0	0.0	0.0113*
26	259.00	479	38086.	0.1	0.1	0.0214*	81	137.00	175	39882.	0.1	0.1	0.0224*
27	247.00	703	57256.	0.1	0.1	0.0322*	82	136.00	29	1033448.	0.3	0.3	0.0582*
28	246.00	831	59041.	0.1	0.1	0.0332*	83	135.00	43	2139392.	5.2	5.2	1.2030*
29	239.00	959	86660.	0.2	0.2	0.0499*	84	134.00	59	6001.	0.0	0.0	0.0034*
30	235.00	103	7603.	0.0	0.0	0.0043*	85	133.00	43	16847.	0.0	0.0	0.0095*
31	232.00	479	37925.	0.1	0.1	0.0213*	86	132.00	143	23771.	0.1	0.1	0.0134*
32	232.00	143	9548.	0.0	0.0	0.0054*	87	131.00	35	99268.	0.2	0.2	0.0558*
33	231.00	8	6987.	0.0	0.0	0.0039*	88	130.00	119	24733.	0.1	0.1	0.0139*
34	228.00	287	23112.	0.1	0.1	0.0130*	89	129.00	59	31002.	0.1	0.1	0.0174*
35	223.00	415	38909.	0.1	0.1	0.0219*	90	128.00	25	1606720.	0.2	0.2	0.0403*
36	220.00	479	39819.	0.1	0.1	0.0224*	91	127.00	35	26406.	0.1	0.1	0.0148*
37	219.00	8	12825.	0.0	0.0	0.0072*	92	126.00	175	15729.	0.0	0.0	0.0088*
38	214.00	415	36170.	0.1	0.1	0.0203*	93	125.00	43	25275.	0.1	0.1	0.0142*
39	209.00	959	101584.	0.2	0.2	0.0571*	94	124.00	35	146100.	0.4	0.4	0.0822*
40	207.00	239	20272.	0.0	0.0	0.0114*	95	123.00	35	2684416.	6.6	6.6	1.5094*
41	205.00	959	72996.	0.2	0.2	0.0410*	96	122.00	119	9680.	0.0	0.0	0.0054*
42	197.00	703	58331.	0.1	0.1	0.0328*	97	120.00	71	5970.	0.0	0.0	0.0034*
43	188.00	831	55118.	0.1	0.1	0.0310*	98	120.00	43	145972.	0.4	0.4	0.0821*
44	187.00	831	62319.	0.2	0.2	0.0350*	99	119.00	29	61444.	0.2	0.2	0.0345*
45	185.00	575	47149.	0.1	0.1	0.0255*	100	118.00	29	48290.	0.1	0.1	0.0272*
46	181.00	8	17796.	0.0	0.0	0.0100*	101	117.00	29	14813.	0.0	0.0	0.0083*
47	180.00	287	21547.	0.1	0.1	0.0121*	102	116.00	207	16237.	0.0	0.0	0.0091*
48	178.00	175	12170.	0.0	0.0	0.0068*	103	115.00	207	38890.	0.1	0.1	0.0219*
49	177.00	351	28685.	0.1	0.1	0.0161*	104	114.00	175	251436.	0.6	0.6	0.1414*
50	174.00	287	21296.	0.1	0.1	0.0120*	105	113.00	107	25742.	0.1	0.1	0.0145*
51	173.00	239	48843.	0.1	0.1	0.0275*	106	112.00	187	4381.	0.0	0.0	0.0025*
52	172.00	8	8781.	0.0	0.0	0.0049*	107	111.00	51	104652.	0.3	0.3	0.0588*
53	171.00	25	233552.	0.6	0.6	0.1313*	108	110.00	103	78288.	0.2	0.2	0.0440*
54	170.00	29	203836.	0.5	0.5	0.1146*	109	109.00	71	10776.	0.0	0.0	0.0061*
55	169.00	25	153640.	0.4	0.4	0.0864*	110	108.00	71				

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	187.00	71	37908.	0.1	0.1	0.0213*	166	49.00	71	234388.	0.6	0.6	0.1318*
112	186.00	87	21804.	0.1	0.1	0.0123*	167	48.00	175	49118.	0.1	0.1	0.0276*
113	185.00	43	107600.	0.3	0.3	0.0605*	168	47.00	87	457136.	1.1	1.1	0.2570*
114	184.00	35	49365.	0.1	0.1	0.0278*	169	46.00	43	102460.	0.3	0.3	0.0576*
115	183.00	71	18314.	0.0	0.0	0.0103*	170	45.00	103	1355264.	3.3	3.3	0.7621*
116	182.00	71	39621.	0.1	0.1	0.0223*	171	44.00	71	2437184.	5.9	5.9	1.3704*
117	181.00	43	24109.	0.1	0.1	0.0136*	172	43.00	119	40962048.	100.0	100.0	*23.03*
118	180.00	71	29172.	0.1	0.1	0.0164*	173	42.00	103	11948544.	29.2	29.2	6.7185*
119	99.00	87	32845.	0.1	0.1	0.0185*	174	41.00	103	14533120.	35.5	35.5	8.1718*
120	98.00	175	31831.	0.1	0.1	0.0179*	175	40.00	103	1299392.	3.2	3.2	0.7306*
121	97.00	287	23066.	0.1	0.1	0.0130*	176	39.00	143	8063744.	19.7	19.7	4.5342*
122	96.00	287	25188.	0.1	0.1	0.0142*	177	38.00	87	1062592.	2.6	2.6	0.5975*
123	95.00	239	18776.	0.0	0.0	0.0106*	178	37.00	87	482528.	1.2	1.2	0.2713*
124	93.00	207	93564.	0.2	0.2	0.0526*	179	36.00	87	317808.	0.8	0.8	0.1787*
125	91.00	43	29356.	0.1	0.1	0.0165*	180	35.00	71	125112.	0.3	0.3	0.0703*
126	90.00	119	31637.	0.1	0.1	0.0178*							
127	88.00	207	51560.	0.1	0.1	0.0290*							
128	87.00	43	89852.	0.2	0.2	0.0505*							
129	86.00	71	52355.	0.1	0.1	0.0294*							
130	85.00	43	26786.	0.1	0.1	0.0151*							
131	84.00	51	307040.	0.7	0.7	0.1726*							
132	83.00	71	10868992.	26.5	26.5	6.1115*							
133	82.00	43	52446.	0.1	0.1	0.0295*							
134	81.00	51	138276.	0.3	0.3	0.0778*							
135	80.00	43	1027968.	2.5	2.5	0.5780*							
136	79.00	35	47861.	0.1	0.1	0.0269*							
137	78.00	51	317568.	0.8	0.8	0.1786*							
138	77.00	51	1475200.	3.6	3.6	0.8295*							
139	76.00	71	35649.	0.1	0.1	0.0200*							
140	75.00	43	210189.	0.5	0.5	0.1182*							
141	74.00	43	434512.	1.1	1.1	0.2443*							
142	73.00	51	153284.	0.4	0.4	0.0862*							
143	72.00	51	1040640.	2.5	2.5	0.5851*							
144	71.00	87	22889472.	55.9	55.9	*12.87*							
145	70.00	51	402368.	1.0	1.0	0.2262*							
146	69.00	71	4122752.	10.1	10.1	2.3182*							
147	68.00	43	110940.	0.3	0.3	0.0624*							
148	67.00	207	48459.	0.1	0.1	0.0272*							
149	66.00	71	11631.	0.0	0.0	0.0065*							
150	65.00	51	75568.	0.2	0.2	0.0425*							
151	64.00	71	1429184.	3.5	3.5	0.8036*							
152	63.00	51	652544.	1.6	1.6	0.3669*							
153	62.00	119	28150.	0.1	0.1	0.0158*							
154	61.00	71	375696.	0.9	0.9	0.2113*							
155	60.00	43	130572.	0.3	0.3	0.0734*							
156	59.00	59	350064.	0.9	0.9	0.1968*							
157	58.00	71	184708.	0.5	0.5	0.1039*							
158	57.00	59	338448.	0.8	0.8	0.1303*							
159	56.00	51	362992.	0.9	0.9	0.2041*							
160	55.00	71	6126080.	15.0	15.0	3.4446*							
161	54.00	51	91428.	0.2	0.2	0.0514*							
162	53.00	71	192276.	0.5	0.5	0.1081*							
163	52.00	103	77696.	6.2	6.2	0.0437*							
164	51.00	51	599264.	1.5	1.5	0.3370*							
165	50.00	71	304496.	0.7	0.7	0.1712*							

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	443.00	8	1058.	0.0	0.0	0.0018	56	70.00	14	210680.	0.8	0.8	0.3520
2	293.00	6	1564.	0.0	0.0	0.0026	57	69.00	35	2834432.	11.2	11.2	4.7353
3	281.00	8	16402.	0.1	0.1	0.0274	58	68.00	17	17140.	0.1	0.1	0.0286
4	243.00	6	2435.	0.0	0.0	0.0041	59	67.00	17	11089.	0.0	0.0	0.0185*
5	231.00	8	19873.	0.1	0.1	0.0332	60	65.00	10	15584.	0.1	0.1	0.0260
6	219.00	10	24897.	0.1	0.1	0.0416	61	64.00	17	302248.	1.2	1.2	0.5059
7	193.00	6	1626.	0.0	0.0	0.0027	62	63.00	14	133260.	0.5	0.5	0.2226
8	185.00	17	37777.	0.1	0.1	0.0631	63	61.00	21	318432.	1.3	1.3	0.5286*
9	184.00	12	13132.	0.1	0.1	0.0219	64	60.00	8	3903.	0.0	0.0	0.0065
10	181.00	14	55681.	0.2	0.2	0.0930	65	59.00	21	450512.	1.8	1.8	0.7526*
11	170.00	14	16374.	0.1	0.1	0.0274	66	58.00	29	1018160.	4.0	4.0	1.7010*
12	169.00	21	540224.	2.1	2.1	0.9025	67	57.00	59	25206784.	100.0	100.0	*42.11*
13	168.00	14	25001.	0.1	0.1	0.0418	68	56.00	25	817040.	3.2	3.2	1.3550*
14	167.00	10	15143.	0.1	0.1	0.0253	69	55.00	29	95536.	3.7	3.7	1.5462*
15	166.00	6	2134.	0.0	0.0	0.0036	70	54.00	17	259064.	0.2	0.2	0.0991
16	165.00	17	59579.	0.2	0.2	0.0095	71	53.00	17	20789.	1.0	1.0	0.4328
17	162.00	8	1672.	0.0	0.0	0.0028	72	52.00	17	379696.	0.1	0.1	0.0347
18	155.00	8	7006.	0.0	0.0	0.0117	73	51.00	29	115572.	1.5	1.5	0.6343
19	153.00	10	8381.	0.0	0.0	0.0033	74	50.00	17	375280.	0.5	0.5	0.1931*
20	151.00	8	1985.	0.0	0.0	0.0140	75	49.00	25	19027.	0.1	0.1	0.0318*
21	150.00	12	20457.	0.1	0.1	0.0342	76	48.00	12	160084.	0.6	0.6	0.2674*
22	149.00	17	334144.	1.3	1.3	0.5582	77	47.00	25	184252.	0.7	0.7	0.3078
23	145.00	6	2253.	0.0	0.0	0.0038	78	45.00	21	97592.	0.4	0.4	0.1630
24	143.00	8	4589.	0.0	0.0	0.0077	79	44.00	14	358688.	1.4	1.4	0.5992*
25	142.00	12	48697.	0.2	0.2	0.0814	80	43.00	25	1133184.	4.5	4.5	*19.11*
26	141.00	25	1214720.	4.8	4.8	2.0293	81	42.00	29	11440896.	45.4	45.4	1.0359*
27	139.00	6	1287.	0.0	0.0	0.0022	82	41.00	43	620048.	2.5	2.5	5.7901
28	135.00	10	7670.	0.0	0.0	0.0128	83	40.00	29	3465856.	13.7	13.7	0.1938*
29	133.00	6	1606.	0.0	0.0	0.0027	84	39.00	35	280800.	1.1	1.1	0.4691*
30	131.00	17	123952.	0.5	0.5	0.2071*	85	38.00	21	116004.	0.5	0.5	0.1938*
31	128.00	12	24234.	0.1	0.1	0.0405	86	37.00	21	125784.	0.5	0.5	0.2101
32	127.00	21	750928.	3.0	3.0	1.2545	87	36.00	14	67444.	0.3	0.3	0.1127*
33	123.00	12	13263.	0.1	0.1	0.0222	88	35.00	17				
34	119.00	17	130540.	0.5	0.5	0.2181							
35	113.00	11	59892.	0.2	0.2	0.1001							
36	109.00	14	264240.	1.0	1.0	0.4414							
37	108.00	10	2445.	0.0	0.0	0.0041							
38	107.00	14	138108.	0.5	0.5	0.2307							
39	104.00	6	1486.	0.0	0.0	0.0025							
40	103.00	8	2972.	0.0	0.0	0.0050							
41	100.00	12	20818.	0.1	0.1	0.0348							
42	99.00	8	6936.	0.0	0.0	0.0116							
43	93.00	8	2057.	0.0	0.0	0.0034							
44	88.00	8	10724.	0.0	0.0	0.0179							
45	87.00	17	276656.	1.1	1.1	0.4622*							
46	86.00	21	171364.	0.7	0.7	0.2863*							
47	85.00	25	879552.	3.5	3.5	1.4694*							
48	84.00	21	240968.	1.0	1.0	0.4026*							
49	83.00	35	2592256.	10.3	10.3	4.3307*							
50	82.00	8	3354.	0.0	0.0	0.0056							
51	81.00	21	37916.	0.2	0.2	0.0633							
52	80.00	10	2788.	0.0	0.0	0.0047							
53	77.00	14	5755.	0.0	0.0	0.0096							
54	72.00	8	5568.	0.0	0.0	0.0093							
55	71.00	12	57648.	0.2	0.2	0.0963							

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	481.00	8	1804.	0.0	0.0	0.0016	56	90.00	6	2801.	0.0	0.0	0.0024
2	283.00	10	2538.	0.0	0.0	0.0022	57	88.00	10	6464.	0.0	0.0	0.0056
3	282.00	10	3515.	0.0	0.0	0.0031	58	87.00	10	38363.	0.1	0.0	0.0334
4	281.00	10	38269.	0.1	0.0	0.0333	59	86.00	21	268512.	1.0	1.0	0.2336*
5	231.00	8	10338.	0.0	0.0	0.0090	60	85.00	35	4233216.	15.1	15.1	3.6830*
6	219.00	8	7780.	0.0	0.0	0.0068	61	84.00	21	237100.	0.8	0.8	0.2063*
7	193.00	6	1325.	0.0	0.0	0.0012	62	83.00	35	5845248.	20.8	20.8	5.0856*
8	186.00	6	1678.	0.0	0.0	0.0015	63	82.00	8	8182.	0.0	0.0	0.0071
9	185.00	12	70000.	0.2	0.2	0.0609*	64	81.00	12	79736.	0.3	0.3	0.0694*
10	184.00	10	76868.	0.3	0.3	0.0669	65	80.00	12	87748.	0.3	0.3	0.0763*
11	183.00	8	6656.	0.0	0.0	0.0058	66	79.00	10	3437.	0.0	0.0	0.0030
12	181.00	8	29304.	0.1	0.0	0.0255	67	77.00	12	75012.	0.3	0.3	0.0653*
13	171.00	8	1223.	0.0	0.0	0.0011	68	75.00	6	1828.	0.0	0.0	0.0016
14	170.00	17	177328.	0.6	0.6	0.1543*	69	73.00	10	61289.	0.2	0.2	0.0533*
15	169.00	29	2889856.	10.3	10.3	2.5143*	70	71.00	12	59827.	0.2	0.2	0.0521*
16	168.00	10	1470.	0.0	0.0	0.0013	71	70.00	14	106308.	0.4	0.4	0.0925*
17	167.00	8	4951.	0.0	0.0	0.0043	72	69.00	35	4412928.	15.7	15.7	3.8394
18	166.00	8	2632.	0.0	0.0	0.0023	73	68.00	12	45265.	0.2	0.2	0.0394*
19	165.00	17	195796.	0.7	0.7	0.1703	74	67.00	8	12649.	0.0	0.0	0.0110
20	163.00	6	1807.	0.0	0.0	0.0016	75	65.00	17	9058.	0.0	0.0	0.0079*
21	158.00	12	69692.	0.2	0.2	0.0606	76	64.00	25	581592.	3.1	3.1	0.7696
22	157.00	21	818320.	2.9	2.9	0.7120*	77	63.00	21	373888.	1.3	1.3	0.3253*
23	156.00	51	15398912.	54.8	54.8	*13.39*	78	61.00	17	186708.	0.7	0.7	0.1624
24	155.00	29	515696.	1.8	1.8	0.4487*	79	60.00	6	1399.	0.0	0.0	0.0012
25	154.00	6	1658.	0.0	0.0	0.0014	80	59.00	17	152156.	0.5	0.5	0.1324*
26	153.00	6	2597.	0.0	0.0	0.0023	81	58.00	29	1210496.	4.3	4.3	1.0532
27	151.00	6	1020.	0.0	0.0	0.0009	82	57.00	59	28094464.	100.0	100.0	*24.44*
28	150.00	10	36888.	0.1	0.1	0.0321	83	56.00	43	5915136.	21.1	21.1	5.1464*
29	149.00	21	803584.	2.9	2.9	0.6991	84	55.00	35	4672000.	16.6	16.6	4.0648
30	143.00	8	3051.	0.0	0.0	0.0027	85	54.00	21	239624.	0.9	0.9	0.2085*
31	142.00	14	83672.	0.3	0.3	0.0728	86	53.00	25	820768.	2.9	2.9	0.7141
32	141.00	14	174648.	0.6	0.6	0.1519	87	52.00	17	106972.	0.4	0.4	0.0931
33	139.00	8	1409.	0.0	0.0	0.0012	88	51.00	25	675872.	2.4	2.4	0.5880*
34	137.00	14	82640.	0.3	0.3	0.0719	89	50.00	21	353504.	1.3	1.3	0.3076*
35	136.00	25	1592320.	5.7	5.7	1.3854*	90	49.00	21	241544.	0.9	0.9	0.2102*
36	135.00	25	1010704.	3.6	3.6	0.8793	91	48.00	8	8759.	0.0	0.0	0.0076*
37	134.00	12	15905.	0.1	0.1	0.0138*	92	47.00	25	349504.	1.2	1.2	0.3041*
38	133.00	6	1199.	0.0	0.0	0.0010	93	46.00	6	5572.	0.0	0.0	0.0048
39	131.00	14	102360.	0.4	0.4	0.0891*	94	45.00	35	798512.	2.8	2.8	0.6947*
40	129.00	6	1744.	0.0	0.0	0.0015	95	44.00	25	312528.	1.1	1.1	0.2719*
41	128.00	10	44551.	0.2	0.2	0.0388*	96	43.00	29	622880.	2.2	2.2	0.5419*
42	127.00	25	1378880.	4.9	4.9	1.1997	97	42.00	35	13001760.	4.6	4.6	1.1326*
43	123.00	14	107728.	0.4	0.4	0.0937*	98	41.00	43	170009664.	60.5	60.5	*14.79*
44	119.00	21	128940.	0.5	0.5	0.1122*	99	40.00	35	698608.	2.5	2.5	0.6078*
45	118.00	17	31187.	0.1	0.1	0.0271*	100	39.00	35	5302016.	18.9	18.9	4.6129
46	113.00	14	125692.	0.4	0.4	0.1094*	101	38.00	29	418032.	1.5	1.5	0.3637*
47	110.00	10	19385.	0.1	0.1	0.0169	102	37.00	21	139088.	0.5	0.5	0.1210*
48	109.00	21	1279488.	4.6	4.6	1.1132*	103	36.00	17	224848.	0.8	0.8	0.2042*
49	107.00	8	1648.	0.0	0.0	0.0014	104	35.00	14	79248.	0.3	0.3	0.0689*
50	103.00	6	1443.	0.0	0.0	0.0013							
51	101.00	6	2413.	0.0	0.0	0.0021							
52	100.00	8	7395.	0.0	0.0	0.0064							
53	93.00	6	1552.	0.0	0.0	0.0014							
54	92.00	12	12324.	0.0	0.0	0.0107							
55	91.00	21	747504.	2.7	2.7	0.6504							

2ALPA.1 [TIC=176848896, 188X-28491776] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	10	3076.	0.0	0.0	0.0017	56	100.00	10	4745.	0.0	0.0	0.0027
2	269.00	5	1051.	0.0	0.0	0.0006	57	99.00	8	7684.	0.0	0.0	0.0043
3	231.00	12	2743.	0.0	0.0	0.0016	58	93.00	6	4615.	0.0	0.0	0.0026
4	219.00	8	8630.	0.0	0.0	0.0049	59	92.00	8	2444.	0.0	0.0	0.0014
5	186.00	10	2847.	0.0	0.0	0.0016	60	91.00	14	177592.	0.6	0.6	0.1004
6	185.00	14	111928.	0.4	0.2	0.0633	61	90.00	8	2333.	0.0	0.0	0.0013
7	184.00	10	55238.	0.2	0.2	0.0312	62	87.00	12	55436.	0.2	0.2	0.0313
8	183.00	10	15514.	0.1	0.1	0.0088	63	86.00	21	388912.	1.4	1.4	0.2199
9	181.00	8	14792.	0.1	0.1	0.0084	64	85.00	35	7940864.	27.9	27.9	4.4902*
10	172.00	8	8781.	0.0	0.0	0.0050	65	84.00	21	325744.	1.1	1.1	0.1842*
11	171.00	17	131740.	0.5	0.5	0.0745	66	83.00	35	10503936.	36.9	36.9	5.9395*
12	170.00	12	75344.	0.3	0.3	0.0426	67	82.00	10	24668.	0.1	0.1	0.0139
13	169.00	21	382144.	1.3	1.3	0.2161*	68	81.00	17	124908.	0.4	0.4	0.0706*
14	166.00	8	14440.	0.1	0.1	0.0082	69	80.00	21	1038000.	3.6	3.6	0.5869
15	165.00	17	374208.	1.3	1.3	0.2116	70	79.00	10	21540.	0.1	0.1	0.0122
16	162.00	6	1874.	0.0	0.0	0.0011	71	78.00	21	349728.	1.2	1.2	0.1978
17	157.00	10	43571.	0.2	0.2	0.0246	72	77.00	25	1749120.	6.1	6.1	0.9890
18	156.00	21	487424.	1.7	1.7	0.2756	73	76.00	6	3087.	0.0	0.0	0.0017
19	155.00	43	6988544.	24.5	24.5	3.9517*	74	75.00	17	134128.	0.5	0.5	0.0758
20	154.00	8	2325.	0.0	0.0	0.0013	75	74.00	21	483456.	1.7	1.7	0.2734
21	153.00	8	1922.	0.0	0.0	0.0011	76	73.00	12	97772.	0.3	0.3	0.0553
22	152.00	12	8560.	0.0	0.0	0.0048*	77	72.00	25	409376.	1.4	1.4	0.2315
23	151.00	17	178216.	0.6	0.6	0.1008	78	71.00	21	8972288.	31.5	31.5	5.0734*
24	150.00	10	4635.	0.0	0.0	0.0026	79	70.00	14	151176.	0.5	0.5	0.0855
25	149.00	12	71476.	0.3	0.3	0.0409	80	69.00	35	3219840.	11.3	11.3	1.8207
26	144.00	17	125392.	0.4	0.4	0.0709*	81	68.00	14	56413.	0.2	0.2	0.0319*
27	143.00	25	1219584.	4.3	4.3	0.6896*	82	67.00	10	15987.	0.1	0.1	0.0090
28	142.00	71	25825208.	90.6	90.6	*14.60*	83	65.00	12	49023.	0.2	0.2	0.0277*
29	141.00	25	257760.	0.9	0.2	0.1458*	84	64.00	25	1258176.	4.4	4.4	0.7114
30	140.00	12	47746.	0.2	0.2	0.0270*	85	63.00	21	569824.	2.0	2.0	0.3222
31	139.00	8	14503.	0.1	0.1	0.0082	86	62.00	6	2020.	0.0	0.0	0.0011
32	137.00	12	4034.	0.0	0.0	0.0023	87	61.00	21	352960.	1.2	1.2	0.1996
33	136.00	17	196748.	0.7	0.7	0.1113	88	60.00	14	98616.	0.3	0.3	0.0558
34	135.00	25	2520192.	8.8	8.8	1.4251	89	59.00	21	266096.	0.9	0.9	0.1505*
35	131.00	12	69584.	0.2	0.0	0.0393*	90	58.00	25	508800.	1.8	1.8	0.2877
36	129.00	8	1618.	0.0	0.0	0.0009	91	57.00	35	9089792.	31.9	31.9	5.1399*
37	128.00	14	90920.	0.3	0.3	0.0514	92	56.00	35	4203264.	14.8	14.8	2.3768*
38	127.00	25	2395008.	8.4	8.4	1.3543	93	55.00	43	9447424.	33.2	33.2	5.3421*
39	126.00	8	14915.	0.1	0.1	0.0084	94	54.00	17	258544.	0.9	0.9	0.1462
40	124.00	8	5927.	0.0	0.0	0.0034	95	53.00	25	607584.	2.1	2.1	0.3436
41	123.00	17	179496.	0.6	0.6	0.1015	96	52.00	14	90436.	0.3	0.3	0.0511
42	122.00	35	3157504.	11.1	11.1	1.7854*	97	51.00	25	745824.	2.6	2.6	0.4217
43	119.00	12	82576.	0.3	0.3	0.0467	98	50.00	21	363184.	1.3	1.3	0.2054
44	118.00	14	28114.	0.1	0.1	0.0159*	99	49.00	17	108552.	0.4	0.4	0.0614*
45	117.00	14	39971.	0.1	0.1	0.0226*	100	47.00	21	403536.	1.4	1.4	0.2282*
46	114.00	6	1726.	0.0	0.0	0.0010	101	46.00	12	70064.	0.2	0.2	0.0396*
47	113.00	17	356880.	1.3	1.3	0.2018	102	45.00	35	1062016.	3.7	3.7	0.6005
48	112.00	12	17005.	0.1	0.1	0.0096	103	44.00	35	2055488.	7.2	7.2	1.1623*
49	110.00	14	30820.	0.1	0.1	0.0174	104	43.00	53	28491776.	100.0	100.0	*16.11*
50	109.00	17	149608.	0.5	0.5	0.0846	105	42.00	49	9411328.	33.0	33.0	5.3217*
51	107.00	12	7127.	0.0	0.0	0.0040	106	41.00	51	15272704.	53.6	53.6	8.6360*
52	105.00	21	80192.	0.3	0.3	0.0453*	107	40.00	29	1019936.	3.6	3.6	0.5767*
53	104.00	10	19316.	0.1	0.1	0.0105*	108	39.00	51	7464448.	26.2	26.2	4.2208*
54	102.00	8	8141.	0.0	0.0	0.0046	109	38.00	35	800624.	2.8	2.8	0.4527*
55	101.00	8	2466.	0.0	0.0	0.0014	110	37.00	25	273328.	1.0	1.0	0.1546*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	36.00	21	260924.	0.9	0.9	0.1475
112	35.00	12	37089.	0.1	0.1	0.0210*

8XAV2.1 [TIC=134733824, 166X=37451776] EI

2,2-dimethylbutyric acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	319.00	6	1565.	0.0	0.0	0.0012	56	85.00	10	28666.	0.1	0.1	0.0213
2	275.00	6	1095.	0.0	0.0	0.0008	57	84.00	21	158704.	0.4	0.4	0.1178*
3	231.00	6	1025.	0.0	0.0	0.0008	58	83.00	35	5520384.	14.7	14.7	4.0973*
4	219.00	6	1534.	0.0	0.0	0.0011	59	82.00	10	36375.	0.1	0.1	0.0270*
5	199.00	12	58557.	0.2	0.2	0.00435	60	81.00	14	111200.	0.3	0.3	0.0825*
6	198.00	6	21057.	0.0	0.0	0.0016	61	80.00	6	2103.	0.0	0.0	0.0016
7	197.00	6	1507.	0.0	0.0	0.0011	62	79.00	8	1435.	0.0	0.0	0.0011
8	193.00	6	1164.	0.0	0.0	0.0009	63	77.00	12	60298.	0.2	0.2	0.0448
9	184.00	12	43722.	0.1	0.1	0.0325	64	75.00	6	4795.	0.0	0.0	0.0036
10	183.00	21	728624.	1.9	1.9	0.5408	65	73.00	17	104368.	0.3	0.3	0.0775
11	182.00	8	18727.	0.1	0.1	0.0139	66	72.00	29	1905728.	5.1	5.1	1.4144*
12	181.00	8	27127.	0.1	0.1	0.0201	67	71.00	71	37451776.	100.0	100.0	*27.79*
13	172.00	8	2288.	0.0	0.0	0.0017	68	70.00	43	2340160.	6.2	6.2	1.7369*
14	171.00	17	164000.	0.4	0.4	0.1217	69	69.00	35	3602496.	9.6	9.6	2.6738
15	170.00	29	2459392.	6.6	6.6	1.8254	70	68.00	12	69908.	0.2	0.2	0.0519*
16	169.00	21	286752.	0.8	0.8	0.2128*	71	67.00	12	157792.	0.4	0.4	0.1171*
17	168.00	10	25533.	0.1	0.1	0.0190	72	66.00	14	9620.	0.0	0.0	0.0071*
18	167.00	12	50954.	0.1	0.1	0.0378*	73	65.00	10	42800.	0.1	0.1	0.0318
19	163.00	17	160144.	0.4	0.4	0.1169	74	64.00	21	488880.	1.3	1.3	0.3628
20	162.00	6	997.	0.0	0.0	0.0007	75	63.00	21	280592.	0.7	0.7	0.2083
21	156.00	14	76000.	0.2	0.2	0.0564	76	62.00	8	5657.	0.0	0.0	0.0042
22	155.00	21	627616.	1.7	1.7	0.4658	77	61.00	25	443888.	1.2	1.2	0.3295
23	153.00	8	14069.	0.0	0.0	0.0104	78	60.00	10	21322.	0.1	0.1	0.0158
24	151.00	6	2204.	0.0	0.0	0.0016	79	59.00	25	827728.	2.2	2.2	0.6143
25	150.00	12	52593.	0.1	0.1	0.0390	80	58.00	6	2960.	0.0	0.0	0.0022
26	149.00	17	242368.	0.6	0.6	0.1799	81	57.00	21	182312.	0.5	0.5	0.1353*
27	142.00	6	1419.	0.0	0.0	0.0011	82	56.00	25	616416.	1.6	1.6	0.4575
28	142.00	12	71788.	0.2	0.2	0.0533	83	55.00	35	6608128.	17.6	17.6	4.9046*
29	141.00	21	956096.	2.6	2.6	0.7096	84	54.00	21	239112.	0.6	0.6	0.1775*
30	139.00	8	4030.	0.0	0.0	0.0030	85	53.00	29	1280256.	3.2	3.2	0.8908
31	136.00	10	38851.	0.1	0.1	0.0229	86	52.00	17	137440.	0.4	0.4	0.1020*
32	135.00	21	787072.	2.1	2.1	0.5842	87	51.00	29	552816.	1.5	1.5	0.4103
33	131.00	12	51047.	0.1	0.1	0.0379	88	50.00	21	212320.	0.6	0.6	0.1576*
34	128.00	14	106132.	0.3	0.3	0.0788	89	49.00	14	65860.	0.2	0.2	0.0489*
35	127.00	29	2831744.	7.6	7.6	2.1017*	90	48.00	6	1909.	0.0	0.0	0.0014
36	126.00	8	2603.	0.0	0.0	0.0019	91	47.00	21	309264.	0.8	0.8	0.2295*
37	124.00	14	50627.	0.1	0.1	0.0376*	92	45.00	29	525200.	1.4	1.4	0.3898
38	123.00	25	1593216.	4.3	4.3	1.1825	93	44.00	35	1252288.	3.3	3.3	*26.72*
39	122.00	10	3486.	0.0	0.0	0.0026	94	43.00	71	36012032.	96.2	96.2	2.0341*
40	119.00	12	53036.	0.1	0.1	0.0394*	95	42.00	35	2740672.	7.3	7.3	7.6505*
41	114.00	6	899.	0.0	0.0	0.0007	96	41.00	29	10307840.	27.5	27.5	7.6505*
42	113.00	17	226528.	0.6	0.6	0.1681	97	40.00	35	909936.	2.4	2.4	3.9914*
43	109.00	17	107488.	0.3	0.3	0.0798	98	39.00	51	5377792.	14.4	14.4	0.2759*
44	106.00	6	1145.	0.0	0.0	0.0008	99	38.00	35	371680.	1.0	1.0	0.0861*
45	105.00	10	23245.	0.1	0.1	0.0173	100	37.00	17	116028.	0.3	0.3	0.2299
46	104.00	10	4858.	0.0	0.0	0.0036	101	36.00	21	309792.	0.8	0.8	0.0571*
47	101.00	12	12425.	0.0	0.0	0.0092	102	35.00	17	76960.	0.2	0.2	
48	100.00	14	80844.	0.2	0.2	0.0600*							
49	99.00	21	734096.	2.0	2.0	0.5448							
50	97.00	10	97.	0.0	0.0	0.0003							
51	95.00	8	11239.	0.1	0.1	0.0140							
52	93.00	8	18834.	0.0	0.0	0.0025							
53	91.00	8	3309.	0.0	0.0	0.0038							
54	87.00	17	100000.	0.3	0.3	0.0742							
55	86.00	8	3718.	0.0	0.0	0.0028							

BY2AV.1 [TIC=36323328, 188X=18881792] EI

3,3-dimethylbutyric acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	283.00	8	1767.	0.0	0.0	0.0049	56	54.00	17	81676.	0.8	0.8	0.2249*
2	282.00	10	5759.	0.1	0.1	0.0159	57	53.00	25	289664.	2.9	2.9	0.7975
3	281.00	12	37565.	0.4	0.4	0.1034	58	52.00	10	8269.	0.1	0.1	0.0228
4	267.00	8	1164.	0.0	0.0	0.0032	59	51.00	21	166604.	1.7	1.7	0.4587
5	231.00	6	1474.	0.0	0.0	0.0041	60	50.00	14	55735.	0.6	0.6	0.1534*
6	219.00	10	5970.	0.1	0.1	0.0164	61	49.00	17	59020.	0.6	0.6	0.1625*
7	199.00	6	2116.	0.0	0.0	0.0018	62	47.00	10	22791.	0.2	0.2	0.0627
8	193.00	6	3265.	0.0	0.0	0.0057	63	45.00	14	33242.	0.3	0.3	0.0915*
9	184.00	8	11731.	0.1	0.1	0.0323	64	44.00	21	113636.	1.1	1.1	0.3128*
10	183.00	17	257640.	2.6	2.6	0.7093	65	43.00	35	1297920.	12.9	12.9	3.5732
11	182.00	12	42223.	0.4	0.4	0.1162	66	42.00	35	646912.	6.4	6.4	1.7810*
12	181.00	8	15407.	0.2	0.2	0.0424*	67	41.00	35	3659072.	36.3	36.3	*10.07*
13	169.00	10	20292.	0.2	0.2	0.0559	68	40.00	25	231284.	2.3	2.3	0.6367*
14	155.00	8	14279.	0.1	0.1	0.0393	69	39.00	29	1374144.	13.6	13.6	3.7831
15	154.00	14	56791.	0.6	0.6	0.1563*	70	38.00	17	76800.	0.8	0.8	0.2114*
16	143.00	14	39687.	0.4	0.4	0.1093*	71	37.00	12	6365.	0.1	0.1	0.0175*
17	142.00	25	1087104.	10.8	10.8	2.9929	72	36.00	10	20382.	0.2	0.2	0.0561*
18	141.00	43	6141184.	50.9	50.9	*16.90*	73	35.00	6	2596.	0.0	0.0	0.0071
19	140.00	10	24947.	0.2	0.2	0.0687*							
20	139.00	14	56155.	0.6	0.6	0.1546							
21	131.00	14	32435.	0.3	0.3	0.0893							
22	127.00	12	38756.	0.4	0.4	0.1067*							
23	123.00	12	44004.	0.4	0.4	0.1211*							
24	122.00	17	110840.	1.1	1.1	0.3051							
25	119.00	14	46406.	0.5	0.5	0.1278							
26	113.00	14	54606.	0.5	0.5	0.1503							
27	100.00	12	62708.	0.6	0.6	0.1726							
28	99.00	25	974816.	9.7	9.7	2.6837							
29	98.00	6	2154.	0.0	0.0	0.0059							
30	86.00	8	14569.	0.1	0.1	0.0401							
31	85.00	10	2621.	0.0	0.0	0.0072							
32	84.00	21	143596.	1.4	1.4	0.3953*							
33	83.00	35	2974144.	29.5	29.5	8.1880							
34	82.00	10	43028.	0.4	0.4	0.1185							
35	81.00	12	22464.	0.2	0.2	0.0618*							
36	80.00	14	37212.	0.4	0.4	0.1024*							
37	78.00	8	4090.	0.0	0.0	0.0113							
38	77.00	17	88420.	0.9	0.9	0.2434*							
39	74.00	10	11872.	0.1	0.1	0.0327							
40	73.00	10	7807.	0.1	0.1	0.0215							
41	71.00	21	217120.	2.2	2.2	0.5977							
42	70.00	8	11002.	0.1	0.1	0.0303							
43	69.00	35	605040.	6.0	6.0	1.6657							
44	68.00	8	10931.	0.1	0.1	0.0301							
45	67.00	12	29153.	0.3	0.3	0.0803*							
46	65.00	8	8830.	0.1	0.1	0.0243							
47	64.00	17	113628.	1.1	1.1	0.3128*							
48	63.00	14	65186.	0.6	0.6	0.1795*							
49	61.00	29	436400.	4.3	4.3	1.2014							
50	60.00	10	4974.	0.0	0.0	0.0137							
51	59.00	21	175232.	1.7	1.7	0.4824							
52	58.00	25	410496.	4.1	4.1	1.1301							
53	57.00	43	10081792.	100.0	100.0	*27.75*							
54	56.00	29	682288.	6.8	6.8	1.8784							
55	55.00	35	2781952.	27.6	27.6	7.6589							

TRI1PK.1 [VIC-18461184, 188X-2381952] EI

2-ethylbutyric acid.
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	219.00	6	969.	0.0	0.0	0.0093	56	68.00	17	26917.	1.2	1.2	0.2573*
2	199.00	10	6469.	0.3	0.3	0.0618	57	67.00	14	16848.	0.7	0.7	0.1611*
3	197.00	6	758.	0.0	0.0	0.0072	58	65.00	12	3824.	0.2	0.2	0.0366
4	184.00	10	3182.	0.1	0.1	0.0304	59	64.00	21	57166.	2.5	2.5	0.5465
5	183.00	17	40963.	1.8	1.8	0.3916	60	63.00	17	29979.	1.3	1.3	0.2866*
6	181.00	12	3426.	0.1	0.1	0.0327	61	62.00	8	2667.	0.1	0.1	0.0255
7	179.00	14	22051.	1.0	1.0	0.2108	62	61.00	21	19141.	0.8	0.8	0.1830*
8	175.00	8	566.	0.0	0.0	0.0054	63	60.00	8	1744.	0.1	0.1	0.0167
9	172.00	6	1836.	0.1	0.1	0.0176	64	59.00	14	15215.	0.7	0.7	0.1454
10	171.00	21	65147.	2.8	2.8	0.5227	65	58.00	14	2934.	0.1	0.1	0.0280*
11	170.00	35	916336.	39.8	39.8	8.7594	66	57.00	17	26835.	1.2	1.2	0.2565
12	169.00	43	260032.	11.3	11.3	2.4857*	67	56.00	25	54997.	2.4	2.4	0.5257
13	168.00	12	3937.	0.2	0.2	0.0376*	68	55.00	43	850848.	37.0	37.0	8.1334*
14	166.00	8	1004.	0.0	0.0	0.0096	69	54.00	21	24901.	1.1	1.1	0.2380*
15	163.00	14	17906.	0.8	0.8	0.1712	70	53.00	25	94592.	4.1	4.1	0.9042
16	157.00	8	4564.	0.2	0.2	0.0436	71	52.00	10	9052.	0.4	0.4	0.0865*
17	156.00	17	46533.	2.0	2.0	0.4448	72	51.00	29	52910.	2.3	2.3	0.5058
18	155.00	35	769088.	33.4	33.4	7.3518*	73	50.00	17	18640.	0.8	0.8	0.1782
19	150.00	17	4334.	0.2	0.2	0.0414	74	49.00	12	6559.	0.3	0.3	0.0627
20	149.00	21	72904.	3.2	3.2	0.6969	75	47.00	21	37405.	1.6	1.6	0.3576*
21	148.00	10	2272.	0.1	0.1	0.0217	76	46.00	10	2005.	0.1	0.1	0.0192
22	142.00	25	36818.	1.6	1.6	0.3519*	77	45.00	29	58003.	2.5	2.5	0.5545
23	141.00	35	28878.	1.3	1.3	0.2760*	78	44.00	35	86172.	3.7	3.7	0.8237*
24	137.00	17	21694.	0.9	0.9	0.2074	79	43.00	51	2301952.	100.0	100.0	*22.00*
25	136.00	14	15232.	0.7	0.7	0.1456	80	42.00	35	210244.	9.1	9.1	2.0098*
26	135.00	21	114560.	5.0	5.0	1.0953	81	41.00	43	827472.	35.9	35.9	7.9099*
27	132.00	17	4250.	0.2	0.2	0.0406*	82	40.00	25	78436.	3.4	3.4	0.7498*
28	131.00	14	6412.	0.3	0.3	0.0613*	83	39.00	43	491616.	21.4	21.4	4.6994*
29	128.00	8	6751.	0.3	0.3	0.0645	84	38.00	35	44248.	1.9	1.9	0.4230*
30	127.00	21	107648.	4.7	4.7	1.0290	85	37.00	10	10204.	0.4	0.4	0.0975*
31	122.00	8	2937.	0.1	0.1	0.0281	86	36.00	12	23356.	1.0	1.0	0.2233
32	119.00	12	10213.	0.4	0.4	0.0976	87	35.00	10	9545.	0.4	0.4	0.0912
33	118.00	8	1511.	0.1	0.1	0.0144							
34	113.00	17	19890.	0.9	0.9	0.1901							
35	110.00	8	1977.	0.1	0.1	0.0189							
36	109.00	21	90676.	3.9	3.9	9.8668							
37	105.00	8	1881.	0.1	0.1	0.0180							
38	103.00	8	2805.	0.1	0.1	0.0268							
39	100.00	12	16042.	0.7	0.7	0.1533							
40	99.00	25	190116.	8.3	8.3	1.8173*							
41	97.00	12	3103.	0.1	0.1	0.0297							
42	87.00	10	3862.	0.2	0.2	0.0369							
43	86.00	6	739.	0.0	0.0	0.0071							
44	85.00	8	3636.	0.2	0.2	0.0348							
45	84.00	17	15033.	0.7	0.7	0.1437							
46	83.00	35	447936.	19.5	19.5	4.2819							
47	81.00	14	16235.	0.7	0.7	0.1552							
48	80.00	8	1545.	0.1	0.1	0.0148							
49	78.00	6	1306.	0.1	0.1	0.0125							
50	77.00	10	5911.	0.3	0.3	0.0565							
51	73.00	12	5222.	0.2	0.2	0.0499							
52	72.00	21	50111.	2.2	2.2	0.4790*							
53	71.00	35	869008.	37.8	37.8	8.3070							
54	70.00	29	164552.	7.1	7.1	1.5730							
55	69.00	35	452032.	19.6	19.6	4.3210							

FVIAV.1 [TIC-36274176, 188X-6958488] EI

2-methylisopentanoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	6	369.	0.0	0.0	0.0010	56	100.00	17	51778.	0.7	0.7	0.1427*
2	343.00	6	1654.	0.0	0.0	0.0046	57	99.00	35	586592.	8.4	8.4	1.6171
3	282.00	6	687.	0.0	0.0	0.0019	58	98.00	10	2279.	0.0	0.0	0.0063
4	281.00	12	16928.	0.2	0.2	0.0467	59	97.00	12	23055.	0.3	0.3	0.0636*
5	280.00	6	1820.	0.0	0.0	0.0050	60	96.00	8	1535.	0.0	0.0	0.0042
6	265.00	6	1754.	0.0	0.0	0.0048	61	95.00	8	1632.	0.0	0.0	0.0045
7	231.00	10	3700.	0.1	0.1	0.0102	62	93.00	8	1168.	0.0	0.0	0.0032
8	207.00	6	452.	0.0	0.0	0.0012	63	92.00	10	10037.	0.1	0.1	0.0277
9	205.00	8	1615.	0.0	0.0	0.0045	64	91.00	29	399952.	5.8	5.8	1.1026
10	199.00	10	10357.	0.1	0.1	0.0286	65	90.00	10	3023.	0.0	0.0	0.0083
11	198.00	8	2028.	0.0	0.0	0.0056	66	88.00	10	13228.	0.2	0.2	0.0365
12	193.00	10	3975.	0.1	0.1	0.0110	67	87.00	10	4053.	0.1	0.1	0.0112
13	185.00	8	1369.	0.0	0.0	0.0038	68	86.00	10	6548.	0.1	0.1	0.0181*
14	184.00	10	17427.	0.3	0.3	0.0482	69	85.00	12	7822.	0.1	0.1	0.0216*
15	183.00	25	322784.	4.6	4.6	0.0898	70	84.00	17	59086.	0.9	0.9	0.1629*
16	182.00	8	5936.	0.1	0.1	0.0164	71	83.00	43	1707136.	24.6	24.6	4.7862*
17	181.00	10	8698.	0.1	0.1	0.0240*	72	82.00	12	28220.	0.4	0.4	0.0778*
18	180.00	8	1322.	0.0	0.0	0.0036	73	81.00	17	34948.	0.5	0.5	0.0963*
19	179.00	14	37210.	0.5	0.5	0.1026	74	80.00	14	33472.	0.5	0.5	0.0923*
20	178.00	6	1080.	0.0	0.0	0.0030	75	79.00	6	4622.	0.1	0.1	0.0127
21	169.00	14	32011.	0.5	0.5	0.0882	76	78.00	10	3788.	0.1	0.1	0.0104
22	168.00	6	2182.	0.0	0.0	0.0060	77	77.00	10	23066.	0.3	0.3	0.0636
23	167.00	8	5747.	0.1	0.1	0.0158	78	76.00	6	827.	0.0	0.0	0.0023
24	163.00	21	68660.	1.0	1.0	0.1893*	79	75.00	8	1053.	0.0	0.0	0.0029
25	162.00	6	792.	0.0	0.0	0.0022	80	74.00	10	4135.	0.1	0.1	0.0114*
26	159.00	6	1076.	0.0	0.0	0.0030	81	73.00	12	26510.	0.4	0.4	0.0731
27	158.00	14	33121.	0.5	0.5	0.0913*	82	72.00	25	96756.	1.4	1.4	0.2667*
28	157.00	29	307024.	4.4	4.4	0.8464	83	71.00	35	1571520.	22.6	22.6	4.3323*
29	156.00	59	5768964.	8.3	8.3	15.90*	84	70.00	25	179400.	2.5	2.5	0.4698
30	155.00	35	183764.	2.6	2.6	0.5066*	85	69.00	35	612672.	8.8	8.8	1.6890
31	154.00	12	5793.	0.1	0.1	0.0160*	86	68.00	12	13364.	0.2	0.2	0.0368*
32	153.00	8	719.	0.0	0.0	0.0020	87	67.00	17	53302.	0.8	0.8	0.1469*
33	151.00	8	3026.	0.0	0.0	0.0083	88	66.00	12	5887.	0.1	0.1	0.0162
34	142.00	10	13997.	0.2	0.2	0.0386	89	65.00	10	20001.	0.3	0.3	0.0551*
35	141.00	25	141968.	2.0	2.0	0.3914	90	64.00	29	207460.	3.0	3.0	0.5719*
36	138.00	8	8822.	0.1	0.1	0.0243	91	63.00	21	111824.	1.6	1.6	0.3083
37	137.00	25	230928.	3.3	3.3	0.6366	92	62.00	8	1716.	0.0	0.0	0.0047
38	136.00	35	917200.	13.2	13.2	2.5285	93	61.00	25	69444.	1.0	1.0	0.1914*
39	135.00	35	414752.	6.0	6.0	1.1434*	94	59.00	21	95948.	1.4	1.4	0.2645*
40	134.00	17	24408.	0.4	0.4	0.0673*	95	58.00	21	96004.	1.4	1.4	0.2647
41	131.00	12	20279.	0.3	0.3	0.0559	96	57.00	35	1803136.	25.9	25.9	4.9709*
42	128.00	12	31185.	0.4	0.4	0.0860*	97	56.00	43	1920512.	27.6	27.6	5.2944*
43	127.00	35	816784.	11.8	11.8	2.2517*	98	55.00	43	1982656.	28.5	28.5	5.4658*
44	126.00	8	3937.	0.1	0.1	0.0109	99	54.00	25	116464.	1.7	1.7	0.3211*
45	125.00	6	1253.	0.0	0.0	0.0035	100	53.00	35	355872.	5.1	5.1	0.9811
46	125.00	8	8375.	0.1	0.1	0.0231	101	52.00	14	47241.	0.7	0.7	0.1302*
47	121.00	8	1789.	0.0	0.0	0.0049	102	51.00	29	201040.	2.9	2.9	0.5542*
48	119.00	17	43887.	0.6	0.6	0.1210*	103	50.00	21	82844.	1.2	1.2	0.2284*
49	118.00	25	57594.	0.8	0.8	0.1588*	104	49.00	12	42532.	0.6	0.6	0.1173*
50	114.00	8	1043.	0.0	0.0	0.0029	105	48.00	10	2557.	0.0	0.0	0.0070
51	113.00	17	71136.	1.0	1.0	0.1961	106	47.00	25	109904.	1.6	1.6	0.3030*
52	109.00	25	172256.	2.5	2.5	0.4749*	107	46.00	8	1927.	0.0	0.0	0.0053
53	108.00	6	470.	0.0	0.0	0.0013	108	45.00	35	178764.	2.6	2.6	0.4928*
54	107.00	8	1085.	0.0	0.0	0.0030	109	44.00	35	253840.	3.7	3.7	0.6998
55	101.00	8	2072.	0.0	0.0	0.0057	110	43.00	59	6950400.	100.0	100.0	*19.16*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	42.00	35	413088.	5.9	5.9	1.1388*
112	41.00	51	3606848.	51.9	51.9	9.9433*
113	40.00	35	235588.	3.4	3.4	0.6495*
114	39.00	59	1629888.	23.5	23.5	4.4932*
115	38.00	35	157172.	2.3	2.3	0.4333*
116	37.00	14	41186.	0.6	0.6	0.1135*
117	36.00	21	109704.	1.6	1.6	0.3024*
118	35.00	12	26033.	0.4	0.4	0.0718*

BH3AV.1 [TIC-142815232, 150X-25740288] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	341.00	6	1348.	0.0	0.0	0.0009	56	91.00	25	1255488.	4.9	4.9	0.8791
2	281.00	10	9491.	0.0	0.0	0.0066	57	90.00	8	8506.	0.0	0.0	0.0060
3	231.00	8	5371.	0.0	0.0	0.0038	58	89.00	6	2102.	0.0	0.0	0.0015
4	200.00	8	1883.	0.0	0.0	0.0013	59	88.00	10	7121.	0.0	0.0	0.0050
5	199.00	12	87084.	0.3	0.3	0.0610	60	87.00	10	5723.	0.0	0.0	0.0040
6	198.00	8	5923.	0.0	0.0	0.0041	61	86.00	6	1275.	0.0	0.0	0.0009
7	197.00	8	2037.	0.0	0.0	0.0014	62	85.00	8	2977.	0.0	0.0	0.0021
8	184.00	10	19176.	0.1	0.1	0.0134	63	84.00	17	160600.	0.6	0.6	0.1125
9	182.00	21	486720.	1.9	1.9	0.0340	64	83.00	35	6383360.	24.8	24.8	4.4697*
10	181.00	10	26195.	0.1	0.1	0.0183	65	82.00	10	21529.	0.1	0.1	0.0151
11	180.00	10	5613.	0.0	0.0	0.0039	66	81.00	21	262256.	1.0	1.0	0.1836*
12	179.00	17	183792.	0.7	0.7	0.01287	67	80.00	14	97676.	0.4	0.4	0.0684*
13	171.00	8	4012.	0.0	0.0	0.0028	68	79.00	10	19992.	0.1	0.1	0.0140*
14	170.00	17	219424.	0.9	0.9	0.01536	69	78.00	8	1585.	0.0	0.0	0.0011
15	169.00	29	3375936.	13.1	13.1	2.3638*	70	77.00	12	90652.	0.4	0.4	0.0635*
16	168.00	6	764.	0.0	0.0	0.0005	71	74.00	6	3272.	0.0	0.0	0.0023
17	167.00	10	2125.	0.0	0.0	0.0015	72	73.00	14	101060.	0.4	0.4	0.0708*
18	165.00	8	1875.	0.0	0.0	0.0013	73	72.00	21	466480.	1.8	1.8	0.3266*
19	163.00	14	127436.	0.5	0.5	0.0082	74	71.00	35	9679360.	37.6	37.6	6.7775*
20	159.00	6	1531.	0.0	0.0	0.0011	75	70.00	25	1148992.	4.5	4.5	0.8045
21	158.00	14	100216.	0.4	0.4	0.00702	76	69.00	35	4445696.	17.3	17.3	3.1129
22	157.00	25	1147456.	4.5	4.5	0.8035*	77	68.00	14	104492.	0.4	0.4	0.0732*
23	156.00	59	22653952.	88.0	88.0	*15.86*	78	67.00	17	251556.	1.0	1.0	0.1761*
24	155.00	35	1361152.	5.3	5.3	0.09531*	79	66.00	10	21394.	0.1	0.1	0.0150*
25	154.00	8	2241.	0.0	0.0	0.0016	80	65.00	17	105656.	0.4	0.4	0.0740*
26	153.00	6	7863.	0.0	0.0	0.0055	81	64.00	25	755936.	2.9	2.9	0.5293
27	151.00	8	2084.	0.0	0.0	0.0015	82	63.00	21	389344.	1.5	1.5	0.2726*
28	149.00	10	41913.	0.2	0.2	0.0293	83	62.00	12	12918.	0.1	0.1	0.0090*
29	149.00	21	740992.	2.9	2.9	0.5188	84	61.00	21	276240.	1.1	1.1	0.1934*
30	142.00	10	41340.	0.2	0.2	0.0289*	85	60.00	6	6436.	0.0	0.0	0.0045
31	141.00	17	273952.	1.1	1.1	0.1918	86	59.00	17	178780.	0.7	0.7	0.1252*
32	140.00	8	5823.	0.0	0.0	0.0041	87	58.00	17	246140.	1.0	1.0	0.1723*
33	139.00	8	8509.	0.0	0.0	0.0060	88	57.00	35	5058048.	19.7	19.7	3.5417*
34	138.00	6	2149.	0.0	0.0	0.0015	89	56.00	35	5692672.	22.1	22.1	3.9860
35	137.00	17	189944.	0.7	0.7	0.1330*	90	55.00	21	7107584.	27.6	27.6	4.9760*
36	136.00	29	3062848.	11.9	11.9	2.1446	91	54.00	21	226016.	0.9	0.9	0.1583*
37	135.00	29	1749184.	6.8	6.8	1.2248*	92	53.00	29	1031088.	4.0	4.0	0.0761*
38	134.00	17	67240.	0.3	0.3	0.0471*	93	52.00	14	108632.	0.4	0.4	0.0419
39	131.00	12	80028.	0.3	0.3	0.0560*	94	51.00	25	588208.	2.3	2.3	0.0504*
40	128.00	12	37216.	0.1	0.1	0.0261	95	50.00	17	203308.	0.8	0.8	0.1424
41	127.00	25	1638144.	6.4	6.4	1.1470	96	49.00	12	71916.	0.3	0.3	0.0416
42	124.00	8	1474.	0.0	0.0	0.0010	97	47.00	21	345104.	1.3	1.3	0.0513*
43	123.00	14	154904.	0.6	0.6	0.1085*	98	45.00	35	733008.	2.8	2.8	0.5133*
44	121.00	10	3926.	0.0	0.0	0.0027	99	44.00	35	1006288.	3.9	3.9	0.7046*
45	119.00	25	165284.	0.6	0.6	0.1157*	100	43.00	51	25740288.	100.0	100.0	19.02*
46	116.00	17	78184.	0.3	0.3	0.0547*	101	42.00	35	4611840.	17.9	17.9	3.2292*
47	113.00	17	279296.	1.1	1.1	0.1956	102	41.00	43	13186816.	51.2	51.2	9.2335*
48	110.00	10	20602.	0.1	0.1	0.0144	103	40.00	35	1063552.	4.1	4.1	0.7447*
49	109.00	25	1246144.	4.8	4.8	0.8726*	104	39.00	43	6229504.	24.2	24.2	4.3619*
50	101.00	10	27017.	0.1	0.1	0.0189	105	38.00	29	426960.	1.7	1.7	0.2990*
51	100.00	17	151316.	0.6	0.6	0.1060	106	37.00	17	117752.	0.5	0.5	0.0825*
52	99.00	29	2460608.	9.6	9.6	1.7229	107	36.00	17	229352.	0.9	0.9	0.1606*
53	98.00	10	48282.	0.2	0.2	0.0338	108	35.00	14	48546.	0.2	0.2	0.0340*
54	97.00	12	31690.	0.1	0.1	0.0222*							
55	92.00	10	22707.	0.1	0.1	0.0159							

803PA.1 [TIC-68431872, 188X-11631616] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	13899.	0.1	0.1	0.0203	56	84.00	14	69252.	0.6	0.6	0.1012*
2	269.00	6	3027.	0.0	0.0	0.0044	57	83.00	35	4137088.	35.6	35.6	0.0456*
3	267.00	12	5380.	0.0	0.0	0.0079	58	82.00	10	20055.	0.2	0.2	0.0293*
4	231.00	8	7484.	0.1	0.1	0.0108	59	81.00	14	66016.	0.6	0.6	0.0965*
5	219.00	6	8300.	0.1	0.1	0.0121	60	80.00	21	188996.	1.6	1.6	0.2762*
6	207.00	6	1914.	0.0	0.0	0.0028	61	78.00	12	78460.	0.7	0.7	0.1147
7	199.00	12	40185.	0.3	0.3	0.0087	62	77.00	21	444240.	3.8	3.8	0.6492
8	198.00	6	1516.	0.0	0.0	0.0022	63	75.00	12	4479.	0.0	0.0	0.0065
9	193.00	8	1268.	0.0	0.0	0.0019	64	74.00	17	137940.	1.2	1.2	0.0016*
10	183.00	14	115660.	1.0	1.0	0.1690	65	73.00	17	140676.	1.2	1.2	0.2056*
11	181.00	10	44504.	0.4	0.4	0.0650	66	72.00	12	59002.	0.5	0.5	0.0862*
12	179.00	12	20186.	0.2	0.2	0.0295	67	71.00	29	1457152.	12.5	12.5	2.1293
13	171.00	12	5991.	0.1	0.1	0.0088	68	70.00	25	568736.	4.9	4.9	0.8311*
14	170.00	14	103020.	0.9	0.9	0.1505	69	69.00	35	2609280.	22.4	22.4	3.8130
15	169.00	25	1761856.	15.1	15.1	2.5746	70	68.00	12	96748.	0.8	0.8	0.1414
16	168.00	10	9657.	0.1	0.1	0.0141	71	67.00	10	56557.	0.5	0.5	0.0826
17	164.00	6	1534.	0.0	0.0	0.0022	72	66.00	8	4297.	0.0	0.0	0.0063
18	163.00	10	23294.	0.2	0.2	0.0340	73	65.00	17	37494.	0.3	0.3	0.0548*
19	156.00	10	34236.	0.3	0.3	0.0500	74	64.00	21	246360.	2.1	2.1	0.3600*
20	155.00	21	341072.	2.9	2.9	0.4984	75	63.00	17	154508.	1.3	1.3	0.2258*
21	154.00	10	2219.	0.0	0.0	0.0032	76	62.00	8	4062.	0.0	0.0	0.0059
22	153.00	12	22021.	0.2	0.2	0.0322	77	61.00	17	161776.	1.4	1.4	0.2364*
23	151.00	8	1003.	0.0	0.0	0.0015	78	60.00	8	8450.	0.1	0.1	0.0123
24	150.00	8	5420.	0.0	0.0	0.0079	79	59.00	12	66120.	0.6	0.6	0.0966*
25	149.00	21	298320.	2.6	2.6	0.4359	80	58.00	25	260964.	2.2	2.2	0.3813*
26	145.00	8	2252.	0.0	0.0	0.0033	81	57.00	35	5321984.	45.8	45.8	7.7771
27	144.00	14	69456.	0.6	0.6	1.015*	82	56.00	29	1768576.	15.2	15.2	2.5844
28	143.00	25	1075008.	9.2	9.2	1.5709*	83	55.00	35	3518848.	30.3	30.3	5.1421*
29	142.00	43	11631616.	100.0	100.0	*16.99*	84	54.00	17	126516.	1.1	1.1	0.1849*
30	141.00	25	675472.	5.8	5.8	0.9871*	85	53.00	25	504928.	4.3	4.3	0.7379
31	140.00	14	118916.	1.0	1.0	0.1738*	86	52.00	21	37504.	0.3	0.3	0.0548*
32	139.00	10	22783.	0.2	0.2	0.0333	87	51.00	21	285312.	2.5	2.5	0.4169*
33	136.00	6	2340.	0.0	0.0	0.0034	88	50.00	14	99332.	0.9	0.9	0.1452*
34	135.00	14	131048.	1.1	1.1	0.1915*	89	49.00	12	33613.	0.3	0.3	0.0491*
35	131.00	17	107696.	0.9	0.9	0.1574*	90	48.00	8	2745.	0.0	0.0	0.0040
36	128.00	14	120148.	1.0	1.0	0.1756*	91	47.00	25	287200.	2.5	2.5	0.4197*
37	127.00	29	3462784.	29.8	29.8	5.0602	92	46.00	10	3368.	0.0	0.0	0.0049
38	126.00	10	75060.	0.6	0.6	0.1097	93	45.00	21	241980.	2.1	2.1	0.3536*
39	124.00	10	5044.	0.0	0.0	0.0074	94	44.00	35	427984.	3.7	3.7	0.6254*
40	123.00	21	443344.	3.8	3.8	0.6479*	95	43.00	43	6938624.	59.7	59.7	*10.13*
41	122.00	21	1035136.	8.9	8.9	1.5127	96	42.00	35	3060224.	26.3	26.3	4.4719
42	119.00	17	133640.	1.1	1.1	0.1953	97	41.00	35	6828288.	58.7	58.7	9.9782*
43	113.00	21	216720.	1.9	1.9	0.3167	98	40.00	29	465664.	4.0	4.0	0.6805*
44	107.00	6	8611.	0.1	0.1	0.0126	99	39.00	35	2541888.	21.9	21.9	3.7145
45	105.00	12	12998.	0.1	0.1	0.0190*	100	38.00	17	164108.	1.4	1.4	0.2398*
46	104.00	8	1687.	0.0	0.0	0.0025	101	37.00	14	34122.	0.3	0.3	0.0499*
47	103.00	6	2637.	0.0	0.0	0.0039	102	36.00	17	106592.	0.9	0.9	0.1558*
48	101.00	6	1117.	0.0	0.0	0.0016	103	35.00	14	13052.	0.1	0.1	0.0191
49	100.00	17	140328.	1.2	1.2	0.2051*							
50	99.00	29	2070912.	17.8	17.8	3.0262*							
51	98.00	12	30924.	0.3	0.3	0.0452*							
52	97.00	12	54849.	0.5	0.5	0.0802							
53	91.00	6	1290.	0.0	0.0	0.0019							
54	87.00	10	8349.	0.1	0.1	0.0122							
55	85.00	8	5278.	0.0	0.0	0.0077							

8XAV3.1 [TIC-121663488, 188X-19456888] EI

4ALPA.1 [TIC-187287688, 188X-27485312] EI

Hexanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_4\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	269.00	8	2374.	0.0	0.0	0.0013	56	100.00	21	483232.	1.8	1.8	0.2581
2	243.00	6	1350.	0.0	0.0	0.0007	57	99.00	35	7783040.	28.1	28.1	4.1147*
3	231.00	10	5495.	0.0	0.0	0.0029	58	98.00	17	497968.	1.8	1.8	0.2660
4	200.00	6	1751.	0.0	0.0	0.0009	59	97.00	17	233500.	0.9	0.9	0.1247
5	199.00	17	213176.	0.8	0.8	0.1139	60	95.00	8	2413.	0.0	0.0	0.0013
6	198.00	14	144584.	0.5	0.5	0.0772	61	91.00	17	251080.	0.9	0.9	0.1341
7	197.00	8	5925.	0.0	0.0	0.0032	62	87.00	14	4480.	0.0	0.0	0.0024*
8	183.00	6	10783.	0.0	0.0	0.0058	63	85.00	8	8172.	0.0	0.0	0.0044
9	181.00	10	29189.	0.1	0.1	0.0156	64	84.00	17	199724.	0.7	0.7	0.1067
10	180.00	10	57190.	0.2	0.2	0.0305	65	83.00	43	9497600.	34.7	34.7	5.0733*
11	179.00	17	553040.	2.0	2.0	0.2954*	66	82.00	10	37444.	0.1	0.1	0.0200
12	171.00	10	16467.	0.1	0.1	0.0088	67	81.00	25	417264.	1.5	1.5	0.2229
13	170.00	17	249020.	0.9	0.9	0.1330	68	80.00	25	1077184.	3.9	3.9	0.5754
14	169.00	29	3372224.	12.3	12.3	1.8013*	69	79.00	12	50979.	0.2	0.2	0.0272*
15	167.00	10	3173.	0.0	0.0	0.0017	70	78.00	21	306448.	1.1	1.1	0.1637*
16	165.00	8	13985.	0.1	0.1	0.0075	71	77.00	21	1561792.	5.7	5.7	0.8343
17	157.00	12	70568.	0.3	0.3	0.0377	72	75.00	17	49132.	0.2	0.2	0.0262
18	156.00	21	1060160.	3.9	3.9	0.5603*	73	74.00	21	482288.	1.8	1.8	0.2576
19	155.00	51	11368448.	41.5	41.5	6.0726*	74	73.00	14	90792.	0.3	0.3	0.0485*
20	154.00	12	14580.	0.1	0.1	0.0078*	75	72.00	17	212740.	0.8	0.8	0.1136*
21	153.00	8	12316.	0.0	0.0	0.0065	76	71.00	29	4133952.	15.1	15.1	2.2082
22	152.00	6	1402.	0.0	0.0	0.0007	77	70.00	29	3481600.	12.7	12.7	1.8598
23	151.00	8	2339.	0.0	0.0	0.0012	78	69.00	35	3955776.	14.4	14.4	2.1130*
24	150.00	8	1653.	0.0	0.0	0.0009	79	68.00	21	272688.	1.0	1.0	0.1457
25	149.00	17	168768.	0.6	0.6	0.0902	80	67.00	21	277824.	1.0	1.0	0.1484*
26	145.00	5	811.	0.0	0.0	0.0004	81	66.00	10	35480.	0.1	0.1	0.0190*
27	144.00	17	156580.	0.6	0.6	0.0836	82	65.00	17	126216.	0.5	0.5	0.0672
28	143.00	35	2061312.	7.5	7.5	1.1011*	83	64.00	21	804480.	2.9	2.9	0.2490
29	142.00	59	26999808.	98.5	98.5	*14.42*	84	63.00	25	466128.	1.7	1.7	0.0122
30	141.00	29	558736.	2.0	2.0	0.2985*	85	62.00	8	22866.	0.1	0.1	0.01854*
31	140.00	14	73240.	0.3	0.3	0.0391	86	61.00	25	347040.	1.3	1.3	0.0341*
32	139.00	12	65153.	0.2	0.2	0.0348	87	60.00	12	63897.	0.2	0.2	0.0769*
33	137.00	12	51064.	0.2	0.2	0.0273*	88	59.00	17	144024.	0.5	0.5	0.1655*
34	136.00	17	358976.	1.3	1.3	0.1918	89	58.00	25	309904.	1.1	1.1	0.0769*
35	135.00	25	2491264.	9.1	9.1	0.1307*	90	57.00	35	5153792.	18.8	18.8	2.7530*
36	131.00	10	49855.	0.2	0.2	0.0266*	91	56.00	35	3029760.	11.1	11.1	1.6184*
37	129.00	8	15828.	0.1	0.1	0.0085	92	55.00	51	12298496.	44.9	44.9	6.5694*
38	128.00	17	195656.	0.7	0.7	0.1045	93	54.00	21	383968.	1.4	1.4	0.2051
39	127.00	35	5405952.	19.7	19.7	2.8877*	94	53.00	25	973568.	3.6	3.6	0.5200
40	126.00	14	86124.	0.3	0.3	0.0460*	95	52.00	17	136448.	0.5	0.5	0.0729*
41	125.00	6	1667.	0.0	0.0	0.0009	96	51.00	25	657040.	2.4	2.4	0.3510*
42	124.00	8	5370.	0.0	0.0	0.0029	97	50.00	21	216848.	0.8	0.8	0.1158*
43	123.00	17	257280.	0.9	0.9	0.1374	98	49.00	8	31299.	0.1	0.1	0.0167
44	122.00	25	3017856.	11.0	11.0	1.6120*	99	48.00	14	96440.	0.4	0.4	0.0515*
45	119.00	12	81264.	0.3	0.3	0.0434	100	47.00	21	487024.	1.8	1.8	0.2602
46	118.00	21	77708.	0.3	0.3	0.0415*	101	46.00	12	45953.	0.2	0.2	0.0245
47	117.00	12	29857.	0.1	0.1	0.0159	102	45.00	29	670928.	2.4	2.4	0.3584
48	113.00	17	505216.	1.8	1.8	0.2699	103	44.00	35	1653760.	6.0	6.0	0.8834
49	109.00	17	332512.	1.2	1.2	0.1776	104	43.00	59	27405312.	100.0	100.0	*14.63*
50	107.00	10	25766.	0.1	0.1	0.0138*	105	42.00	43	11640320.	42.5	42.5	6.2179*
51	106.00	8	6624.	0.0	0.0	0.0035	106	41.00	43	15408640.	56.2	56.2	8.2308*
52	105.00	21	55836.	0.2	0.2	0.0298*	107	40.00	29	1184000.	4.3	4.3	0.6325*
53	104.00	6	2948.	0.0	0.0	0.0016	108	39.00	43	7021568.	25.6	25.6	3.7507*
54	103.00	6	1336.	0.0	0.0	0.0007	109	38.00	29	422400.	1.5	1.5	0.2256*
55	101.00	12	22152.	0.1	0.1	0.0118*	110	37.00	17	112204.	0.4	0.4	0.0599*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	36.00	21	182000.	0.7	0.7	0.0973*
112	35.00	8	10577.	0.0	0.0	0.0056

8H4AV.1 [TIC=142831616, 188X=24838976] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	231.00	10	1889.	0.0	0.0	0.0013	56	109.00	21	835056.	3.4	3.4	0.5846
2	214.00	8	2679.	0.0	0.0	0.0019	57	107.00	8	4765.	0.0	0.0	0.0033
3	213.00	14	99136.	0.4	0.4	0.0694*	58	99.00	6	1278.	0.0	0.0	0.0009
4	212.00	12	91488.	0.4	0.4	0.0641	59	97.00	14	129140.	0.5	0.5	0.0904
5	192.00	8	1282.	0.0	0.0	0.0009	60	95.00	17	255628.	1.0	1.0	0.1790*
6	190.00	17	188840.	0.8	0.8	0.1322	61	94.00	8	12606.	0.1	0.1	0.0088
7	194.00	8	1708.	0.0	0.0	0.0012	62	92.00	6	2413.	0.0	0.0	0.0017
8	193.00	17	161248.	0.6	0.6	0.1129*	63	92.00	8	26150.	0.1	0.1	0.0183
9	184.00	10	62990.	0.3	0.3	0.0441	64	91.00	25	1189952.	4.8	4.8	0.8331
10	183.00	21	940528.	3.8	3.8	0.6585	65	90.00	8	10305.	0.0	0.0	0.0072
11	181.00	8	19643.	0.1	0.1	0.0138	66	88.00	8	6348.	0.0	0.0	0.0044
12	179.00	6	3387.	0.0	0.0	0.0024	67	87.00	8	17717.	0.1	0.1	0.0124
13	171.00	10	27425.	0.1	0.1	0.0192	68	86.00	17	293600.	1.2	1.2	0.2056
14	170.00	21	473920.	0.1	0.1	0.3318*	69	85.00	35	5329664.	1.2	1.2	0.2056
15	169.00	35	6556416.	26.4	26.4	4.5903*	70	84.00	29	589600.	2.4	2.4	0.4128*
16	168.00	6	2229.	0.0	0.0	0.0016	71	83.00	35	6217472.	25.0	25.0	4.3530*
17	167.00	8	15835.	0.1	0.1	0.0111	72	82.00	10	47069.	0.2	0.2	0.0330*
18	165.00	6	1256.	0.0	0.0	0.0009	73	81.00	17	135244.	0.5	0.5	0.0947*
19	164.00	6	3989.	0.0	0.0	0.0028	74	80.00	14	90576.	0.4	0.4	0.0634
20	163.00	10	48559.	0.2	0.2	0.0340	75	79.00	12	73716.	0.3	0.3	0.0516*
21	159.00	6	1487.	0.0	0.0	0.0010	76	78.00	10	9086.	0.0	0.0	0.0064
22	158.00	17	118300.	0.5	0.5	0.0828*	77	77.00	14	138828.	0.6	0.6	0.0972
23	157.00	29	1260480.	5.1	5.1	0.8825*	78	75.00	8	7370.	0.0	0.0	0.0052
24	156.00	71	24830976.	100.0	100.0	*17.38*	79	74.00	8	8689.	0.0	0.0	0.0061
25	155.00	35	1417408.	5.7	5.7	0.9924*	80	73.00	14	114716.	0.5	0.5	0.0803*
26	154.00	8	1582.	0.0	0.0	0.0011	81	72.00	6	1834.	0.0	0.0	0.0013
27	153.00	8	21442.	0.1	0.1	0.0150	82	71.00	17	175980.	0.7	0.7	0.1232
28	151.00	10	25425.	0.1	0.1	0.0178	83	70.00	25	1261184.	5.1	5.1	0.8830
29	150.00	10	42321.	0.2	0.2	0.0296	84	69.00	35	4201472.	16.9	16.9	2.9416*
30	149.00	21	1093824.	4.4	4.4	0.7658	85	68.00	21	260508.	1.0	1.0	0.1824*
31	142.00	12	74354.	0.3	0.3	0.0521*	86	67.00	21	368992.	1.5	1.5	0.2583*
32	141.00	17	404544.	1.6	1.6	0.2832	87	66.00	8	30465.	0.1	0.1	0.0213
33	140.00	8	6802.	0.0	0.0	0.0048	88	65.00	14	127212.	0.5	0.5	0.0891
34	139.00	10	21932.	0.1	0.1	0.0154	89	64.00	25	575984.	2.3	2.3	0.4033
35	138.00	6	1934.	0.0	0.0	0.0014	90	63.00	21	283808.	1.1	1.1	0.1987*
36	137.00	14	184104.	0.7	0.7	0.1289	91	62.00	10	8795.	0.0	0.0	0.0062
37	136.00	35	3148160.	12.7	12.7	2.2041*	92	61.00	17	236592.	1.0	1.0	0.1656
38	135.00	35	1781184.	7.2	7.2	1.2471*	93	59.00	21	195196.	0.8	0.8	0.1367*
39	134.00	14	39165.	0.2	0.2	0.0274*	94	58.00	25	392224.	1.6	1.6	0.2746*
40	132.00	8	6051.	0.0	0.0	0.0042	95	57.00	43	7908608.	31.8	31.8	5.5370*
41	131.00	14	67392.	0.3	0.3	0.0472*	96	56.00	35	6942720.	28.0	28.0	4.8608
42	129.00	8	15111.	0.1	0.1	0.0106	97	55.00	35	8180480.	32.9	32.9	5.7274*
43	128.00	14	90340.	0.4	0.4	0.0632*	98	54.00	25	334752.	1.3	1.3	0.2344*
44	127.00	25	2449344.	9.9	9.9	1.7148	99	53.00	29	1036320.	4.2	4.2	0.7256
45	123.00	14	94344.	0.4	0.4	0.0661	100	52.00	14	118816.	0.5	0.5	0.0832*
46	121.00	8	7817.	0.0	0.0	0.0055	101	51.00	25	506544.	2.0	2.0	0.3546
47	120.00	6	2171.	0.0	0.0	0.0015	102	50.00	17	177340.	0.7	0.7	0.1242*
48	119.00	29	209596.	0.8	0.8	0.1467*	103	49.00	8	19320.	0.1	0.1	0.0135*
49	118.00	17	60686.	0.2	0.2	0.0425*	104	47.00	21	330432.	1.3	1.3	0.2313*
50	115.00	6	2232.	0.0	0.0	0.0016	105	45.00	29	534432.	2.2	2.2	0.3742*
51	114.00	14	115988.	0.5	0.5	0.0812*	106	44.00	35	817120.	3.3	3.3	0.5721*
52	113.00	29	2075840.	8.4	8.4	1.4533	107	43.00	51	18590720.	74.9	74.9	*13.01*
53	112.00	12	123340.	0.5	0.5	0.0864	108	42.00	35	3405056.	13.7	13.7	2.3840
54	111.00	10	32907.	0.1	0.1	0.0230	109	41.00	43	14731008.	59.3	59.3	*10.31*
55	110.00	10	5855.	0.0	0.0	0.0041	110	40.00	35	1013376.	4.1	4.1	0.7095*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	39.00	35	5375488.	21.6	21.6	3.7635*
112	38.00	25	284432.	1.1	1.1	0.1991*
113	37.00	14	83624.	0.3	0.3	0.0585*
114	36.00	14	193420.	0.8	0.8	0.1354*
115	35.00	17	42289.	0.2	0.2	0.0296*

FV2AV.1 [TIC-71667712, 100X-12842249] E1

5-methylhexanoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	267.00	6	1212.	0.0	0.0	0.0017	56	107.00	8	4197.	0.0	0.0	0.0059
2	243.00	6	1289.	0.0	0.0	0.0018	57	105.00	8	5222.	0.0	0.0	0.0073
3	231.00	6	1150.	0.0	0.0	0.0016	58	104.00	6	3018.	0.0	0.0	0.0042
4	213.00	10	30303.	0.3	0.0	0.00423	59	99.00	8	3677.	0.0	0.0	0.0051
5	211.00	8	1964.	0.0	0.0	0.0027	60	98.00	17	84120.	0.7	0.7	0.1174*
6	201.00	6	754.	0.0	0.0	0.0011	61	97.00	35	1100096.	9.1	9.1	1.5350*
7	197.00	17	72912.	0.6	0.6	0.1017*	62	96.00	21	157784.	1.3	1.3	0.2222*
8	196.00	8	976.	0.0	0.0	0.0014	63	95.00	35	1930944.	16.0	16.0	2.6943*
9	195.00	12	10092.	0.1	0.1	0.0141	64	94.00	29	607808.	5.0	5.0	0.8481*
10	194.00	21	179256.	1.5	1.5	0.2501	65	93.00	8	3358.	0.0	0.0	0.0047
11	193.00	8	7097.	0.1	0.1	0.0099	66	91.00	8	9757.	0.1	0.1	0.0136
12	184.00	10	10007.	0.1	0.1	0.0140	67	85.00	21	102800.	0.9	0.9	0.1434*
13	181.00	8	11112.	0.1	0.1	0.0155	68	84.00	25	198440.	1.6	1.6	0.2769
14	179.00	17	89016.	0.7	0.7	0.1242	69	83.00	43	2503744.	20.8	20.8	3.4935*
15	172.00	8	2185.	0.0	0.0	0.0030	70	82.00	10	29064.	0.2	0.2	0.0406*
16	171.00	21	158992.	1.3	1.3	0.2218*	71	81.00	17	96312.	0.8	0.8	0.1344*
17	170.00	25	290688.	2.4	2.4	0.4056*	72	80.00	29	181156.	1.5	1.5	0.2528*
18	169.00	35	18624.	20.1	20.1	3.3748*	73	79.00	21	149268.	1.2	1.2	0.2083*
19	168.00	12	18795.	0.2	0.2	0.0262*	74	78.00	17	74604.	0.6	0.6	0.1041*
20	157.00	6	1091.	0.0	0.0	0.0015	75	77.00	29	307040.	2.5	2.5	0.4284*
21	156.00	21	176848.	1.5	1.5	0.2468	76	76.00	8	1819.	0.0	0.0	0.0025
22	155.00	35	1487936.	12.4	12.4	2.0762*	77	75.00	10	6179.	0.1	0.1	0.0086
23	154.00	14	5005.	0.0	0.0	0.0070*	78	74.00	17	87964.	0.7	0.7	0.1227*
24	153.00	12	33753.	0.3	0.0	0.0471*	79	73.00	12	43014.	0.4	0.4	0.0600*
25	152.00	8	4639.	0.0	0.0	0.0065	80	72.00	21	160896.	1.3	1.3	0.2245
26	151.00	12	45151.	0.4	0.4	0.0630*	81	71.00	43	3304384.	27.4	27.4	4.6107*
27	149.00	8	5106.	0.0	0.0	0.0071*	82	70.00	35	705168.	5.9	5.9	0.9839*
28	145.00	8	1246.	0.0	0.0	0.0017	83	69.00	43	6826752.	56.7	56.7	9.5256*
29	144.00	10	9822.	0.1	0.1	0.0137	84	68.00	29	330128.	2.7	2.7	0.4136*
30	143.00	25	320032.	2.7	2.7	0.4577	85	67.00	25	296384.	2.5	2.5	0.4136*
31	142.00	43	6480384.	53.8	53.8	9.0423*	86	66.00	12	32819.	0.3	0.3	0.0458*
32	141.00	17	38036.	0.3	0.3	0.0542*	87	65.00	17	81690.	0.7	0.7	0.1140*
33	140.00	8	13543.	0.1	0.1	0.0189*	88	64.00	25	218912.	1.8	1.8	0.3055*
34	139.00	8	13478.	0.0	0.0	0.0188	89	63.00	25	162356.	1.3	1.3	0.2264
35	138.00	6	2094.	0.0	0.0	0.0029	90	62.00	6	2593.	0.0	0.0	0.0036
36	137.00	10	10000.	0.1	0.1	0.0140	91	61.00	21	112732.	0.9	0.9	0.1573*
37	136.00	14	51552.	0.4	0.4	0.0719*	92	60.00	10	18024.	0.1	0.1	0.0251*
38	135.00	25	257560.	2.1	2.1	0.3594	93	59.00	12	36415.	0.3	0.3	0.0500*
39	131.00	12	30020.	0.2	0.2	0.0419*	94	58.00	17	49478.	0.4	0.4	0.0690*
40	130.00	6	1065.	0.0	0.0	0.0015	95	57.00	35	808064.	6.7	6.7	1.1275
41	129.00	10	7797.	0.1	0.1	0.0109*	96	56.00	35	861440.	7.2	7.2	1.2020*
42	128.00	14	54046.	0.4	0.4	0.0754*	97	55.00	43	3748928.	31.1	31.1	5.2310*
43	127.00	35	1279488.	10.6	10.6	1.7853	98	54.00	21	147888.	1.2	1.2	0.2064*
44	126.00	12	13965.	0.1	0.1	0.0195*	99	53.00	29	480560.	4.0	4.0	0.6705*
45	123.00	12	34870.	0.3	0.3	0.0475	100	52.00	17	51532.	0.4	0.4	0.0719*
46	122.00	29	594912.	4.9	4.9	0.8301	101	51.00	35	254980.	2.1	2.1	0.3558*
47	119.00	10	21122.	0.2	0.2	0.0295	102	50.00	21	86460.	0.7	0.7	0.1206*
48	118.00	8	2534.	0.0	0.0	0.0035	103	49.00	12	47130.	0.4	0.4	0.0658*
49	117.00	8	2060.	0.0	0.0	0.0029	104	48.00	25	223632.	1.9	1.9	0.3120*
50	114.00	14	59711.	0.5	0.5	0.0033*	105	47.00	21	141792.	1.2	1.2	0.1978*
51	113.00	35	937216.	7.8	7.8	1.3077	106	46.00	8	2106.	0.0	0.0	0.0029
52	112.00	25	176100.	1.5	1.5	0.2457*	107	45.00	29	214260.	1.8	1.8	0.2990*
53	111.00	17	84192.	0.7	0.7	0.1175*	108	44.00	43	541264.	4.5	4.5	0.7552*
54	110.00	8	3259.	0.0	0.0	0.0045	109	43.00	59	12042240.	100.0	100.0	*16.80*
55	109.00	21	135796.	1.1	1.1	0.1895*	110	42.00	51	3936896.	32.7	32.7	5.4933*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	41.00	51	8314112.	69.0	69.0	*11.60*
112	40.00	35	637872.	5.3	5.3	0.8900*
113	39.00	43	2971968.	24.7	24.7	4.1469*
114	38.00	35	189436.	1.6	1.6	0.2643*
115	37.00	17	36586.	0.3	0.3	0.0510*
116	36.00	25	148940.	1.2	1.2	0.2078*
117	35.00	17	42969.	0.4	0.4	0.0600*

SALPA.1 [TIC-181813248, 180X-26882848] EI

Heptanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_5\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	201.00	8	2052.	0.0	0.0	0.0011	56	113.00	35	6099968.	22.7	22.7	3.3551*
2	231.00	6	2106.	0.0	0.0	0.0012	57	112.00	14	97600.	0.4	0.4	0.0537
3	219.00	12	5487.	0.0	0.0	0.0030	58	111.00	14	112788.	0.4	0.4	0.0620
4	214.00	8	14907.	0.1	0.1	0.0082	59	110.00	8	7924.	0.0	0.0	0.0044
5	213.00	17	203500.	0.8	0.8	0.1119	60	109.00	17	332272.	1.2	1.2	0.1828
6	212.00	17	408928.	1.5	1.5	0.2249	61	107.00	8	6943.	0.0	0.0	0.0038
7	211.00	8	3043.	0.0	0.0	0.0017	62	106.00	6	2019.	0.0	0.0	0.0011
8	197.00	10	56151.	0.2	0.2	0.0309	63	105.00	25	85272.	0.3	0.3	0.0439*
9	195.00	6	2639.	0.0	0.0	0.0015	64	104.00	6	1574.	0.0	0.0	0.0009
10	194.00	10	41425.	0.2	0.2	0.0228	65	102.00	10	3846.	0.0	0.0	0.0021
11	193.00	21	41328.	1.5	1.5	0.2273*	66	100.00	8	2925.	0.0	0.0	0.0016
12	185.00	8	1935.	0.0	0.0	0.0011	67	99.00	8	4938.	0.0	0.0	0.0027
13	184.00	14	125100.	0.5	0.5	0.0688	68	98.00	8	2048.	0.0	0.0	0.0011
14	183.00	21	1490176.	5.5	5.5	0.8196	69	97.00	17	185748.	0.7	0.7	0.1022
15	181.00	8	20495.	0.1	0.1	0.0113	70	96.00	10	30050.	0.1	0.1	0.0165
16	171.00	10	27231.	0.1	0.1	0.0150	71	95.00	21	522256.	1.9	1.9	0.2872
17	170.00	17	382832.	1.4	1.4	0.2106*	72	94.00	17	168288.	0.6	0.6	0.0926
18	169.00	35	5478656.	20.4	20.4	3.0133*	73	93.00	8	6393.	0.0	0.0	0.0035
19	168.00	8	9696.	0.0	0.0	0.0053	74	91.00	17	180204.	0.7	0.7	0.0991*
20	167.00	8	2789.	0.0	0.0	0.0015	75	86.00	14	94896.	0.4	0.4	0.0522
21	165.00	10	32392.	0.1	0.1	0.0178	76	85.00	29	1671360.	6.2	6.2	0.9193*
22	163.00	10	56697.	0.2	0.2	0.0312	77	84.00	29	2798848.	10.4	10.4	1.5394
23	157.00	12	81080.	0.3	0.3	0.0446	78	83.00	14	8467712.	31.5	31.5	4.6574*
24	156.00	21	817920.	3.0	3.0	0.4499*	79	82.00	13	74220.	0.3	0.3	0.0408*
25	155.00	43	10998784.	40.9	40.9	6.0495*	80	81.00	21	195672.	0.7	0.7	0.1076*
26	154.00	12	13256.	0.0	0.0	0.0073	81	80.00	21	555216.	2.1	2.1	0.3054
27	153.00	12	29981.	0.1	0.1	0.0165	82	79.00	17	110512.	0.4	0.4	0.0608
28	151.00	6	1744.	0.0	0.0	0.0010	83	78.00	17	272480.	1.0	1.0	0.1499
29	150.00	6	2376.	0.0	0.0	0.0013	84	77.00	25	1250432.	4.7	4.7	0.6878
30	149.00	14	104352.	0.4	0.4	0.0574*	85	75.00	12	48094.	0.2	0.2	0.0265*
31	145.00	6	688.	0.0	0.0	0.0004	86	74.00	21	382976.	1.4	1.4	0.2106
32	144.00	17	156260.	0.6	0.6	0.0059	87	73.00	14	73116.	0.3	0.3	0.0402*
33	143.00	35	2328064.	8.7	8.7	1.2805*	88	72.00	17	223204.	0.8	0.8	0.1228
34	142.00	71	24602624.	91.5	91.5	*13.53*	89	71.00	29	4489472.	16.7	16.7	2.4693
35	141.00	29	1058112.	3.9	3.9	0.5820*	90	70.00	35	2459584.	9.1	9.1	1.3528
36	140.00	12	106576.	0.4	0.4	0.0586*	91	69.00	35	4458240.	16.6	16.6	2.4521
37	139.00	14	91368.	0.3	0.3	0.0503	92	68.00	25	1444416.	5.4	5.4	0.7945
38	137.00	10	34226.	0.1	0.1	0.0188	93	67.00	21	503680.	1.9	1.9	0.2770
39	136.00	17	320048.	1.2	1.2	0.1760	94	66.00	14	60299.	0.2	0.2	0.0332*
40	135.00	35	2520768.	9.4	9.4	1.3855*	95	65.00	17	137804.	0.5	0.5	0.0758
41	134.00	8	1372.	0.0	0.0	0.0008	96	64.00	25	593216.	2.2	2.2	0.3263*
42	131.00	10	46808.	0.2	0.2	0.0257	97	63.00	21	341488.	1.3	1.3	0.1878
43	125.00	8	5619.	0.0	0.0	0.0031	98	62.00	10	21207.	0.1	0.1	0.0117
44	128.00	25	119700.	0.4	0.4	0.0658	99	61.00	21	303296.	1.1	1.1	0.1668
45	127.00	25	3086720.	11.5	11.5	1.6977	100	60.00	10	35071.	0.1	0.1	0.0193*
46	126.00	8	42349.	0.2	0.2	0.0233	101	59.00	17	146328.	0.5	0.5	0.0805*
47	125.00	8	4485.	0.0	0.0	0.0025	102	58.00	25	267568.	1.0	1.0	0.1472
48	124.00	8	7952.	0.0	0.0	0.0044	103	57.00	29	3023104.	11.2	11.2	1.6628
49	123.00	17	284784.	1.1	1.1	0.1566	104	56.00	35	3142592.	11.7	11.7	1.7285*
50	122.00	25	2713024.	10.1	10.1	1.4922*	105	55.00	43	15378176.	57.2	57.2	8.4582*
51	119.00	12	55527.	0.2	0.2	0.0335	106	54.00	21	595664.	2.2	2.2	0.3276
52	118.00	25	82896.	0.3	0.3	0.0456*	107	53.00	25	1064256.	4.0	4.0	0.5854
53	117.00	12	37905.	0.1	0.1	0.0208*	108	52.00	17	136740.	0.5	0.5	0.0752
54	115.00	10	13286.	0.0	0.0	0.0073	109	51.00	21	465680.	1.7	1.7	0.2561
55	114.00	17	403952.	1.5	1.5	0.2222	110	50.00	21	181004.	0.7	0.7	0.0996

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	49.00	10	14414.	0.1	0.1	0.0079
112	48.00	14	118560.	0.4	0.4	0.0652*
113	47.00	21	326640.	1.2	1.2	0.1797*
114	46.00	12	23269.	0.1	0.1	0.0128
115	45.00	29	496992.	1.8	1.8	0.2734
116	44.00	35	1408000.	5.2	5.2	0.7744
117	43.00	59	26882048.	100.0	100.0	*14.78*
118	42.00	35	6747136.	25.1	25.1	3.7110*
119	41.00	51	16256512.	60.5	60.5	8.9413*
120	40.00	25	1025904.	3.8	3.8	0.5643*
121	39.00	43	5688320.	21.2	21.2	3.1287*
122	38.00	25	277984.	1.0	1.0	0.1529*
123	37.00	17	70244.	0.3	0.3	0.0386*
124	36.00	21	191920.	0.7	0.7	0.1056*
125	35.00	8	9296.	0.0	0.0	0.0051

6ALPA.1 [TIC=172855296, 100X-21587968] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	1144.	0.0	0.0	0.0007	56	118.00	25	99040.	0.5	0.5	0.0573*
2	228.00	8	7287.	0.0	0.0	0.0042	57	117.00	10	14513.	0.1	0.1	0.0084*
3	227.00	17	230680.	1.1	0.1335	0.1335	58	113.00	17	525264.	2.4	2.4	0.3039
4	226.00	21	816528.	3.8	0.4724*	0.4724*	59	111.00	10	47245.	0.2	0.2	0.0273*
5	211.00	14	112132.	0.5	0.0649	0.0649	60	110.00	8	14831.	0.1	0.1	0.0086
6	208.00	10	30221.	0.1	0.0175	0.0175	61	109.00	25	593280.	2.7	2.7	0.3432
7	207.00	17	329760.	1.5	0.1908	0.1908	62	108.00	17	99492.	0.5	0.5	0.0576
8	199.00	8	3866.	0.0	0.0	0.0022	63	107.00	10	23132.	0.1	0.1	0.0134
9	198.00	14	143444.	0.7	0.0830	0.0830	64	105.00	17	46636.	0.2	0.2	0.0270*
10	197.00	21	1497024.	6.9	0.8661	0.8661	65	104.00	8	7902.	0.0	0.0	0.0046
11	185.00	10	31293.	0.1	0.0181	0.0181	66	102.00	10	10016.	0.0	0.0	0.0058
12	184.00	17	307968.	1.4	0.1782	0.1782	67	100.00	6	3999.	0.3	0.3	0.0023
13	193.00	29	3720640.	17.2	2.1525*	2.1525*	68	99.00	14	73636.	0.4	0.4	0.0426
14	182.00	9	2266.	0.0	0.0	0.0013	69	98.00	21	892848.	4.1	4.1	0.5165
15	181.00	8	25092.	0.1	0.0145	0.0145	70	97.00	21	676432.	3.1	3.1	0.3913
16	179.00	6	3117.	0.0	0.0	0.0018	71	96.00	10	11432.	0.1	0.1	0.0066
17	177.00	10	26719.	0.1	0.0155	0.0155	72	95.00	12	38204.	0.2	0.2	0.0221
18	171.00	8	5625.	0.0	0.0	0.0033	73	94.00	6	1728.	0.0	0.0	0.0010
19	170.00	14	165064.	0.8	0.08	0.08	74	93.00	10	31402.	0.1	0.1	0.0182
20	169.00	21	2013120.	9.3	1.1646*	1.1646*	75	91.00	17	140740.	0.7	0.7	0.0814
21	168.00	12	6834.	0.0	0.0	0.0040	76	89.00	8	2822.	0.0	0.0	0.0016
22	167.00	8	10912.	0.1	0.0063	0.0063	77	87.00	10	12341.	0.1	0.1	0.0071
23	166.00	6	1346.	0.0	0.0	0.0008	78	86.00	17	303088.	1.4	1.4	0.1753
24	165.00	10	38689.	0.2	0.0224	0.0224	79	85.00	35	5575936.	25.8	25.8	3.2258*
25	163.00	10	33850.	0.2	0.0196	0.0196	80	84.00	35	3546432.	16.4	16.4	2.0517*
26	157.00	12	55477.	0.3	0.0321	0.0321	81	83.00	43	7818496.	36.2	36.2	4.5231*
27	156.00	25	852176.	3.9	0.4930*	0.4930*	82	82.00	25	1447424.	6.7	6.7	0.8374*
28	155.00	51	11932160.	55.3	6.9030*	6.9030*	83	81.00	21	318784.	1.5	1.5	0.1844
29	154.00	8	7023.	0.0	0.0041	0.0041	84	80.00	25	503168.	2.3	2.3	0.2911
30	153.00	14	75944.	0.4	0.0439	0.0439	85	79.00	17	186896.	0.9	0.9	0.1081*
31	152.00	8	19336.	0.1	0.0112	0.0112	86	78.00	21	224032.	1.0	1.0	0.1296
32	151.00	6	1105.	0.0	0.0006	0.0006	87	77.00	21	946000.	4.4	4.4	0.5473
33	150.00	8	1242.	0.0	0.0007	0.0007	88	75.00	10	32818.	0.2	0.2	0.0190
34	149.00	14	64321.	0.3	0.0372*	0.0372*	89	74.00	21	279392.	1.3	1.3	0.1616
35	148.00	6	1554.	0.0	0.0046	0.0046	90	73.00	14	54357.	0.3	0.3	0.0314*
36	145.00	6	1554.	0.0	0.0009	0.0009	91	72.00	17	5579.	0.0	0.0	0.0032*
37	144.00	17	135312.	0.6	0.0783*	0.0783*	92	71.00	21	266272.	1.2	1.2	0.1540
38	143.00	35	2137400.	9.9	1.2365*	1.2365*	93	70.00	25	801200.	3.7	3.7	0.4635
39	142.00	59	20984832.	97.2	*12.14*	*12.14*	94	69.00	35	5327872.	24.7	24.7	3.0823*
40	141.00	25	706384.	3.3	0.4087*	0.4087*	95	68.00	21	373488.	1.7	1.7	0.2161
41	140.00	14	102044.	0.5	0.0590	0.0590	96	67.00	25	1069824.	5.0	5.0	0.6109*
42	139.00	12	86820.	0.4	0.0502	0.0502	97	66.00	14	49605.	0.2	0.2	0.0287*
43	137.00	10	28915.	0.1	0.0167	0.0167	98	65.00	17	157004.	0.7	0.7	0.0908*
44	136.00	17	264864.	1.2	0.1532	0.1532	99	64.00	21	358144.	1.7	1.7	0.2072
45	135.00	25	2450240.	11.4	1.4175*	1.4175*	100	63.00	21	256924.	1.2	1.2	0.1486
46	131.00	10	31635.	0.1	0.0183	0.0183	101	62.00	12	13897.	0.1	0.1	0.0080*
47	129.00	10	21548.	0.1	0.0125	0.0125	102	61.00	25	244508.	1.1	1.1	0.1415
48	128.00	21	402112.	1.9	0.02326*	0.02326*	103	60.00	12	48741.	0.2	0.2	0.0282
49	127.00	43	6427136.	29.8	3.7182*	3.7182*	104	59.00	17	150904.	0.7	0.7	0.0873
50	126.00	17	74356.	0.3	0.0428*	0.0428*	105	58.00	25	419120.	1.9	1.9	0.2425*
51	125.00	14	92956.	0.4	0.0538	0.0538	106	57.00	43	8383232.	38.8	38.8	4.8499*
52	124.00	8	7899.	0.0	0.0046	0.0046	107	56.00	35	2679104.	12.4	12.4	1.5499*
53	123.00	17	27896.	1.3	0.1613	0.1613	108	55.00	51	15237120.	70.6	70.6	8.8150*
54	122.00	25	2204544.	10.2	1.2754	1.2754	109	54.00	25	626928.	2.9	2.9	0.3627
55	119.00	12	54797.	0.3	0.0317*	0.0317*	110	53.00	25	1044928.	4.8	4.8	0.6045

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	52.00	17	118456.	0.5	0.5	0.0685
112	51.00	21	359984.	1.7	1.7	0.2083
113	50.00	17	133088.	0.6	0.6	0.0770*
114	49.00	6	1495.	0.0	0.0	0.0009
115	48.00	12	36190.	0.2	0.2	0.0209*
116	47.00	21	283888.	1.3	1.3	0.1642
117	46.00	8	18825.	0.1	0.1	0.0109
118	45.00	25	360016.	1.7	1.7	0.2083
119	44.00	35	1054016.	4.9	4.9	0.6098
120	43.00	59	21587968.	100.0	100.0	*12.48*
121	42.00	43	6248704.	28.9	28.9	3.6150*
122	41.00	51	15472128.	71.7	71.7	8.9509*
123	40.00	25	920512.	4.3	4.3	0.5325
124	39.00	43	4660224.	21.6	21.6	2.6960*
125	38.00	25	202692.	0.9	0.9	0.1173*
126	37.00	14	30206.	0.1	0.1	0.0175*
127	36.00	21	162528.	0.8	0.8	0.0940*
128	35.00	8	9523.	0.0	0.0	0.0055*

7ALPA.1 [TIC-179781632, 188X-28163584] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	431.00	6	1574.	0.0	0.0	0.0009	129.00	0.0	0.0	0.0036
2	281.00	6	3785.	0.0	0.0	0.0021	128.00	0.4	0.4	0.0443
3	269.00	6	2028.	0.0	0.0	0.0011	127.00	10.1	10.1	1.1329
4	242.00	10	18189.	0.1	0.0	0.0011	126.00	0.1	0.1	0.0108
5	241.00	14	258456.	1.3	1.3	0.1438	125.00	0.2	0.2	0.0172
6	240.00	21	1230336.	6.1	6.1	0.6844	124.00	0.1	0.1	0.0095*
7	239.00	8	10999.	0.0	0.0	0.0026	123.00	2.3	2.3	0.2621
8	225.00	8	3142.	0.0	0.0	0.0017	122.00	10.2	10.2	1.1471
9	223.00	8	1845.	0.0	0.0	0.0010	121.00	0.1	0.1	0.0160*
10	222.00	10	59914.	0.3	0.0	0.0333	119.00	0.2	0.2	0.0252*
11	221.00	17	333840.	1.7	1.7	0.1857*	118.00	0.4	0.4	0.0429*
12	213.00	8	22162.	0.1	0.1	0.0123	117.00	0.2	0.2	0.0173*
13	212.00	17	297568.	1.5	1.5	0.1655*	114.00	0.0	0.0	0.0011
14	211.00	25	2874176.	14.3	14.3	1.5987	113.00	2.3	2.3	0.2532
15	199.00	8	11115.	0.1	0.1	0.0062	112.00	1.4	1.4	0.1530
16	198.00	17	301872.	1.5	1.5	0.1679	111.00	0.9	0.9	0.1024*
17	197.00	25	3503936.	17.4	17.4	1.9490	110.00	0.0	0.0	0.0052
18	193.00	8	3123.	0.0	0.0	0.0017	109.00	1.2	1.2	0.1308
19	186.00	6	9256.	0.0	0.0	0.0051	107.00	0.2	0.2	0.0200
20	185.00	8	16266.	0.1	0.1	0.0090*	106.00	0.0	0.0	0.0034*
21	184.00	12	106720.	0.5	0.5	0.0594	105.00	0.3	0.3	0.0302*
22	183.00	17	719440.	3.6	3.6	0.4002	104.00	0.0	0.0	0.0016
23	181.00	8	26675.	0.1	0.1	0.0148	102.00	0.0	0.0	0.0020
24	180.00	6	1709.	0.0	0.0	0.0010	101.00	0.0	0.0	0.0014
25	179.00	10	11112.	0.1	0.1	0.0062	100.00	0.2	0.2	0.0242*
26	177.00	8	11707.	0.1	0.1	0.0065	99.00	4.3	4.3	0.4806*
27	171.00	8	6191.	0.0	0.0	0.0034	98.00	9.4	9.4	1.0554
28	170.00	14	119608.	0.6	0.6	0.0665*	97.00	5.8	5.8	0.6468
29	169.00	21	1656768.	8.2	8.2	0.9215*	96.00	8.0	8.0	0.8947*
30	168.00	8	27769.	0.1	0.1	0.0154	95.00	0.6	0.6	0.0693
31	167.00	10	8097.	0.0	0.0	0.0045	94.00	0.5	0.5	0.0601
32	166.00	8	12016.	0.1	0.1	0.0067	93.00	0.6	0.6	0.0630
33	165.00	10	43304.	0.2	0.2	0.0241	91.00	0.6	0.6	0.0715
34	163.00	6	1772.	0.0	0.0	0.0010	90.00	0.0	0.0	0.0010
35	162.00	8	5623.	0.0	0.0	0.0031	89.00	0.0	0.0	0.0011
36	161.00	6	3336.	0.0	0.0	0.0019	87.00	0.0	0.0	0.0017
37	157.00	12	61921.	0.3	0.3	0.0344	86.00	0.0	0.0	0.0022
38	156.00	21	923200.	4.6	4.6	0.5135*	85.00	0.9	0.9	0.1018*
39	155.00	43	12774912.	63.4	63.4	7.1058*	84.00	8.3	8.3	0.9349
40	154.00	12	24455.	0.1	0.1	0.0136*	83.00	35.6	35.6	3.9886*
41	153.00	12	70780.	0.4	0.4	0.0394*	82.00	1.0	1.0	0.1177*
42	152.00	10	25355.	0.1	0.1	0.0141	81.00	5.2	5.2	0.5818
43	149.00	14	80976.	0.4	0.4	0.0495*	80.00	1.6	1.6	0.1849
44	148.00	6	2586.	0.0	0.0	0.0014	79.00	1.0	1.0	0.1143
45	145.00	10	5883.	0.0	0.0	0.0033	78.00	0.9	0.9	0.1009*
46	144.00	14	148628.	0.7	0.7	0.0827	77.00	3.7	3.7	0.4206
47	143.00	35	2276416.	11.3	11.3	1.2662*	75.00	0.1	0.1	0.0147*
48	142.00	51	20163584.	100.0	100.0	*11.21*	74.00	1.0	1.0	0.1146
49	141.00	43	4105792.	20.4	20.4	2.2838*	73.00	0.4	0.4	0.0431
50	140.00	17	127396.	0.6	0.6	0.0709*	72.00	0.5	0.5	0.0615*
51	139.00	17	172816.	0.9	0.9	0.0961	71.00	10.4	10.4	1.1647
52	137.00	10	26488.	0.1	0.1	0.0147	70.00	6.0	6.0	0.6765
53	136.00	17	259632.	1.3	1.3	0.1444*	69.00	30.4	30.4	3.4049*
54	135.00	25	2511360.	12.5	12.5	1.3969*	68.00	5.0	5.0	0.5608*
55	131.00	10	28090.	0.1	0.1	0.0161	67.00	5.3	5.3	0.5911

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	66.00	12	73672.	0.4	0.4	0.0410
112	65.00	17	168976.	0.8	0.2	0.0940
113	64.00	21	329808.	1.6	1.6	0.1834
114	63.00	21	216484.	0.9	1.1	0.1204
115	61.00	21	190000.	0.1	0.9	0.1057
116	60.00	12	23090.	0.1	0.1	0.0128
117	59.00	17	125928.	0.6	0.6	0.0700*
118	58.00	25	768240.	3.8	3.8	0.4273*
119	57.00	43	16128000.	80.0	80.0	8.9709*
120	56.00	29	3261248.	16.2	16.2	1.8140
121	55.00	51	15435264.	76.6	76.6	8.5856*
122	54.00	25	1062144.	5.3	5.3	0.5908
123	53.00	25	1051200.	5.2	5.2	0.5847
124	52.00	17	102316.	0.5	0.5	0.0569*
125	51.00	21	312736.	1.6	1.6	0.1740*
126	50.00	17	101684.	0.5	0.5	0.0566*
127	49.00	10	7856.	0.0	0.0	0.0044
128	48.00	8	12999.	0.1	0.1	0.0072
129	47.00	21	227292.	1.1	1.1	0.1264*
130	46.00	10	26318.	0.1	0.1	0.0146
131	45.00	25	324880.	1.6	1.6	0.1807*
132	44.00	35	971440.	4.8	4.8	0.5403*
133	43.00	51	20043776.	99.4	99.4	*11.14*
134	42.00	35	5515520.	27.4	27.4	3.0679*
135	41.00	43	16344576.	81.1	81.1	9.0913*
136	40.00	29	880704.	4.4	4.4	0.4899*
137	39.00	35	4322048.	21.4	21.4	2.4041*
138	38.00	25	139180.	0.7	0.7	0.0774*
139	37.00	10	26434.	0.1	0.1	0.0147*
140	36.00	21	143240.	0.7	0.7	0.0797*
141	35.00	8	6440.	0.0	0.0	0.0036

8ALPA.1 [TIC=163135488, 199X=18742272] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	2005.	0.0	0.0	0.0012	56	135.00	25	2190272.	11.7	11.7	1.3425
2	256.00	8	19008.	0.1	0.0	0.0117	57	134.00	6	1563.	0.0	0.0	0.0010
3	255.00	17	309648.	1.7	1.7	0.1898	58	131.00	8	16435.	0.1	0.1	0.0101
4	254.00	25	1811456.	9.7	9.7	1.1104*	59	129.00	8	7056.	0.0	0.0	0.0043
5	253.00	8	4194.	0.0	0.0	0.0026	60	128.00	12	51796.	0.3	0.3	0.0318
6	239.00	8	2146.	0.0	0.0	0.0013	61	127.00	21	1625728.	8.7	8.7	0.9966
7	236.00	10	44321.	0.2	0.0	0.0272	62	126.00	12	60846.	0.3	0.3	0.0373*
8	235.00	17	304544.	1.6	1.6	0.1867	63	125.00	12	72860.	0.4	0.4	0.0442*
9	236.00	12	75820.	0.4	0.4	0.0465	64	124.00	10	10592.	0.1	0.1	0.0065
10	225.00	17	682592.	3.6	3.6	0.4184	65	123.00	21	311920.	1.7	1.7	0.1912
11	213.00	10	39372.	0.2	0.0	0.0241	66	122.00	21	1583168.	8.4	8.4	0.9705*
12	212.00	21	476176.	2.5	2.5	0.2919*	67	121.00	10	28222.	0.2	0.2	0.0173*
13	211.00	29	4686336.	25.0	25.0	2.8727*	68	119.00	12	34484.	0.2	0.2	0.0211
14	201.00	6	1234.	0.0	0.0	0.0008	69	118.00	21	87544.	0.5	0.5	0.0537*
15	200.00	6	4849.	0.0	0.0	0.0030	70	117.00	14	31553.	0.2	0.2	0.0193*
16	199.00	6	5058.	0.0	0.0	0.0031	71	116.00	12	31812.	0.2	0.2	0.0195
17	198.00	14	131808.	0.7	0.7	0.0888	72	113.00	29	894688.	4.8	4.8	0.5484
18	197.00	21	1198400.	5.4	6.4	0.7346	73	112.00	21	899008.	4.7	4.7	0.5388*
19	193.00	8	4748.	0.0	0.0	0.0029	74	111.00	21	393440.	2.1	2.1	0.2412
20	185.00	6	1374.	0.0	0.0	0.0029	75	110.00	25	1525888.	8.1	8.1	0.9354
21	184.00	12	89880.	0.5	0.5	0.0008	76	109.00	17	199708.	1.1	1.1	0.1224
22	183.00	17	569472.	3.0	3.0	0.0551	77	108.00	6	12799.	0.1	0.1	0.0078
23	182.00	6	1568.	0.0	0.0	0.0010	78	107.00	14	89268.	0.5	0.5	0.0547*
24	181.00	10	19527.	0.1	0.1	0.0120	79	105.00	14	31960.	0.2	0.2	0.0196*
25	180.00	8	4100.	0.1	0.1	0.0025	80	104.00	8	2769.	0.0	0.0	0.0017
26	179.00	8	20401.	0.1	0.1	0.0125	81	99.00	12	61226.	0.3	0.3	0.0375
27	177.00	8	7952.	0.0	0.0	0.0049	82	98.00	21	926640.	4.9	4.9	0.5680
28	176.00	14	3426.	0.0	0.0	0.0021*	83	97.00	25	1061696.	5.7	5.7	0.6500
29	175.00	10	10230.	0.1	0.1	0.0063	84	96.00	17	117324.	0.6	0.6	0.0719*
30	171.00	10	6193.	0.0	0.0	0.0038	85	95.00	21	585664.	3.1	3.1	0.3590
31	170.00	14	130184.	0.7	0.7	0.0798	86	94.00	12	70512.	0.4	0.4	0.0432*
32	169.00	25	1823168.	9.7	9.7	1.1176	87	93.00	14	87260.	0.5	0.5	0.0535*
33	168.00	12	56072.	0.3	0.3	0.0344	88	91.00	17	87324.	0.5	0.5	0.0535*
34	167.00	10	11527.	0.1	0.1	0.0071	89	89.00	8	823.	0.0	0.0	0.0005
35	166.00	8	16580.	0.1	0.1	0.0102	90	87.00	10	8495.	0.0	0.0	0.0052*
36	165.00	10	33952.	0.2	0.2	0.0208	91	86.00	17	57101.	0.3	0.3	0.0350*
37	157.00	17	82956.	0.4	0.4	0.0509*	92	85.00	25	814080.	4.3	4.3	0.4990
38	156.00	35	1320896.	7.0	7.0	0.8097*	93	84.00	29	1752512.	9.4	9.4	1.0743
39	155.00	51	14601728.	77.9	77.9	8.9507*	94	83.00	43	6637056.	35.4	35.4	4.0684
40	154.00	17	30424.	0.2	0.2	0.0186*	95	82.00	21	558448.	3.0	3.0	0.3423
41	153.00	17	127900.	0.7	0.7	0.0785*	96	81.00	25	993552.	5.3	5.3	0.6090
42	152.00	10	16951.	0.1	0.1	0.0104	97	80.00	21	268336.	1.4	1.4	0.1645
43	151.00	6	1426.	0.0	0.0	0.0009	98	79.00	17	219636.	1.2	1.2	0.1346
44	150.00	6	1451.	0.0	0.0	0.0009	99	78.00	17	142104.	0.8	0.8	0.0871*
45	149.00	12	82088.	0.4	0.4	0.0503*	100	77.00	21	559712.	3.0	3.0	0.3431
46	148.00	6	1668.	0.0	0.0	0.0010	101	75.00	10	14528.	0.1	0.1	0.0089
47	145.00	12	3147.	0.0	0.0	0.0019	102	74.00	17	161188.	0.9	0.9	0.0988*
48	144.00	17	125480.	0.7	0.7	0.0769	103	73.00	14	56135.	0.3	0.3	0.0344*
49	143.00	25	2044032.	10.9	10.9	1.2530*	104	72.00	21	337280.	1.8	1.8	0.2067
50	142.00	51	17372160.	92.7	92.7	*10.64*	105	71.00	35	6969088.	37.2	37.2	4.2720*
51	141.00	21	586576.	3.1	3.1	0.3596*	106	70.00	25	1271232.	6.8	6.8	0.7792*
52	140.00	10	57452.	0.3	0.3	0.0352	107	69.00	35	5871616.	31.3	31.3	3.5992*
53	139.00	14	108484.	0.6	0.6	0.0665*	108	68.00	25	1047072.	5.6	5.6	0.6418
54	137.00	17	89952.	0.5	0.5	0.0551	109	67.00	21	995024.	5.3	5.3	0.6099
55	136.00	21	327824.	1.7	1.7	0.2010*	110	66.00	14	46511.	0.2	0.2	0.0285

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	65.00	17	136992.	0.7	0.7	0.0840
112	64.00	17	229020.	1.2	1.2	0.1404
113	63.00	17	152196.	0.8	0.8	0.0933*
114	62.00	6	2868.	0.0	0.0	0.0018
115	61.00	21	157228.	0.8	0.8	0.0964*
116	60.00	10	22323.	0.1	0.1	0.0137
117	59.00	14	92292.	0.5	0.5	0.0566*
118	58.00	25	418720.	2.2	2.2	0.2567
119	57.00	35	9980160.	53.2	53.2	6.1177*
120	56.00	35	2460416.	13.1	13.1	1.5882
121	55.00	43	13431809.	71.7	71.7	8.2335*
122	54.00	25	932032.	5.0	5.0	0.5713
123	53.00	21	925392.	4.9	4.9	0.5673
124	52.00	12	78644.	0.4	0.4	0.0482*
125	51.00	21	224072.	1.2	1.2	0.1374*
126	50.00	17	45476.	0.2	0.2	0.0279
127	49.00	6	901.	0.0	0.0	0.0006
128	48.00	8	12990.	0.1	0.1	0.0080*
129	47.00	17	186604.	1.0	1.0	0.1156
130	46.00	8	13272.	0.1	0.1	0.0081
131	45.00	25	249828.	1.3	1.3	0.1531*
132	44.00	35	797600.	4.3	4.3	0.4889
133	43.00	51	18742272.	100.0	100.0	0.4889
134	42.00	35	4344064.	23.2	23.2	*11.48*
135	41.00	43	13856512.	73.9	73.9	2.6629*
136	40.00	25	638128.	3.4	3.4	8.4939*
137	39.00	35	3211520.	17.1	17.1	0.3912*
138	38.00	17	97372.	0.5	0.5	1.9686*
139	37.00	12	13253.	0.1	0.1	0.0597*
140	36.00	21	126776.	0.7	0.7	0.0081*
141	35.00	10	6770.	0.0	0.0	0.0777*
						0.0041

18ALPA.1 [TIC-142882848, 188X-17348688] EI

Undecanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_9\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	8	2062.	0.0	0.0	0.0015	56	139.00	17	132504.	0.8	0.8	0.0933
2	270.00	8	24029.	0.1	0.1	0.0169	57	137.00	10	14273.	0.1	0.1	0.0100*
3	269.00	17	344064.	2.0	2.0	0.2422*	58	136.00	17	169540.	1.0	1.0	0.1193*
4	268.00	25	1910656.	11.0	11.0	1.3448*	59	135.00	25	1716416.	0.9	0.9	1.2080*
5	267.00	6	1134.	0.0	0.0	0.0008	60	131.00	10	16911.	0.1	0.1	0.0119
6	253.00	10	7109.	0.0	0.0	0.0050	61	129.00	8	2682.	0.0	0.0	0.0019
7	251.00	8	2409.	0.0	0.0	0.0017	62	128.00	14	65888.	0.4	0.4	0.0464*
8	250.00	12	35640.	0.2	0.2	0.0251*	63	127.00	29	1629568.	9.4	9.4	1.1469
9	249.00	17	295936.	1.7	1.7	0.2083	64	126.00	17	425056.	2.5	2.5	0.2992
10	240.00	10	58802.	0.3	0.3	0.0414	65	125.00	17	212880.	1.2	1.2	0.1498
11	239.00	17	455280.	2.6	2.6	0.3204	66	124.00	21	1025040.	5.9	5.9	0.7214*
12	227.00	8	9456.	0.1	0.1	0.0067	67	123.00	17	274512.	1.6	1.6	0.1932
13	226.00	14	206268.	1.2	1.2	0.1452	68	122.00	25	1287680.	7.4	7.4	0.9063
14	225.00	21	1914752.	11.0	11.0	1.3476	69	121.00	14	237452.	1.4	1.4	0.1671
15	213.00	10	16086.	0.1	0.1	0.0113	70	119.00	10	29382.	0.2	0.2	0.0207*
16	212.00	17	230228.	1.3	1.3	0.1120	71	118.00	14	42762.	0.2	0.2	0.0301*
17	211.00	25	2360768.	13.6	13.6	1.6616*	72	117.00	8	9746.	0.1	0.1	0.0069
18	207.00	6	815.	0.0	0.0	0.0006	73	115.00	8	4266.	0.0	0.0	0.0030
19	199.00	8	4491.	0.0	0.0	0.0032	74	114.00	8	2939.	0.0	0.0	0.0021
20	198.00	14	111756.	0.6	0.6	0.0787	75	113.00	17	325088.	1.9	1.9	0.2288*
21	197.00	17	907024.	5.2	5.2	0.6384	76	112.00	14	142332.	0.8	0.8	0.11002
22	193.00	10	9221.	0.1	0.1	0.0065	77	111.00	17	277088.	1.6	1.6	0.1950
23	190.00	6	2103.	0.0	0.0	0.0015	78	110.00	14	75464.	0.4	0.4	0.0531*
24	189.00	8	4567.	0.0	0.0	0.0032	79	109.00	21	296368.	1.7	1.7	0.2086
25	185.00	8	4734.	0.0	0.0	0.0033	80	108.00	10	15068.	0.1	0.1	0.0106
26	184.00	12	113904.	0.7	0.7	0.0802	81	107.00	14	64138.	0.4	0.4	0.0451*
27	183.00	17	757776.	4.4	4.4	0.5333	82	106.00	17	8272.	0.0	0.0	0.0058*
28	182.00	10	8971.	0.1	0.1	0.0063	83	105.00	21	44000.	0.3	0.3	0.0310*
29	181.00	8	18786.	0.1	0.1	0.0132	84	104.00	10	3593.	0.0	0.0	0.0025
30	180.00	12	18663.	0.1	0.1	0.0131	85	102.00	6	2104.	0.0	0.0	0.0015
31	179.00	10	8969.	0.1	0.1	0.0063	86	101.00	8	1506.	0.0	0.0	0.0011
32	177.00	6	1970.	0.0	0.0	0.0014	87	100.00	6	4128.	0.0	0.0	0.0029
33	171.00	10	16401.	0.1	0.1	0.0115	88	99.00	17	132968.	0.8	0.8	0.0936*
34	170.00	21	454848.	2.6	2.6	0.3201	89	98.00	25	1102080.	6.4	6.4	0.7757
35	169.00	35	3554048.	29.5	20.5	2.5014*	90	97.00	25	1351872.	7.8	7.8	0.9515
36	168.00	17	46023.	0.3	0.3	0.0330*	91	96.00	17	309056.	1.8	1.8	0.2175*
37	167.00	14	55523.	0.3	0.3	0.0391*	92	95.00	21	615376.	3.5	3.5	0.4331
38	166.00	14	38643.	0.2	0.2	0.0272*	93	94.00	12	60739.	0.4	0.4	0.0427*
39	165.00	10	16044.	0.1	0.1	0.0113	94	93.00	14	112252.	0.6	0.6	0.0790
40	157.00	12	63354.	0.4	0.4	0.0446	95	92.00	6	5400.	0.0	0.0	0.0038
41	156.00	21	983664.	5.7	5.7	0.6923*	96	91.00	12	51731.	0.3	0.3	0.0364
42	155.00	35	9802496.	56.5	56.5	6.8992*	97	90.00	14	9553.	0.1	0.1	0.0067*
43	154.00	8	4576.	0.0	0.0	0.0032*	98	89.00	17	181456.	1.0	1.0	0.1277*
44	153.00	12	71752.	0.4	0.4	0.0505*	99	88.00	29	3171776.	18.3	18.3	2.2324*
45	152.00	10	23900.	0.1	0.1	0.0168	100	87.00	29	1630400.	9.4	9.4	1.1475*
46	151.00	8	28724.	0.2	0.2	0.0202	101	86.00	35	5574144.	32.1	32.1	3.9232*
47	150.00	14	131712.	0.8	0.8	0.0927	102	85.00	21	618608.	3.6	3.6	0.4354
48	149.00	17	84560.	0.5	0.5	0.0595*	103	84.00	25	650864.	3.8	3.8	0.4581
49	148.00	6	746.	0.0	0.0	0.0005	104	83.00	21	195656.	1.1	1.1	0.1377*
50	146.00	6	1160.	0.0	0.0	0.0008	105	82.00	21	224208.	1.3	1.3	0.1578
51	144.00	12	94636.	0.5	0.5	0.0666*	106	81.00	14	125036.	0.7	0.7	0.0880
52	143.00	25	1907008.	11.0	11.0	1.3422*	107	80.00	21	392384.	2.3	2.3	0.2762*
53	142.00	43	14138368.	81.5	81.5	9.9508*	108	79.00	10	5544.	0.0	0.0	0.0039
54	141.00	17	451568.	2.6	2.6	0.3178*	109	78.00	14	121152.	0.7	0.7	0.0853
55	140.00	14	60141.	0.3	0.3	0.0423*	110	77.00	10	62817.	0.4	0.4	0.0442

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	72.00	17	277568.	1.6	1.6	0.1954
112	71.00	29	5339392.	30.8	30.8	3.7580
113	70.00	25	1000944.	5.8	5.8	0.7045
114	69.00	35	5095424.	29.4	29.4	3.5863
115	68.00	21	828592.	4.8	4.8	0.5832
116	67.00	21	898448.	5.2	5.2	0.6323
117	66.00	12	49932.	0.3	0.3	0.0351*
118	65.00	14	100256.	0.6	0.6	0.0706*
119	64.00	17	176276.	1.0	1.0	0.1241
120	63.00	17	104264.	0.6	0.6	0.0734*
121	62.00	6	2010.	0.0	0.0	0.0014
122	61.00	14	126436.	0.7	0.7	0.0890
123	60.00	10	12249.	0.1	0.1	0.0086
124	59.00	10	64383.	0.4	0.4	0.0453
125	58.00	21	340560.	2.0	2.0	0.2397
126	57.00	35	7738368.	44.6	44.6	5.4464*
127	56.00	29	2232640.	12.9	12.9	1.5714
128	55.00	43	11485184.	66.2	66.2	8.0835*
129	54.00	21	808400.	4.7	4.7	0.5690
130	53.00	21	711824.	4.1	4.1	0.5010
131	52.00	12	64968.	0.4	0.4	0.0457
132	51.00	17	180092.	1.0	1.0	0.1268*
133	50.00	12	39923.	0.2	0.2	0.0281
134	49.00	12	3755.	0.0	0.0	0.0026
135	48.00	17	7461.	0.0	0.0	0.0053
136	47.00	17	149500.	0.9	0.9	0.1052*
137	46.00	8	5520.	0.0	0.0	0.0039
138	45.00	17	172644.	1.0	1.0	0.1215
139	44.00	35	708336.	4.1	4.1	0.4985*
140	43.00	43	17348608.	100.0	100.0	*12.21*
141	42.00	35	3614656.	20.8	20.8	2.5441
142	41.00	35	11999488.	69.2	69.2	8.4455*
143	40.00	25	522624.	3.0	3.0	0.3678*
144	39.00	29	2536832.	14.6	14.6	1.7855*
145	38.00	14	75460.	0.4	0.4	0.0531*
146	37.00	12	15478.	0.1	0.1	0.0109*
147	36.00	17	99736.	0.5	0.6	0.0702*
148	35.00	6	1222.	0.0	0.0	0.0009

11ALPA.1 [TIC=17888784, 100X=21198848] EI

Dodecanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_{10}\text{COOCH}_2\text{CF}_3$

PAGE	1	PAGE	2			
PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	285.00	10	3839.	0.3	0.3	0.0021
2	284.00	12	54398.	0.3	0.3	0.0304*
3	282.00	17	542368.	2.6	2.6	0.3032
4	282.00	29	3006464.	14.2	14.2	1.6806*
5	281.00	10	14448.	0.1	0.1	0.0081*
6	267.00	6	7620.	0.3	0.3	0.0043
7	264.00	10	68132.	0.3	0.3	0.0381
8	263.00	17	375536.	1.8	1.8	0.2099
9	254.00	12	96620.	0.5	0.5	0.0540
10	253.00	17	710096.	3.3	3.3	0.3969
11	241.00	10	18035.	0.1	0.1	0.0101
12	240.00	14	260132.	1.2	1.2	0.1454
13	239.00	25	2162240.	10.2	10.2	1.2087*
14	228.00	6	899.	0.2	0.2	0.0005
15	227.00	12	5328.	0.3	0.3	0.0030
16	226.00	12	65108.	0.3	0.3	0.0364
17	225.00	17	525296.	2.5	2.5	0.2936
18	219.00	8	3679.	0.1	0.1	0.0021
19	213.00	10	13159.	0.1	0.1	0.0074
20	212.00	17	292752.	1.4	1.4	0.1637
21	211.00	25	3134976.	14.8	14.8	1.7525
22	207.00	6	1350.	0.3	0.3	0.0008
23	203.00	10	3930.	0.3	0.3	0.0022
24	199.00	8	10375.	0.9	0.9	0.0058
25	198.00	17	201208.	0.9	0.9	0.1125
26	197.00	21	1496768.	7.1	7.1	0.8367*
27	196.00	8	2523.	0.3	0.3	0.0014
28	195.00	8	4759.	0.3	0.3	0.0027
29	193.00	6	1452.	0.3	0.3	0.0008
30	185.00	10	20062.	0.1	0.1	0.0112
31	184.00	21	543248.	2.6	2.6	0.3037
32	183.00	29	3243072.	15.3	15.3	1.8129*
33	182.00	10	31950.	0.2	0.2	0.0179*
34	181.00	14	54457.	0.3	0.3	0.0304*
35	180.00	12	45458.	0.2	0.2	0.0254*
36	179.00	12	36515.	0.2	0.2	0.0204
37	177.00	8	11777.	0.1	0.1	0.0066
38	171.00	10	33714.	0.2	0.2	0.0188
39	170.00	17	291400.	1.4	1.4	0.1629
40	169.00	21	158800.	7.5	7.5	0.8881
41	168.00	10	53431.	0.3	0.3	0.0299
42	167.00	10	21420.	0.1	0.1	0.0120
43	166.00	10	27073.	0.1	0.1	0.0151
44	165.00	14	53955.	0.3	0.3	0.0302*
45	164.00	17	128932.	0.6	0.6	0.0721
46	163.00	10	21766.	0.1	0.1	0.0122*
47	158.00	14	6699.	0.3	0.3	0.0037*
48	157.00	14	79420.	0.4	0.4	0.0444*
49	156.00	21	1080256.	5.1	5.1	0.6039*
50	155.00	43	12194048.	57.5	57.5	6.8166*
51	154.00	10	12929.	0.1	0.1	0.0072*
52	153.00	14	109556.	0.5	0.5	0.0612
53	152.00	10	35241.	0.2	0.2	0.0197
54	151.00	10	5051.	0.2	0.2	0.0028*
55	149.00	14	91916.	0.4	0.4	0.0514
56	148.00	8	3797.	0.3	0.3	0.0021
57	145.00	8	6726.	0.3	0.3	0.0038
58	144.00	14	151400.	0.7	0.7	0.0846
59	143.00	29	2613888.	80.5	80.5	1.4612*
60	142.00	51	17058816.	80.5	80.5	9.5360*
61	141.00	29	901216.	4.3	4.3	0.5038*
62	140.00	21	426336.	2.0	2.0	0.2383*
63	139.00	21	296384.	1.4	1.4	0.1657
64	138.00	21	1210752.	5.7	5.7	0.6768*
65	137.00	10	23908.	0.1	0.1	0.0134*
66	136.00	17	178668.	0.8	0.8	0.0999*
67	135.00	25	1877504.	8.9	8.9	1.0495*
68	131.00	8	19705.	0.1	0.1	0.0110
69	129.00	10	6990.	0.3	0.3	0.0039
70	128.00	10	35879.	0.2	0.2	0.0201
71	127.00	21	1488448.	7.0	7.0	0.8321
72	126.00	12	65544.	0.3	0.3	0.0366
73	125.00	17	155460.	0.7	0.7	0.0869
74	124.00	12	38503.	0.2	0.2	0.0215
75	123.00	21	355120.	1.7	1.7	0.1985
76	122.00	21	1269440.	6.0	6.0	0.7096
77	121.00	17	134180.	0.6	0.6	0.0750*
78	119.00	10	37094.	0.2	0.2	0.0207*
79	118.00	21	55535.	0.3	0.3	0.0310*
80	117.00	8	16004.	0.1	0.1	0.0089*
81	115.00	6	1483.	0.3	0.3	0.0008
82	114.00	6	1855.	0.3	0.3	0.0010
83	113.00	21	364240.	1.7	1.7	0.2036
84	112.00	21	356560.	1.7	1.7	0.1993
85	111.00	21	701104.	3.3	3.3	0.3919
86	110.00	17	372896.	1.8	1.8	0.2085
87	109.00	25	471008.	2.2	2.2	0.2633
88	108.00	10	29941.	0.1	0.1	0.0167
89	107.00	14	110804.	0.5	0.5	0.0619*
90	106.00	8	2634.	0.3	0.3	0.0015
91	105.00	12	14946.	0.1	0.1	0.0084*
92	103.00	8	1661.	0.3	0.3	0.0009
93	101.00	10	2717.	0.3	0.3	0.0015
94	100.00	17	62621.	5.0	5.0	0.8350
95	99.00	21	1059520.	5.0	5.0	0.5923
96	98.00	21	1484672.	7.0	7.0	0.8299
97	97.00	25	2072448.	9.8	9.8	1.1585
98	96.00	21	634352.	3.0	3.0	0.3546*
99	95.00	21	702496.	3.3	3.3	0.3927
100	94.00	14	80396.	0.4	0.4	0.0449*
101	93.00	17	133232.	0.7	0.7	0.0857
102	91.00	14	91420.	0.4	0.4	0.0511*
103	87.00	8	6978.	0.3	0.3	0.0039*
104	86.00	17	271040.	1.3	1.3	0.1515
105	85.00	29	4534784.	21.4	21.4	2.5350
106	84.00	25	1925376.	9.1	9.1	1.0763
107	83.00	35	6785280.	32.0	32.0	3.7930*
108	82.00	21	680608.	3.2	3.2	0.3805
109	81.00	21	872640.	4.1	4.1	0.4878
110	80.00	21	263568.	1.2	1.2	0.1473

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	79.00	17	282640.	1.3	1.3	0.1580
112	78.00	17	107820.	0.5	0.5	0.0603
113	77.00	21	429712.	2.0	2.0	0.2402
114	75.00	14	4468.	0.0	0.0	0.0025
115	74.00	14	120248.	0.6	0.6	0.0672*
116	73.00	12	70272.	0.3	0.3	0.0393
117	72.00	17	255636.	1.2	1.2	0.1429
118	71.00	35	5373184.	25.3	25.3	3.0036*
119	70.00	35	1369984.	6.5	6.5	0.7658
120	69.00	35	6485504.	30.6	30.6	3.6254*
121	68.00	25	1095872.	5.2	5.2	0.6126
122	67.00	21	1173632.	5.5	5.5	0.6561
123	66.00	12	81112.	0.4	0.4	0.0453
124	65.00	17	149244.	0.7	0.7	0.0834
125	64.00	17	170540.	0.8	0.8	0.0953*
126	63.00	17	129860.	0.6	0.6	0.0726*
127	61.00	17	138120.	0.7	0.7	0.0772*
128	60.00	10	14161.	0.1	0.1	0.0079
129	59.00	14	86656.	0.4	0.4	0.0484*
130	58.00	25	516992.	2.4	2.4	0.2890
131	57.00	43	11385344.	53.7	53.7	6.3645*
132	56.00	29	2901248.	13.7	13.7	1.6218
133	55.00	43	14320128.	67.6	67.6	8.0050*
134	54.00	25	938576.	4.4	4.4	0.5247
135	53.00	21	902720.	4.3	4.3	0.5046
136	52.00	21	54219.	0.3	0.3	0.0303
137	51.00	21	167120.	0.8	0.8	0.0934*
138	50.00	12	40534.	0.2	0.2	0.0227*
139	48.00	14	2558.	0.0	0.0	0.0014*
140	47.00	17	162104.	0.8	0.8	0.0906
141	46.00	6	2195.	0.0	0.0	0.0012
142	45.00	21	196740.	0.0	0.9	0.1100*
143	44.00	35	766880.	0.0	3.6	0.4287*
144	43.00	51	21198848.	100.0	100.0	*11.85*
145	42.00	35	4134000.	19.5	19.5	2.3110
146	41.00	43	14692864.	69.3	69.3	8.2134*
147	40.00	25	535584.	2.5	2.5	0.2994
148	39.00	35	2789696.	13.2	13.2	1.5595*
149	38.00	17	61162.	0.3	0.3	0.0342*
150	37.00	8	13722.	0.1	0.1	0.0077
151	36.00	17	119076.	0.6	0.6	0.0666*
152	35.00	6	1868.	0.0	0.0	0.0010

12ALPA.1 [TIC-167346176, 100X-20188160] EI

Tridecanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_{11}\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	298.00	12	57174.	0.3	0.3	0.0342*	56	153.00	21	228216.	1.1	1.1	0.1354*
2	297.00	17	571600.	2.8	2.8	0.3416*	57	152.00	25	968224.	4.8	4.8	0.5786*
3	296.00	29	3176064.	15.7	15.7	1.8979*	58	151.00	10	7887.	0.0	0.0	0.0047
4	295.00	8	5282.	0.0	0.0	0.0032	59	150.00	10	7928.	0.0	0.0	0.0047
5	293.00	6	713.	0.0	0.0	0.0004	60	149.00	12	98492.	0.5	0.5	0.0589*
6	291.00	8	9187.	0.0	0.0	0.0055	61	145.00	10	6182.	0.0	0.0	0.0037
7	278.00	12	60976.	0.3	0.3	0.0364	62	144.00	14	137420.	0.7	0.7	0.0821*
8	277.00	17	353952.	1.8	1.8	0.2115	63	143.00	29	2739968.	13.6	13.6	1.6373*
9	269.00	8	4624.	0.0	0.0	0.0028	64	142.00	43	15502336.	76.8	76.8	9.2638*
10	268.00	12	93064.	0.5	0.5	0.0556	65	141.00	21	541472.	2.7	2.7	0.3236*
11	267.00	17	675296.	3.3	3.3	0.4035	66	140.00	12	7512.	0.4	0.4	0.0449
12	255.00	10	13444.	0.1	0.1	0.0080	67	139.00	21	199688.	1.0	1.0	0.1193*
13	254.00	14	262640.	1.3	1.3	0.1569	68	138.00	10	14851.	0.1	0.1	0.0089
14	253.00	21	2101440.	10.4	10.4	1.2557	69	137.00	14	49824.	0.2	0.2	0.0238*
15	241.00	8	7537.	0.0	0.0	0.0045	70	136.00	17	172492.	0.9	0.9	0.1031
16	240.00	12	70672.	0.4	0.4	0.0422	71	135.00	25	1588416.	7.9	7.9	0.9492*
17	239.00	17	337456.	1.7	1.7	0.2017	72	132.00	8	2063.	0.0	0.0	0.0012
18	227.00	6	780.	0.0	0.0	0.0005	73	131.00	10	31540.	0.2	0.2	0.0188*
19	226.00	10	55566.	0.3	0.3	0.0332	74	129.00	10	9250.	0.0	0.0	0.0055
20	225.00	17	336752.	1.7	1.7	0.2012	75	128.00	10	40039.	0.2	0.2	0.0239
21	217.00	12	5791.	0.0	0.0	0.0035	76	127.00	21	1296768.	6.4	6.4	0.7749*
22	213.00	10	28961.	0.1	0.1	0.0173*	77	126.00	14	140920.	0.7	0.7	0.0842
23	212.00	17	309296.	1.5	1.5	0.1848	78	125.00	17	318144.	1.6	1.6	0.1901
24	211.00	25	3132672.	15.5	15.5	1.8720*	79	124.00	17	243688.	1.2	1.2	0.1456*
25	210.00	10	2797.	0.0	0.0	0.0017	80	123.00	21	394256.	2.0	2.0	0.2356
26	207.00	8	4609.	0.0	0.0	0.0028	81	122.00	25	1051392.	5.2	5.2	0.6283
27	199.00	12	49708.	0.2	0.2	0.0297*	82	121.00	14	128528.	0.5	0.5	0.0770
28	198.00	21	650896.	3.2	3.2	0.3890*	83	119.00	10	30232.	0.1	0.1	0.0181
29	197.00	29	3336192.	16.5	16.5	1.9936	84	118.00	17	34185.	0.2	0.2	0.0224*
30	196.00	17	11785.	0.1	0.1	0.0070*	85	117.00	12	9989.	0.0	0.0	0.0060*
31	195.00	10	15675.	0.1	0.1	0.0094	86	115.00	8	1579.	0.0	0.0	0.0009
32	194.00	8	2804.	0.0	0.0	0.0017	87	114.00	12	31948.	0.2	0.2	0.0191
33	193.00	10	18368.	0.1	0.1	0.0110	88	113.00	29	773520.	3.8	3.8	0.4622
34	191.00	8	1614.	0.0	0.0	0.0010	89	112.00	17	325936.	1.6	1.6	0.1948
35	185.00	10	11607.	0.1	0.1	0.0069	90	111.00	21	796336.	3.9	3.9	0.4759
36	184.00	17	246988.	1.2	1.2	0.1476	91	110.00	17	300448.	1.5	1.5	0.1795
37	183.00	17	532816.	2.6	2.6	0.3184	92	109.00	25	396736.	2.0	2.0	0.2371*
38	182.00	10	11589.	0.1	0.1	0.0069	93	108.00	12	31489.	0.2	0.2	0.0188
39	181.00	8	32778.	0.2	0.2	0.0196*	94	107.00	17	90856.	0.5	0.5	0.0543*
40	180.00	10	34374.	0.2	0.2	0.0205	95	106.00	8	1388.	0.0	0.0	0.0008
41	179.00	12	62973.	0.3	0.3	0.0376*	96	105.00	10	16045.	0.1	0.1	0.0096*
42	178.00	14	114276.	0.6	0.6	0.0683	97	104.00	8	3180.	0.0	0.0	0.0019
43	177.00	12	21701.	0.1	0.1	0.0130	98	100.00	14	98864.	0.5	0.5	0.0591*
44	171.00	8	8380.	0.0	0.0	0.0050	99	99.00	25	1261888.	6.3	6.3	0.7541
45	170.00	17	138812.	0.7	0.7	0.0829	100	98.00	25	1328768.	6.6	6.6	0.7940
46	169.00	21	1489856.	7.4	7.4	0.8903	101	97.00	25	2155008.	10.7	10.7	1.2878*
47	168.00	10	32644.	0.2	0.2	0.0195	102	96.00	21	629840.	3.1	3.1	0.3764
48	167.00	10	28317.	0.1	0.1	0.0169	103	95.00	21	595920.	3.0	3.0	0.3561
49	166.00	12	21010.	0.1	0.1	0.0126	104	94.00	14	95484.	0.5	0.5	0.0571
50	165.00	10	17419.	0.1	0.1	0.0104	105	93.00	17	136576.	0.7	0.7	0.0816*
51	163.00	8	3426.	0.0	0.0	0.0020	106	92.00	8	1571.	0.0	0.0	0.0009
52	157.00	12	83800.	0.4	0.4	0.0501	107	91.00	12	69200.	0.3	0.3	0.0414
53	156.00	25	1074240.	5.3	5.3	0.6419*	108	87.00	6	4543.	0.0	0.0	0.0027
54	155.00	13	11117824.	55.1	55.1	6.6436*	109	86.00	17	206344.	1.0	1.0	0.1233
55	154.00	17	264496.	1.3	1.3	0.1581*	110	85.00	29	3632192.	18.0	18.0	2.1705

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	84.00	25	1847296.	9.2	9.2	1.1039
112	83.00	35	6059776.	30.0	30.0	3.6211*
113	82.00	25	702608.	3.5	3.5	0.4199*
114	81.00	21	860784.	4.3	4.3	0.5144
115	80.00	21	222788.	1.1	1.1	0.1331*
116	79.00	17	271600.	1.3	1.3	0.1623*
117	78.00	17	114612.	0.6	0.6	0.0685*
118	77.00	21	344432.	1.7	1.7	0.2058*
119	75.00	10	11839.	0.1	0.1	0.0071*
120	74.00	12	85988.	0.4	0.4	0.0514*
121	73.00	12	39935.	0.2	0.2	0.0239*
122	72.00	21	213888.	1.1	1.1	0.1278*
123	71.00	29	5051904.	25.0	25.0	3.0188*
124	70.00	25	1362688.	6.7	6.7	0.8143
125	69.00	35	6527488.	32.3	32.3	3.9006
126	68.00	21	1001088.	5.0	5.0	0.5982
127	67.00	25	1190016.	5.9	5.9	0.7111
128	66.00	14	79872.	0.4	0.4	0.0477*
129	65.00	14	116292.	0.6	0.6	0.0695
130	64.00	17	142144.	0.7	0.7	0.0849*
131	63.00	14	92408.	0.5	0.5	0.0552*
132	61.00	17	122352.	0.6	0.6	0.0731
133	60.00	12	14678.	0.1	0.1	0.0088*
134	59.00	14	91220.	0.5	0.5	0.0545
135	58.00	21	525296.	2.6	2.6	0.3139
136	57.00	43	11698176.	57.9	57.9	6.9904*
137	56.00	29	2693184.	13.3	13.3	1.6093
138	55.00	43	13031168.	64.5	64.5	7.7870*
139	54.00	25	941568.	4.7	4.7	0.5626
140	53.00	21	780496.	3.9	3.9	0.4664
141	52.00	10	39860.	0.2	0.2	0.0238*
142	51.00	17	111224.	0.6	0.6	0.0665*
143	50.00	10	21393.	0.1	0.1	0.0128*
144	48.00	6	2406.	0.0	0.0	0.0014
145	47.00	17	135572.	0.7	0.7	0.0810*
146	46.00	12	2782.	0.0	0.0	0.0017
147	45.00	17	143052.	0.7	0.7	0.0855*
148	44.00	35	740512.	3.7	3.7	0.4425
149	43.00	43	20188160.	100.0	100.0	*12.06*
150	42.00	35	3648384.	18.1	18.1	2.1801*
151	41.00	43	13136128.	65.1	65.1	7.8497*
152	40.00	25	473232.	2.3	2.3	0.2828
153	39.00	29	2128000.	10.5	10.5	1.2716*
154	38.00	17	59252.	0.3	0.3	0.0354*
155	37.00	12	7229.	0.0	0.0	0.0043*
156	36.00	14	97056.	0.5	0.5	0.0580*
157	35.00	6	1861.	0.0	0.0	0.0011

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 5/24/98
 L156EA.2494 [TIC=2158848, 105X=176888] EI

2,6,10-trimethylundecanoic acid,
 2,2,2-trifluoroethyl ester

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	310.00	8	2825.	2.4	2.4	0.3047	104.00	10	2011.	1.7	1.7	0.2169
2	278.00	8	1516.	1.3	1.3	0.1635	103.00	12	2366.	2.0	2.0	0.2552
3	274.00	6	1025.	0.9	0.9	0.1106	99.00	12	5664.	4.9	4.9	0.6109
4	267.00	8	1199.	1.0	1.0	0.1293	98.00	17	4264.	3.7	3.7	0.4599
5	250.00	8	650.	0.6	0.6	0.0701	97.00	29	41946.	36.1	36.1	4.5245
6	239.00	8	1072.	0.9	0.9	0.1156	95.00	25	1023.	0.9	0.9	0.1103
7	237.00	8	1562.	1.3	1.3	0.1685	92.00	17	7070.	6.1	6.1	0.7626*
8	225.00	17	7249.	6.2	6.2	0.7819	89.00	17	3350.	2.9	2.9	0.3613
9	221.00	8	2209.	1.9	1.9	0.2383	85.00	12	9000.	7.8	7.8	0.9708*
10	211.00	21	9684.	8.3	8.3	1.0446*	84.00	25	3137.	2.7	2.7	0.3384
11	210.00	8	482.	0.4	0.4	0.0520	83.00	35	19199.	16.5	16.5	2.0709
12	209.00	10	2843.	2.4	2.4	0.3067	83.00	17	5029.	4.3	4.3	0.5425
13	198.00	12	2958.	2.5	2.5	0.3191	73.00	10	1351.	1.2	1.2	0.1457
14	197.00	10	2288.	0.2	0.2	0.0311	72.00	17	2839.	2.4	2.4	0.3062
15	196.00	10	2243.	1.9	1.9	0.2419	71.00	25	44078.	38.0	38.0	4.7545
16	193.00	8	1581.	1.4	1.4	0.1705	69.00	25	2637.	2.3	2.3	0.2844
17	192.00	10	546.	0.5	0.5	0.0589	69.00	35	34130.	29.4	29.4	3.6814
18	181.00	12	2264.	1.9	1.9	0.2442	68.00	25	678.	0.6	0.6	0.0731
19	178.00	6	1655.	1.4	1.4	0.1785	65.00	12	470.	0.4	0.4	0.0507
20	177.00	8	548.	0.5	0.5	0.0591*	64.00	8	3562.	3.1	3.1	0.3842*
21	175.00	17	3604.	3.1	3.1	0.3887	63.00	12	958.	0.8	0.8	0.1033*
22	169.00	21	5959.	5.1	5.1	0.6428	58.00	17	10007.	8.6	8.6	1.0794*
23	168.00	6	1206.	0.1	0.1	0.0129	57.00	35	64661.	55.7	55.7	6.9746
24	167.00	14	2896.	2.5	2.5	0.3124	56.00	29	20759.	17.9	17.9	2.2392
25	164.00	17	27.	0.0	0.0	0.0029	55.00	35	51664.	44.5	44.5	5.5727
26	162.00	8	2006.	1.7	1.7	0.2164	54.00	21	1363.	1.2	1.2	0.1470
27	158.00	6	1352.	1.2	1.2	0.1458	53.00	25	1930.	1.7	1.7	0.2082
28	157.00	17	4308.	3.7	3.7	0.4647	52.00	14	3433.	3.0	3.0	0.3703
29	156.00	25	63953.	55.1	55.1	6.8983	51.00	17	9519.	8.2	8.2	1.0268*
30	155.00	21	5972.	5.1	5.1	0.6442	50.00	8	1935.	1.7	1.7	0.2087*
31	153.00	25	4222.	3.6	3.6	0.4554	47.00	6	3839.	3.3	3.3	0.4141
32	152.00	21	18859.	16.2	16.2	2.0342	45.00	21	4256.	3.7	3.7	0.4591*
33	151.00	21	850.	0.7	0.7	0.0917	43.00	35	116108.	100.0	100.0	*12.52
34	149.00	17	4565.	3.9	3.9	0.4924	42.00	29	13265.	11.4	11.4	1.4308
35	148.00	12	184.	0.2	0.2	0.0198	41.00	35	79964.	68.9	68.9	8.6253
36	141.00	12	5274.	4.5	4.5	0.5689	40.00	21	3033.	2.6	2.6	0.3272
37	140.00	12	4723.	4.1	4.1	0.5094*	39.00	25	17462.	15.0	15.0	1.8835
38	139.00	12	2902.	2.5	2.5	0.3130*	33.00	17	1439.	1.2	1.2	0.1552
39	138.00	8	2202.	1.9	1.9	0.2375*	30.00	14	4619.	4.0	4.0	0.4982
40	131.00	10	2862.	2.5	2.5	0.3087	29.00	35	34119.	29.4	29.4	3.6802
41	127.00	21	12852.	11.1	11.1	1.3863	28.00	25	10921.	9.4	9.4	1.1780*
42	126.00	8	1409.	1.2	1.2	0.1520	27.00	29	28822.	24.8	24.8	3.1089
43	125.00	21	9763.	8.4	8.4	1.0531						
44	124.00	12	3251.	0.0	0.0	0.0009*						
45	123.00	21	2834.	2.8	2.8	0.3507						
46	121.00	25	1312.	2.4	2.4	0.3057						
47	119.00	14	1415.	1.1	1.1	0.1415						
48	118.00	6	1415.	1.2	1.2	0.1526						
49	113.00	17	5907.	5.1	5.1	0.6372						
50	112.00	12	1942.	1.7	1.7	0.2095						
51	111.00	21	6604.	5.7	5.7	0.7123						
52	110.00	21	3477.	3.0	3.0	0.3750						
53	109.00	29	12318.	10.6	10.6	1.3287						
54	107.00	21	4656.	4.0	4.0	0.5022						
55	105.00	17	219.	0.2	0.2	0.0236						

13ALPA.1 [TIC-174888192, 188X-28319232] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	313.00	8	1533.	0.0	0.0	0.0009	56	164.00	8	2803.	0.0	0.0	0.0016
2	312.00	12	73496.	0.4	0.4	0.0422	57	163.00	10	36905.	0.2	0.2	0.0212
3	311.00	21	762368.	3.8	0.4	0.4379*	58	157.00	14	78684.	0.4	0.4	0.0452
4	310.00	35	4000640.	19.7	3.8	2.2981*	59	156.00	21	1208512.	5.9	5.9	0.6942*
5	309.00	10	15400.	0.1	0.1	0.0088*	60	155.00	35	11432448.	56.3	56.3	6.5670*
6	293.00	6	3501.	0.0	0.0	0.0020	61	154.00	10	21815.	0.1	0.1	0.0125*
7	292.00	12	85508.	0.4	0.4	0.0491	62	153.00	17	145812.	0.7	0.7	0.0838
8	291.00	17	404144.	2.0	2.0	0.2321	63	152.00	14	54998.	0.3	0.3	0.0316*
9	282.00	12	66624.	0.3	0.3	0.0383	64	151.00	12	3481.	0.0	0.0	0.0020
10	281.00	17	376608.	1.9	1.9	0.2163	65	150.00	8	709.	0.0	0.0	0.0041
11	269.00	10	24683.	0.1	0.1	0.0142	66	149.00	17	108556.	0.5	0.5	0.0624*
12	268.00	17	288352.	1.4	1.4	0.1656	67	145.00	12	1333.	0.1	0.1	0.0075*
13	267.00	21	2193856.	10.8	10.8	1.2602*	68	144.00	17	161780.	0.8	0.8	0.0929*
14	255.00	12	2744.	0.0	0.0	0.0016	69	143.00	35	3233792.	15.9	15.9	1.8576*
15	254.00	12	103688.	0.5	0.5	0.0596	70	142.00	43	15599872.	76.8	76.8	8.9609*
16	253.00	17	605168.	3.0	3.0	0.3476	71	141.00	21	547904.	2.7	2.7	0.3147*
17	241.00	8	4700.	0.0	0.0	0.0027	72	140.00	17	133560.	0.7	0.7	0.0768*
18	240.00	12	62409.	0.3	0.3	0.0358	73	139.00	21	265552.	1.3	1.3	0.1525
19	239.00	14	248692.	1.2	1.2	0.1429	74	138.00	17	218148.	1.1	1.1	0.1253
20	231.00	14	6907.	0.0	0.0	0.0040*	75	137.00	12	81952.	0.4	0.4	0.0471
21	230.00	17	7894.	0.0	0.0	0.0045*	76	136.00	17	144648.	0.7	0.7	0.0831
22	227.00	8	4405.	0.0	0.0	0.0025	77	135.00	25	1471744.	7.2	7.2	0.8454*
23	226.00	12	110064.	0.5	0.5	0.0632	78	133.00	6	4376.	0.0	0.0	0.0025
24	225.00	17	679136.	3.3	3.3	0.3901	79	131.00	10	12092.	0.1	0.1	0.0069
25	224.00	6	1628.	0.0	0.0	0.0009	80	129.00	6	9491.	0.0	0.0	0.0055
26	213.00	12	54532.	0.3	0.3	0.0313*	81	128.00	14	74204.	0.4	0.4	0.0426
27	212.00	25	703504.	3.5	3.5	0.4041*	82	127.00	35	1614720.	7.9	7.9	0.9275*
28	211.00	35	5516544.	27.1	27.1	3.1688*	83	126.00	17	151944.	0.7	0.7	0.0873
29	210.00	8	14880.	0.1	0.1	0.0085	84	125.00	21	384864.	1.9	1.9	0.2211
30	209.00	8	17975.	0.1	0.1	0.0103	85	124.00	17	220732.	1.1	1.1	0.1268
31	208.00	12	6559.	0.0	0.0	0.0038	86	123.00	21	377024.	1.9	1.9	0.2166*
32	207.00	10	25169.	0.1	0.1	0.0145	87	122.00	25	981552.	4.8	4.8	0.5638
33	199.00	8	34078.	0.2	0.2	0.0196	88	121.00	14	157944.	0.8	0.8	0.0907*
34	198.00	17	542512.	2.7	2.7	0.3116	89	119.00	12	18717.	0.1	0.1	0.0108*
35	197.00	17	1047728.	5.2	5.2	0.6018	90	118.00	14	38376.	0.2	0.2	0.0220*
36	195.00	6	735.	0.0	0.0	0.0004	91	117.00	8	6465.	0.0	0.0	0.0037
37	193.00	12	43385.	0.2	0.2	0.0249	92	115.00	8	4508.	0.0	0.0	0.0026
38	192.00	14	111560.	0.5	0.5	0.0641	93	114.00	10	59497.	0.3	0.3	0.0342*
39	191.00	8	5702.	0.0	0.0	0.0033	94	113.00	29	1015952.	5.0	5.0	0.5836
40	185.00	10	16394.	0.1	0.1	0.0060	95	112.00	21	367136.	1.8	1.8	0.2109
41	184.00	17	208688.	1.0	1.0	0.1199*	96	111.00	21	949280.	4.7	4.7	0.5453
42	183.00	17	611824.	3.0	3.0	0.3514*	97	110.00	21	326064.	1.6	1.6	0.1873
43	182.00	10	14514.	0.1	0.1	0.0083	98	109.00	25	368832.	1.8	1.8	0.2119*
44	181.00	12	50836.	0.3	0.3	0.0292*	99	108.00	12	49218.	0.2	0.2	0.0283
45	180.00	12	56090.	0.3	0.3	0.0322	100	107.00	17	124776.	0.6	0.6	0.0717*
46	179.00	10	39529.	0.2	0.2	0.0227	101	106.00	8	4670.	0.0	0.0	0.0027
47	178.00	5	500.	0.0	0.0	0.0003	102	105.00	10	14130.	0.1	0.1	0.0081
48	177.00	10	18449.	0.1	0.1	0.0106	103	103.00	6	1431.	0.0	0.0	0.0008
49	171.00	8	8515.	0.0	0.0	0.0049	104	100.00	17	97208.	0.5	0.5	0.0558*
50	170.00	17	217808.	1.1	1.1	0.1251	105	99.00	25	1184128.	5.8	5.8	0.6802
51	169.00	29	1907584.	9.4	9.4	1.0958	106	98.00	25	1421696.	7.0	7.0	0.8167
52	168.00	17	230648.	1.1	1.1	0.1325	107	97.00	25	2379968.	11.7	11.7	1.3671
53	167.00	17	173384.	0.9	0.9	0.0996*	108	96.00	21	621952.	3.1	3.1	0.3573
54	166.00	21	847168.	4.2	4.2	0.4866*	109	95.00	21	649744.	3.2	3.2	0.3732
55	165.00	10	28581.	0.1	0.1	0.0164	110	94.00	14	106024.	0.5	0.5	0.0609

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	93.00	17	166416.	0.8	0.8	0.0956*
112	92.00	8	1833.	0.0	0.0	0.0011
113	91.00	12	69804.	0.3	0.3	0.0401*
114	87.00	10	5856.	0.0	0.0	0.0034
115	86.00	17	218220.	1.1	1.1	0.1254
116	85.00	29	3401920.	16.7	16.7	1.9541
117	84.00	25	1892224.	9.3	9.3	1.0869
118	83.00	35	6203648.	30.5	30.5	3.5635*
119	82.00	21	754400.	3.7	3.7	0.4333
120	81.00	25	940752.	4.6	4.6	0.5404
121	80.00	21	221216.	1.1	1.1	0.1271
122	79.00	17	288656.	1.4	1.4	0.1658
123	78.00	14	97772.	0.5	0.5	0.0562
124	77.00	21	338080.	1.7	1.7	0.1942*
125	75.00	6	1353.	0.0	0.0	0.0008
126	74.00	10	69604.	0.3	0.3	0.0400
127	73.00	12	63005.	0.3	0.3	0.0362*
128	72.00	21	276544.	1.4	1.4	0.1589
129	71.00	29	5635840.	27.7	27.7	3.2373*
130	70.00	25	1436160.	7.1	7.1	0.8250
131	69.00	35	6917632.	34.0	34.0	3.9736*
132	68.00	25	1057600.	5.2	5.2	0.6075
133	67.00	21	1150016.	5.7	5.7	0.6606
134	66.00	14	78084.	0.4	0.4	0.0449
135	65.00	17	134644.	0.7	0.7	0.0773*
136	64.00	17	143732.	0.7	0.7	0.0826
137	63.00	10	63716.	0.3	0.3	0.0366*
138	61.00	14	99624.	0.5	0.5	0.0572
139	60.00	14	12659.	0.1	0.1	0.0073
140	59.00	10	80348.	0.4	0.4	0.0462*
141	58.00	25	556224.	2.7	2.7	0.3195
142	57.00	43	12436992.	61.2	61.2	7.1441*
143	56.00	29	2675328.	13.2	13.2	1.5368
144	55.00	43	12827904.	63.1	63.1	7.3686*
145	54.00	25	901600.	4.4	4.4	0.5179
146	53.00	21	716512.	3.5	3.5	0.4116
147	52.00	10	34892.	0.2	0.2	0.0200*
148	51.00	1	113916.	0.6	0.6	0.0654
149	50.00	12	33920.	0.2	0.2	0.0195
150	48.00	8	1613.	0.0	0.0	0.0009
151	47.00	17	131288.	0.6	0.6	0.0754*
152	46.00	8	3807.	0.0	0.0	0.0022
153	45.00	21	156900.	0.8	0.8	0.0901*
154	44.00	35	758240.	3.7	3.7	0.4355*
155	43.00	51	20319232.	100.0	100.0	*11.67*
156	42.00	35	3442880.	16.9	16.9	1.9777
157	41.00	43	13061632.	64.3	64.3	7.5029*
158	40.00	25	473648.	2.3	2.3	0.2721*
159	39.00	29	2016704.	9.9	9.9	1.1584*
160	38.00	12	49508.	0.2	0.2	0.3284*
161	37.00	12	10092.	0.0	0.0	0.0058*
162	36.00	17	88512.	0.4	0.4	0.0508*

S2681.2681 [TIC-2288328, 188X-289312] EI

$$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \quad \text{CH}_3 \\ | \quad | \quad | \\ \text{CH}_3\text{CH}(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{COCH}_2\text{CF}_3 \\ || \quad \text{O} \end{array}$$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	324.00	14	4370.	1.5	1.5	0.1986	55	152.00	17	3192.	1.1	1.1	0.1451
2	309.00	8	1018.	0.4	0.4	0.0463	57	150.00	14	939.	0.3	0.3	0.0427
3	308.00	6	979.	0.3	0.3	0.0445	58	149.00	25	1590.	0.5	0.5	0.0723
4	306.00	17	6094.	2.1	2.1	0.2770	59	143.00	17	8197.	2.8	2.8	0.3725
5	305.00	14	4864.	1.7	1.7	0.2211	60	142.00	21	26868.	9.3	9.3	1.2211
6	295.00	10	1367.	0.5	0.5	0.0621	61	141.00	25	17810.	6.2	6.2	0.8094
7	288.00	6	1252.	0.4	0.4	0.0569	62	140.00	17	4421.	1.5	1.5	0.2009
8	282.00	8	1317.	0.5	0.5	0.0599	63	139.00	29	21474.	7.4	7.4	0.7759
9	275.00	8	2051.	0.7	0.7	0.0932	64	137.00	21	8463.	2.9	2.9	0.3846
10	269.00	6	1554.	0.5	0.5	0.0706	65	136.00	17	4255.	1.5	1.5	0.1934*
11	266.00	6	1346.	0.5	0.5	0.0612	66	135.00	29	1510.	0.5	0.5	0.0686
12	249.00	10	1575.	0.5	0.5	0.0716	67	134.00	8	755.	0.3	0.3	0.0343*
13	247.00	8	1697.	0.6	0.6	0.0771	68	133.00	17	47.	0.0	0.0	0.0021
14	240.00	8	2535.	0.9	0.9	0.1152	69	128.00	17	3495.	1.2	1.2	0.1588
15	239.00	17	16097.	5.6	5.6	0.7316	70	127.00	21	21495.	7.4	7.4	0.9769
16	238.00	17	3734.	1.3	1.3	0.1697	71	126.00	14	2619.	0.9	0.9	0.1190
17	236.00	6	1001.	0.3	0.3	0.0455	72	125.00	17	1120.	0.4	0.4	0.0509
18	235.00	8	2906.	1.0	1.0	0.1321	73	124.00	12	1447.	0.5	0.5	0.0658*
19	225.00	14	3274.	1.1	1.1	0.1488	74	122.00	21	2993.	1.0	1.0	0.1360
20	222.00	10	2187.	0.8	0.8	0.0994	75	121.00	25	440.	0.2	0.2	0.0200
21	221.00	12	2741.	0.9	0.9	0.1246	76	119.00	25	2018.	0.7	0.7	0.0917
22	213.00	10	1744.	0.6	0.6	0.0793	77	118.00	8	1051.	0.4	0.4	0.0478
23	211.00	17	8053.	2.8	2.8	0.3660	78	117.00	12	4938.	1.7	1.7	0.2244
24	210.00	10	1248.	0.4	0.4	0.0567	79	115.00	8	1020.	0.6	0.6	0.0827
25	209.00	10	4014.	1.4	1.4	0.1824	80	114.00	8	2146.	0.7	0.7	0.0975
26	207.00	14	3920.	1.3	1.3	0.1772*	81	113.00	25	14245.	4.9	4.9	0.6474
27	206.00	17	5057.	1.7	1.7	0.2298	82	112.00	17	9168.	3.2	3.2	0.4167
28	205.00	8	1397.	0.5	0.5	0.0535	83	111.00	21	34868.	12.1	12.1	1.5847*
29	198.00	10	3307.	1.1	1.1	0.1503	84	110.00	29	6021.	2.1	2.1	0.2736
30	197.00	17	3281.	1.1	1.1	0.1491	85	109.00	35	12093.	4.2	4.2	0.5496
31	196.00	21	4356.	1.5	1.5	0.1980	86	106.00	21	6603.	2.3	2.3	0.3001
32	195.00	17	396.	0.1	0.1	0.0180	87	105.00	17	475.	0.2	0.2	0.0216
33	194.00	12	866.	0.3	0.3	0.0394	88	103.00	10	2298.	0.8	0.8	0.1044
34	192.00	12	3120.	1.1	1.1	0.1418	89	100.00	10	1517.	0.5	0.5	0.0689
35	191.00	14	3615.	1.2	1.2	0.1643	90	99.00	21	8013.	2.8	2.8	0.3642
36	184.00	14	2493.	0.9	0.9	0.1133	91	98.00	21	14588.	5.0	5.0	0.6630
37	183.00	21	5087.	2.0	2.0	0.2676	92	97.00	35	64007.	22.2	22.2	2.9126
38	181.00	8	498.	0.2	0.2	0.0226*	93	96.00	35	21019.	7.3	7.3	0.9553
39	180.00	25	17211.	5.9	5.9	0.7822	94	95.00	25	9868.	3.4	3.4	0.4485
40	179.00	17	2156.	0.7	0.7	0.0980	95	94.00	17	703.	0.2	0.2	0.0319
41	178.00	21	6254.	2.2	2.2	0.2842	96	92.00	8	471.	0.2	0.2	0.0214
42	176.00	12	2098.	0.7	0.7	0.0953	97	91.00	21	898.	0.3	0.3	0.0408
43	173.00	6	1600.	0.6	0.6	0.0727	98	86.00	17	4557.	1.6	1.6	0.2071
44	171.00	10	2636.	0.9	0.9	0.1190	99	85.00	29	20554.	7.1	7.1	0.9341
45	170.00	25	10128.	3.5	3.5	0.4503	100	84.00	25	3619.	1.3	1.3	0.1645
46	169.00	29	98352.	34.0	34.0	4.4699	101	83.00	35	66192.	22.9	22.9	3.0083
47	168.00	10	818.	0.3	0.3	0.0372	102	82.00	25	7331.	2.5	2.5	0.3332
48	167.00	21	7444.	2.6	2.6	0.3383	103	81.00	25	5256.	1.8	1.8	0.2389
49	166.00	29	4220.	1.5	1.5	0.1918	104	77.00	25	7268.	2.5	2.5	0.3303
50	165.00	21	3223.	1.1	1.1	0.1465	105	76.00	8	1888.	0.7	0.7	0.0858
51	163.00	17	3351.	1.2	1.2	0.1523	106	74.00	8	2689.	0.9	0.9	0.1222
52	159.00	8	1522.	0.5	0.5	0.0692	107	73.00	12	2458.	0.8	0.8	0.1117
53	156.00	17	2136.	0.7	0.7	0.0971	108	72.00	14	6749.	2.3	2.3	0.3067
54	154.00	8	1150.	0.4	0.4	0.0523	109	71.00	35	128108.	44.3	44.3	5.8222
55	153.00	17	5151.	1.8	1.8	0.2341	110	70.00	25	24203.	8.4	8.4	1.1000*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	69.00	35	107456.	37.1	37.1	4.8837
112	68.00	21	4192.	1.4	1.4	0.1985
113	66.00	21	3806.	1.3	1.3	0.1730
114	65.00	21	7062.	2.4	2.4	0.3210
115	63.00	12	6858.	2.4	2.4	0.3117
116	61.00	17	9207.	3.2	3.2	0.4184
117	60.00	6	711.	0.2	0.2	0.0323
118	59.00	12	1768.	0.6	0.6	0.0804
119	58.00	29	15556.	5.4	5.4	0.7070
120	57.00	35	187912.	65.0	65.0	8.5402
121	56.00	29	67820.	23.4	23.4	3.0823
122	55.00	35	107512.	37.2	37.2	4.8862
123	54.00	25	3369.	1.2	1.2	0.1531
124	53.00	25	14428.	5.0	5.0	0.6557*
125	52.00	14	4951.	1.7	1.7	0.2250
126	51.00	17	331.	0.1	0.1	0.0150
127	50.00	10	1054.	0.4	0.4	0.0479
128	47.00	8	2314.	1.0	1.0	0.1324*
129	44.00	29	13960.	4.8	4.8	0.6345*
130	43.00	43	289312.	100.0	100.0	*13.14*
131	42.00	35	58271.	20.1	20.1	2.6483
132	41.00	35	175636.	60.7	60.7	7.9823
133	40.00	25	6985.	2.4	2.4	0.3175*
134	39.00	29	42733.	14.8	14.8	1.9421
135	38.00	12	1265.	0.4	0.4	0.0575
136	36.00	10	2277.	0.8	0.8	0.1035
137	33.00	14	1956.	0.7	0.7	0.0889*
138	32.00	12	6611.	2.3	2.3	0.3005
139	31.00	17	5226.	1.8	1.8	0.2375
140	30.00	14	3743.	1.3	1.3	0.1701
141	29.00	43	83260.	28.8	28.8	3.7840
142	28.00	43	19292.	6.7	6.7	0.8768
143	27.00	29	23321.	8.1	8.1	1.0599

CS3068.1 [TIC-1870336, 188X-385568] EI

Pentadecanoic acid,
2,2,2,-trifluoroethyl ester

PAGE 1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	346.00	8	62.	0.2	0.2	0.0033	56	132.00	17	2687.	0.7	0.7	0.1431
2	334.00	10	768.	0.2	0.2	0.0409	57	127.00	35	17848.	4.6	4.6	0.9502
3	330.00	8	1441.	0.4	0.4	0.0767	58	118.00	21	2655.	0.7	0.7	0.1413*
4	326.00	8	799.	0.2	0.2	0.0425	59	113.00	29	2231.	0.6	0.6	0.1188
5	325.00	21	10559.	2.7	2.7	0.5621	60	100.00	6	1767.	0.5	0.5	0.0941
6	324.00	17	36464.	9.5	9.5	1.9413	61	99.00	21	5824.	1.5	1.5	0.3101*
7	323.00	6	1190.	0.3	0.3	0.0634	62	98.00	21	14730.	3.8	3.8	0.7842
8	317.00	8	1135.	0.3	0.3	0.0604	63	90.00	21	5309.	1.4	1.4	0.2826*
9	309.00	8	2047.	0.5	0.5	0.1090	64	86.00	25	4269.	1.1	1.1	0.2273*
10	308.00	6	1167.	0.3	0.3	0.0621	65	85.00	25	28611.	7.4	7.4	1.5232
11	306.00	10	2344.	0.6	0.6	0.1248	66	84.00	29	23835.	6.2	6.2	1.2689
12	305.00	17	2668.	0.7	0.7	0.1420	67	83.00	35	15104.	3.9	3.9	0.8041
13	304.00	8	502.	0.1	0.1	0.0267	68	75.00	21	3607.	0.9	0.9	0.1920
14	295.00	10	5138.	1.3	1.3	0.2735	69	72.00	21	1559.	0.4	0.4	0.0830*
15	290.00	8	1726.	0.4	0.4	0.0919	70	71.00	29	72324.	18.8	18.8	3.8504
16	289.00	12	1403.	0.4	0.4	0.0747	71	70.00	25	3661.	0.9	0.9	0.1949
17	287.00	8	409.	0.1	0.1	0.0218	72	69.00	35	8864.	2.3	2.3	0.4719
18	282.00	14	9664.	2.5	2.5	0.5145	73	64.00	21	3923.	1.0	1.0	0.2089
19	281.00	17	17603.	4.6	4.6	0.9372	74	62.00	6	2683.	0.7	0.7	0.1428
20	276.00	12	1274.	0.3	0.3	0.0678	75	61.00	14	2455.	0.6	0.6	0.1307
21	274.00	6	1338.	0.3	0.3	0.0712	75	59.00	21	3676.	1.0	1.0	0.1957
22	268.00	12	2884.	0.7	0.7	0.1535	77	58.00	29	858.	0.2	0.2	0.0457
23	267.00	17	6842.	1.8	1.8	0.3643	78	57.00	51	183204.	47.5	47.5	9.7535*
24	259.00	8	1735.	0.4	0.4	0.0924	79	56.00	35	40988.	10.6	10.6	2.1821
25	254.00	10	2263.	0.6	0.6	0.1205	80	55.00	51	120176.	31.2	31.2	6.3980*
26	253.00	14	9716.	2.5	2.5	0.5173	81	47.00	17	6642.	1.7	1.7	0.3536
27	241.00	8	2282.	0.6	0.6	0.1215	82	45.00	29	8058.	2.1	2.1	0.4290
28	240.00	6	710.	0.2	0.2	0.0378	83	44.00	35	9873.	2.6	2.6	0.5256
29	239.00	21	5623.	1.5	1.5	0.2994	84	43.00	43	385568.	100.0	100.0	*20.52
30	232.00	8	37.	0.0	0.0	0.0020	85	42.00	35	46556.	12.1	12.1	2.4807
31	231.00	10	198.	0.1	0.1	0.0105	86	41.00	43	135520.	35.1	35.1	7.2149*
32	226.00	25	7683.	2.0	2.0	0.4090*	87	32.00	12	3944.	1.0	1.0	0.2100*
33	225.00	25	33369.	8.7	8.7	1.7765	88	29.00	51	43500.	11.3	11.3	2.3159*
34	222.00	12	746.	0.2	0.2	0.0397	89	27.00	35	32192.	8.3	8.3	1.7139
35	215.00	10	3501.	0.9	0.9	0.1864							
36	212.00	21	6126.	1.6	1.6	0.3261							
37	211.00	21	36799.	9.5	9.5	1.9591							
38	198.00	25	11348.	2.9	2.9	0.6042*							
39	197.00	17	5758.	1.5	1.5	0.3065							
40	196.00	10	2395.	0.6	0.6	0.1275							
41	188.00	6	648.	0.2	0.2	0.0345							
42	184.00	14	1410.	0.4	0.4	0.0751							
43	183.00	21	8382.	2.2	2.2	0.4462							
44	182.00	21	44.	0.0	0.0	0.0023							
45	180.00	21	3803.	1.0	1.0	0.2025							
46	172.00	10	400.	0.1	0.1	0.0213							
47	170.00	21	1700.	0.5	0.5	0.0948							
48	166.00	21	1030.	0.3	0.3	0.0548							
49	156.00	21	420.	0.1	0.1	0.0224							
50	155.00	29	123212.	32.0	32.0	6.5596							
51	150.00	17	1100.	0.3	0.3	0.0586							
52	144.00	12	3569.	0.9	0.9	0.1900							
53	143.00	43	47665.	12.4	12.4	*10.28							
54	142.00	29	193264.	50.1	50.1	0.3817							
55	141.00	25	7170.	1.9	1.9								

PAGE 2

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 5/24/98
S2936.2936 [TIC=1098556, 100X=211972] EI

4,8,12-trimethyltridecanoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	351.00	6	658.	0.3	0.3	0.347	56	169.00	21	4255.	2.0	2.0	0.2241
2	350.00	6	747.	0.4	0.4	0.0393	57	168.00	10	5759.	2.7	2.7	0.3033*
3	339.00	12	2251.	1.1	1.1	0.1186	58	167.00	12	1188.	0.6	0.6	0.0626
4	338.00	12	7339.	3.5	3.5	0.3866	59	165.00	17	690.	0.3	0.3	0.0363
5	332.00	8	1905.	0.9	0.9	0.1003	60	164.00	17	2813.	1.3	1.3	0.1482
6	321.00	8	1052.	0.5	0.5	0.0554	61	163.00	25	3398.	1.6	1.6	0.1790
7	309.00	10	2262.	1.1	1.1	0.1191	62	162.00	12	2039.	1.0	1.0	0.1074
8	299.00	8	932.	0.4	0.4	0.0491	63	159.00	14	161.	0.1	0.1	0.0085
9	292.00	12	1395.	0.7	0.7	0.0735	64	157.00	10	3361.	1.6	1.6	0.1770*
10	291.00	8	2790.	1.3	1.3	0.1470	65	156.00	17	1528.	0.7	0.7	0.0805
11	281.00	17	9532.	4.5	4.5	0.5021	66	155.00	25	49676.	23.4	23.4	2.6165
12	278.00	10	1287.	0.6	0.6	0.0678	67	153.00	29	13209.	6.2	6.2	0.6957
13	277.00	17	3234.	1.5	1.5	0.1703	68	151.00	21	3801.	1.8	1.8	0.2002
14	276.00	8	2940.	1.4	1.4	0.1549*	69	150.00	17	11.	0.0	0.0	0.0006
15	275.00	14	2656.	1.3	1.3	0.1399	70	147.00	17	630.	0.3	0.3	0.0332
16	267.00	8	1130.	0.5	0.5	0.0595	71	144.00	8	1759.	0.8	0.8	0.0926
17	264.00	12	3585.	1.7	1.7	0.1888	72	143.00	17	10165.	4.8	4.8	0.5354
18	260.00	8	880.	0.4	0.4	0.0464	73	142.00	21	24789.	11.7	11.7	1.3057
19	253.00	14	7347.	3.5	3.5	0.3870	74	141.00	21	21089.	9.9	9.9	1.1108
20	251.00	12	1619.	0.8	0.8	0.0853	75	139.00	21	3307.	1.6	1.6	0.1742
21	249.00	14	255.	0.1	0.1	0.0134	76	137.00	21	2714.	1.3	1.3	0.1430
22	247.00	6	66.	0.0	0.0	0.0035	77	135.00	29	5633.	2.7	2.7	0.2967
23	239.00	21	6528.	3.1	3.1	0.3438	78	134.00	14	1655.	0.8	0.8	0.0872
24	235.00	10	5508.	2.6	2.6	0.2901	79	133.00	21	1275.	0.6	0.6	0.0672
25	234.00	12	1266.	0.6	0.6	0.0667	80	132.00	10	2577.	1.2	1.2	0.1357
26	233.00	10	6.	0.0	0.0	0.0003	81	131.00	17	2135.	1.0	1.0	0.1125
27	226.00	12	3365.	1.6	1.6	0.1772	82	129.00	14	2125.	1.0	1.0	0.1119
28	225.00	17	10282.	4.9	4.9	0.5415	83	128.00	10	2405.	1.1	1.1	0.1267*
29	223.00	17	5665.	2.7	2.7	0.2984	84	127.00	35	24911.	11.8	11.8	1.3121
30	221.00	17	3933.	1.9	1.9	0.2072	85	126.00	21	5598.	2.6	2.6	0.2949
31	220.00	8	647.	0.3	0.3	0.0341	86	125.00	21	5301.	2.5	2.5	0.2792
32	219.00	17	486.	0.2	0.2	0.0256	87	123.00	25	9253.	4.4	4.4	0.4874
33	217.00	10	1787.	0.8	0.8	0.0941	88	122.00	25	746.	0.4	0.4	0.0393
34	216.00	10	1249.	0.6	0.6	0.0658	89	120.00	12	3387.	1.6	1.6	0.1784*
35	211.00	14	6782.	3.2	3.2	0.3572	90	119.00	17	5079.	2.4	2.4	0.2675
36	210.00	8	751.	0.4	0.4	0.0396	91	118.00	10	2031.	1.0	1.0	0.0925*
37	209.00	14	2735.	1.3	1.3	0.1441	92	116.00	8	1756.	0.8	0.8	0.1118
38	205.00	17	4420.	2.1	2.1	0.2328	93	115.00	17	2122.	1.0	1.0	0.1566
39	203.00	10	245.	0.1	0.1	0.0129	94	114.00	14	2974.	1.4	1.4	0.13833
40	201.00	8	2007.	0.9	0.9	0.1057	95	113.00	29	26263.	12.4	12.4	1.3833
41	200.00	6	1138.	0.5	0.5	0.0599	96	112.00	25	9100.	4.3	4.3	0.4793
42	198.00	6	1698.	0.8	0.8	0.0894	97	111.00	25	12787.	6.0	6.0	0.6735
43	197.00	25	10499.	5.0	5.0	0.5530	98	110.00	21	6398.	3.0	3.0	0.3370
44	196.00	17	4604.	2.2	2.2	0.2425	99	109.00	29	13840.	6.5	6.5	0.7290
45	195.00	21	6032.	2.8	2.8	0.3177	100	108.00	25	5295.	2.5	2.5	0.2789
46	193.00	25	436.	0.2	0.2	0.0230	101	107.00	25	2771.	1.3	1.3	0.1460
47	191.00	21	2107.	1.0	1.0	0.1110	102	105.00	21	2658.	1.3	1.3	0.1400*
48	187.00	8	4728.	2.2	2.2	0.2490*	103	103.00	21	3535.	1.7	1.7	0.1862*
49	183.00	21	7230.	3.4	3.4	0.3808	104	99.00	25	17757.	8.4	8.4	0.9353
50	181.00	29	9277.	4.4	4.4	0.4886	105	98.00	21	7962.	3.8	3.8	0.4194
51	179.00	25	1555.	0.7	0.7	0.0819	106	97.00	25	19190.	9.1	9.1	1.0108
52	173.00	14	94.	0.0	0.0	0.0050	107	96.00	25	6634.	3.1	3.1	0.3494
53	172.00	8	1814.	0.9	0.9	0.0955	108	94.00	25	1022.	0.5	0.5	0.0538
54	171.00	14	3503.	1.7	1.7	0.1845	109	93.00	25	12832.	6.1	6.1	0.6759
55	170.00	10	146.	0.1	0.1	0.0077	110	92.00	21	6147.	2.9	2.9	0.3238

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	91.00	25	11603.	5.5	5.5	0.6111
112	89.00	10	74.	0.0	0.0	0.0039
113	86.00	12	3906.	1.8	1.8	0.2057
114	85.00	25	26251.	13.2	13.2	1.4775
115	84.00	25	3600.	1.7	1.7	0.1896
116	83.00	43	63240.	29.8	29.8	3.3309
117	82.00	29	5709.	2.7	2.7	0.3007
118	78.00	12	11.	0.0	0.0	0.0006
119	77.00	29	14489.	6.8	6.8	0.7632
120	73.00	21	2099.	1.0	1.0	0.1106
121	72.00	17	6639.	3.1	3.1	0.3497
122	71.00	35	134924.	63.7	63.7	7.1066
123	70.00	29	21417.	10.1	10.1	1.1281
124	69.00	43	78660.	37.1	37.1	4.1431
125	68.00	25	18880.	8.9	8.9	0.9944
126	67.00	35	39100.	18.4	18.4	2.0599
127	66.00	21	4513.	2.1	2.1	0.2377*
128	65.00	21	4076.	1.9	1.9	0.2147
129	64.00	6	2781.	1.3	1.3	0.1465
130	61.00	21	349.	0.2	0.2	0.0184
131	60.00	12	2899.	1.4	1.4	0.1527
132	59.00	12	1683.	0.8	0.8	0.0886
133	58.00	17	4845.	2.3	2.3	0.2552*
134	57.00	29	18882.	89.1	89.1	9.9492
135	56.00	29	19831.	9.4	9.4	1.0445
136	55.00	43	133568.	63.0	63.0	7.0352
137	54.00	29	9586.	4.5	4.5	0.5049
138	53.00	29	7073.	3.3	3.3	0.3725
139	47.00	21	1527.	0.7	0.7	0.0804
140	45.00	25	6281.	3.0	3.0	0.3308
141	44.00	25	8997.	4.2	4.2	0.4739*
142	43.00	43	211972.	100.0	100.0	*11.16*
143	42.00	35	31688.	14.9	14.9	1.6691
144	41.00	35	116952.	55.2	55.2	6.1600*
145	39.00	29	20582.	9.7	9.7	1.0841
146	36.00	12	3464.	1.6	1.6	0.1825
147	33.00	29	5798.	2.7	2.7	0.3054
148	31.00	17	2447.	1.2	1.2	0.1289
149	29.00	35	65328.	30.8	30.8	3.4409
150	28.00	35	8816.	4.2	4.2	0.4644
151	27.00	29	42361.	20.0	20.0	2.2312

14ALPA.1 [TIC=172678976, 188X=21356544] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	430.00	8	1395.	0.0	0.0	0.0008	56	191.00	10	11611.	0.1	0.1	0.0067
2	429.00	6	2579.	0.0	0.0	0.0015	57	190.00	6	1056.	0.0	0.0	0.0006
3	341.00	8	6404.	0.0	0.0	0.0037	58	185.00	8	15962.	0.1	0.1	0.0092
4	340.00	14	150108.	0.7	0.7	0.0869*	59	184.00	17	347744.	1.6	1.6	0.2014
5	339.00	21	1205248.	5.6	5.6	0.6980*	60	183.00	21	637648.	3.0	3.0	0.3693
6	338.00	35	4449280.	20.8	20.8	2.5767*	61	182.00	10	18177.	0.1	0.1	0.0105
7	337.00	12	2446.	0.0	0.0	0.0014*	62	181.00	12	50231.	0.2	0.2	0.0291
8	336.00	10	1929.	0.0	0.0	0.0011	63	180.00	10	59134.	0.3	0.3	0.0342
9	321.00	10	9359.	0.0	0.0	0.0058	64	179.00	10	44636.	0.2	0.2	0.0259
10	320.00	12	104556.	0.5	0.5	0.0606*	65	177.00	10	24556.	0.1	0.1	0.0142
11	319.00	17	385072.	1.8	1.8	0.2230	66	171.00	8	11162.	0.1	0.1	0.0065
12	311.00	6	6298.	0.0	0.0	0.0036	67	170.00	17	243816.	1.1	1.1	0.1412
13	310.00	12	78056.	0.4	0.4	0.0452*	68	169.00	25	1471552.	6.9	6.9	0.8522*
14	309.00	17	319328.	1.5	1.5	0.1849	69	168.00	17	97008.	0.5	0.5	0.0562*
15	297.00	6	15778.	0.1	0.1	0.0091	70	167.00	17	93840.	0.4	0.4	0.0543*
16	296.00	17	248728.	1.2	1.2	0.1440*	71	166.00	17	143780.	0.7	0.7	0.0833*
17	295.00	21	1502272.	7.0	7.0	0.8700	72	165.00	12	48906.	0.2	0.2	0.0283
18	283.00	6	11186.	0.1	0.1	0.0065	73	164.00	6	1090.	0.0	0.0	0.0006
19	282.00	12	71304.	0.3	0.3	0.0413	74	163.00	12	40362.	0.2	0.2	0.0234*
20	281.00	17	265520.	1.2	1.2	0.1538	75	157.00	12	63606.	0.3	0.3	0.0368
21	269.00	8	3787.	0.0	0.0	0.0022	76	156.00	25	1022720.	4.8	4.8	0.5923*
22	268.00	12	82676.	0.4	0.4	0.0479	77	155.00	35	10001408.	46.8	46.8	5.7922*
23	267.00	17	578320.	2.7	2.7	0.3349	78	154.00	12	68480.	0.3	0.3	0.0397
24	258.00	6	11729.	0.0	0.0	0.0010	79	153.00	21	207876.	1.0	1.0	0.1204*
25	255.00	8	11345.	0.1	0.1	0.0066	80	152.00	17	182708.	0.9	0.9	0.1058
26	254.00	12	138940.	0.7	0.7	0.0805	81	151.00	10	30446.	0.1	0.1	0.0079
27	253.00	17	731744.	3.4	3.4	0.4238	82	150.00	8	13639.	0.1	0.1	0.0079
28	241.00	12	34140.	0.2	0.2	0.0198	83	149.00	17	122244.	0.6	0.6	0.0708
29	240.00	21	508416.	2.4	2.4	0.2944*	84	148.00	8	5906.	0.0	0.0	0.0034
30	239.00	25	1980544.	9.3	9.3	0.1470	85	147.00	6	1886.	0.0	0.0	0.0011
31	238.00	10	21453.	0.1	0.1	0.0124	86	144.00	17	193748.	0.9	0.9	0.1122
32	237.00	10	4353.	0.0	0.0	0.0025	87	143.00	25	3448128.	16.1	16.1	1.9969*
33	227.00	8	9863.	0.0	0.0	0.0057	88	142.00	43	13665792.	64.0	64.0	7.9144*
34	226.00	12	135656.	0.6	0.6	0.0786	89	141.00	25	740848.	3.5	3.5	0.4291
35	225.00	17	304848.	1.4	1.4	0.1765	90	140.00	17	126056.	0.6	0.6	0.0730*
36	223.00	6	990.	0.0	0.0	0.0006	91	139.00	17	321920.	1.5	1.5	0.1864
37	221.00	8	21873.	0.1	0.1	0.0127	92	138.00	17	174700.	0.8	0.8	0.1012
38	220.00	14	113932.	0.5	0.5	0.0660	93	137.00	14	86864.	0.4	0.4	0.0503*
39	219.00	8	1885.	0.0	0.0	0.0011	94	136.00	17	128332.	0.6	0.6	0.0743
40	213.00	10	29417.	0.1	0.1	0.0170	95	135.00	25	1225088.	5.7	5.7	0.7095*
41	212.00	17	366096.	1.7	1.7	0.2120*	96	133.00	14	5331.	0.0	0.0	0.0031
42	211.00	25	2897024.	13.6	13.6	1.6778*	97	132.00	6	1272.	0.0	0.0	0.0007
43	210.00	8	4197.	0.0	0.0	0.0024	98	131.00	10	14054.	0.1	0.1	0.0081
44	209.00	10	13746.	0.1	0.1	0.0080	99	129.00	8	3680.	0.0	0.0	0.0021
45	208.00	6	4194.	0.0	0.0	0.0005	100	125.00	14	70276.	0.3	0.3	0.0407*
46	207.00	14	102284.	0.5	0.5	0.0592	101	126.00	29	1512960.	7.1	7.1	0.8762
47	205.00	6	896.	0.0	0.0	0.0005	102	125.00	17	148668.	0.7	0.7	0.0861*
48	199.00	10	50542.	0.2	0.2	0.0293	103	125.00	21	472720.	2.2	2.2	0.2738
49	198.00	21	694112.	3.3	3.3	0.4020	104	124.00	17	206788.	1.0	1.0	0.1198
50	197.00	25	1246464.	5.8	5.8	0.7219*	105	123.00	25	381504.	1.8	1.8	0.2209
51	196.00	14	123572.	0.6	0.6	0.0716	106	122.00	21	724576.	3.4	3.4	0.4196
52	195.00	14	102592.	0.5	0.5	0.0594*	107	121.00	17	164748.	0.8	0.8	0.0954*
53	194.00	17	615184.	2.9	2.9	0.3563	108	120.00	6	1375.	0.0	0.0	0.0008
54	193.00	8	19641.	0.1	0.1	0.0114	109	119.00	8	19228.	0.1	0.1	0.0111
55	192.00	8	2097.	0.0	0.0	0.0012	110	118.00	25	27399.	0.1	0.1	0.0159*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	116.00	10	4780.	0.0	0.0	0.0028*
112	115.00	6	1952.	0.0	0.0	0.0011
113	114.00	12	41939.	0.2	0.0	0.0243
114	113.00	29	853360.	4.0	4.0	0.4942
115	112.00	21	413328.	1.9	1.9	0.2394
116	111.00	21	1037328.	4.9	4.9	0.6008
117	110.00	17	292464.	1.4	1.4	0.1694
118	109.00	21	364464.	1.7	1.7	0.2111
119	108.00	12	42354.	0.2	0.2	0.0245
120	107.00	14	130184.	0.6	0.6	0.0754
121	106.00	8	3964.	0.0	0.0	0.0023
122	105.00	10	21478.	0.1	0.1	0.0124*
123	104.00	6	1636.	0.0	0.0	0.0089
124	103.00	14	72736.	0.3	0.3	0.0421*
125	99.00	21	1023760.	4.8	4.8	0.5929
126	98.00	25	1422080.	6.7	6.7	0.8236*
127	97.00	29	2765376.	12.9	12.9	1.6015*
128	96.00	21	706304.	3.3	3.3	0.4090*
129	95.00	21	675440.	3.2	3.2	0.3912
130	94.00	14	95932.	0.4	0.4	0.0556*
131	93.00	17	162232.	0.8	0.8	0.0940
132	91.00	14	67460.	0.3	0.3	0.0391
133	87.00	12	7579.	0.0	0.0	0.0044*
134	86.00	17	244436.	1.1	1.1	0.1416*
135	85.00	29	3634368.	17.0	17.0	2.1048*
136	84.00	25	1884352.	8.8	8.8	1.0913
137	83.00	35	6003456.	28.1	28.1	3.4768*
138	82.00	25	832528.	3.9	3.9	0.4821
139	81.00	25	940208.	4.4	4.4	0.5445
140	80.00	21	215684.	1.0	1.0	0.1249*
141	79.00	21	272640.	1.3	1.3	0.1579*
142	78.00	12	80716.	0.4	0.4	0.0467*
143	77.00	17	267568.	1.3	1.3	0.1550
144	75.00	10	7099.	0.0	0.0	0.0041
145	74.00	14	46939.	0.2	0.2	0.0272*
146	73.00	14	82192.	0.4	0.4	0.0476
147	72.00	21	313936.	1.5	1.5	0.1818
148	71.00	29	6310144.	29.5	29.5	3.6544*
149	70.00	25	1524736.	7.1	7.1	0.8830
150	69.00	35	6832896.	32.0	32.0	3.9572
151	68.00	21	1156032.	5.4	5.4	0.6695
152	67.00	21	1151936.	5.4	5.4	0.6671
153	66.00	10	50741.	0.2	0.2	0.0294*
154	65.00	17	77744.	0.4	0.4	0.0450*
155	64.00	14	85144.	0.4	0.4	0.0493
156	63.00	14	60173.	0.3	0.3	0.0348*
157	61.00	14	76104.	0.4	0.4	0.0441*
158	60.00	8	5409.	0.0	0.0	0.0031
159	59.00	12	72944.	0.3	0.3	0.0422
160	58.00	25	660576.	3.1	3.1	0.3826
161	57.00	43	13820416.	64.7	64.7	8.0039*
162	56.00	29	2827392.	13.2	13.2	1.6374
163	55.00	43	12601344.	59.0	59.0	7.2979*
164	54.00	21	937136.	4.4	4.4	0.5427
165	53.00	21	617712.	2.9	2.9	0.3577

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
166	52.00	10	13774.	0.1	0.1	0.0080*
167	51.00	14	118192.	0.6	0.6	0.0684*
168	50.00	12	20677.	0.1	0.1	0.0120*
169	48.00	6	1921.	0.0	0.0	0.0011
170	47.00	14	104220.	0.5	0.5	0.0604
171	46.00	17	118484.	0.6	0.6	0.0686*
172	45.00	35	786992.	3.7	3.7	0.4558*
173	44.00	43	21356544.	100.0	100.0	*12.36*
174	42.00	35	3148480.	14.7	14.7	1.8234
175	41.00	35	12245504.	57.3	57.3	7.0918*
176	40.00	25	358384.	1.7	1.7	0.2076*
177	39.00	29	1589952.	7.4	7.4	0.9208*
178	38.00	14	47548.	0.2	0.2	0.0275*
179	37.00	6	6690.	0.0	0.0	0.0039
180	36.00	21	103252.	0.5	0.5	0.0598*
181	35.00	8	2221.	0.0	0.0	0.0013

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 6/24/98
 S3158.3158 [TIC=2827888, 188X=323528] EI

5,9,13-trimethyltetradecanoic acid,
 2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	372.00	6	779.	0.2	0.2	0.0276	56	196.00	14	1976.	0.6	0.6	0.0599*
2	352.00	17	10450.	3.2	3.2	0.3696	57	195.00	17	1035.	0.3	0.3	0.0366
3	347.00	8	1178.	0.4	0.4	0.0417	58	193.00	25	3455.	1.1	1.1	0.1222
4	342.00	8	650.	0.2	0.2	0.0230	59	189.00	14	4164.	1.3	1.3	0.1473
5	338.00	12	2176.	0.7	0.7	0.0770	60	186.00	6	2659.	0.8	0.8	0.0941
6	337.00	6	1016.	0.3	0.3	0.0359	61	185.00	10	291.	0.1	0.1	0.0103
7	335.00	10	2869.	0.9	0.9	0.1015	62	183.00	21	8204.	2.5	2.5	0.2902
8	334.00	12	606.	0.2	0.2	0.0214	63	192.00	17	4216.	1.3	1.3	0.1491
9	333.00	12	1744.	0.5	0.5	0.0617	64	181.00	21	1026.	0.3	0.3	0.0363
10	332.00	10	2228.	0.7	0.7	0.0788	65	180.00	17	1973.	0.6	0.6	0.0698
11	317.00	8	483.	0.1	0.1	0.0171	66	179.00	29	7300.	2.3	2.3	0.2582
12	315.00	6	1.	0.0	0.0	0.0000	67	178.00	17	3348.	1.0	1.0	0.1184
13	309.00	17	7764.	2.4	2.4	0.2746	68	175.00	21	2567.	0.8	0.8	0.0908
14	308.00	10	1451.	0.4	0.4	0.0513	69	172.00	10	1244.	0.4	0.4	0.0440
15	306.00	6	1617.	0.5	0.5	0.0572	70	171.00	12	3351.	1.0	1.0	0.1185
16	301.00	6	1732.	0.5	0.5	0.0613	71	170.00	14	3278.	1.0	1.0	0.1160*
17	291.00	12	941.	0.3	0.3	0.0333	72	169.00	21	13360.	4.1	4.1	0.4726
18	289.00	10	1529.	0.5	0.5	0.0541	73	168.00	14	3721.	1.2	1.2	0.1316
19	287.00	10	828.	0.3	0.3	0.0293	74	167.00	21	19162.	5.9	5.9	0.6778
20	282.00	10	28.	0.0	0.0	0.0010	75	166.00	12	2989.	0.9	0.9	0.1057
21	281.00	10	3956.	1.2	1.2	0.1399	76	165.00	21	1909.	0.6	0.6	0.0675
22	280.00	8	1151.	0.4	0.4	0.0407	77	164.00	17	4956.	1.5	1.5	0.1753
23	279.00	8	2331.	0.7	0.7	0.0825	78	163.00	21	1515.	0.5	0.5	0.0536
24	275.00	14	1013.	0.3	0.3	0.0358	79	161.00	25	6220.	1.9	1.9	0.2200
25	273.00	8	1232.	0.4	0.4	0.0436	80	159.00	14	1500.	0.5	0.5	0.0531
26	268.00	14	1922.	0.6	0.6	0.0680	81	157.00	6	2054.	0.6	0.6	0.0727
27	267.00	17	6441.	2.0	2.0	0.2278	82	155.00	14	2813.	0.9	0.9	0.0995
28	266.00	12	2882.	0.9	0.9	0.0019	83	152.00	21	21070.	6.5	6.5	0.7453
29	264.00	8	53.	0.0	0.0	0.0019	84	151.00	17	3427.	1.1	1.1	0.1212
30	262.00	14	3593.	1.1	1.1	0.1271	85	148.00	25	4318.	1.3	1.3	0.1527
31	259.00	6	1471.	0.5	0.5	0.0520	86	146.00	25	5322.	1.6	1.6	0.1883
32	253.00	12	1474.	0.5	0.5	0.0521	87	149.00	21	21103.	6.5	6.5	0.7455
33	250.00	10	311.	0.1	0.1	0.0110	88	148.00	14	2081.	0.6	0.6	0.0736
34	249.00	17	842.	0.3	0.3	0.0298	89	145.00	12	4515.	0.2	0.2	0.0229
35	248.00	14	1210.	0.4	0.4	0.0428	90	142.00	25	34357.	10.6	10.6	1.2153
36	245.00	8	1090.	0.6	0.6	0.0669	91	141.00	21	12534.	3.9	3.9	0.4434
37	240.00	6	1497.	0.5	0.5	0.0530	92	139.00	25	7316.	2.3	2.3	0.2588
38	239.00	21	5718.	1.8	1.8	0.2023	93	138.00	21	4596.	1.4	1.4	0.1626
39	238.00	8	3581.	1.1	1.1	0.1267	94	136.00	17	3098.	1.0	1.0	0.1096
40	237.00	17	10269.	3.2	3.2	0.3632	95	135.00	21	4020.	1.2	1.2	0.1422*
41	235.00	17	203.	0.1	0.1	0.0072	96	134.00	14	5977.	1.8	1.8	0.2114
42	234.00	17	2196.	0.7	0.7	0.0777	97	133.00	25	1267.	0.4	0.4	0.0448
43	225.00	14	3522.	1.1	1.1	0.1246	98	132.00	21	8046.	2.5	2.5	0.2846
44	221.00	17	13.	0.0	0.0	0.0005	99	132.00	8	1286.	0.4	0.4	0.0455
45	213.00	14	937.	0.3	0.3	0.0331	100	128.00	17	1584.	0.5	0.5	0.0560
46	216.00	10	2385.	0.7	0.7	0.0844	101	127.00	29	4048.	1.3	1.3	0.1432
47	214.00	6	922.	0.3	0.3	0.0326	102	126.00	17	12089.	3.7	3.7	0.4276
48	211.00	21	941.	0.3	0.3	0.0333	103	125.00	25	3011.	0.9	0.9	0.1065
49	210.00	14	9830.	3.0	3.0	0.3477	104	125.00	25	24236.	7.5	7.5	0.8573
50	209.00	21	56.	0.0	0.0	0.0020	105	124.00	25	8138.	2.5	2.5	0.2879
51	208.00	21	2028.	0.6	0.6	0.0717	106	124.00	25	3417.	1.1	1.1	0.1209
52	205.00	17	1276.	0.4	0.4	0.0451	107	121.00	25	12400.	3.8	3.8	0.4386
53	199.00	12	1782.	0.6	0.6	0.0630	108	119.00	21	9734.	3.0	3.0	0.3443
54	198.00	12	5112.	1.6	1.6	0.1808	109	118.00	11	2767.	0.9	0.9	0.0979
55	197.00	25	24155.	7.5	7.5	0.8544							

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	114.00	8	1091.	0.3	0.3	0.0386	166	40.00	25	6631.	2.0	2.0	0.2346
112	113.00	43	23186.	7.2	7.2	0.8202	167	39.00	29	8135.	2.5	2.5	0.2878*
113	112.00	29	10877.	3.4	3.4	0.3848	168	37.00	8	1935.	0.6	0.6	0.0684*
114	111.00	35	26376.	8.2	8.2	0.9330	169	36.00	12	3088.	1.0	1.0	0.1092
115	110.00	21	13404.	4.1	4.1	0.4741	170	33.00	14	3814.	1.2	1.2	0.1349
116	109.00	29	22952.	7.1	7.1	0.8119	171	32.00	8	1863.	0.6	0.6	0.0659*
117	108.00	21	1197.	0.4	0.4	0.0423	172	31.00	14	1847.	0.6	0.6	0.0653
118	107.00	25	16102.	5.0	5.0	0.5696*	173	30.00	17	427.	0.1	0.1	0.0151
119	106.00	17	1638.	0.5	0.5	0.0579	174	29.00	43	87988.	27.2	27.2	3.1124
120	105.00	25	11022.	3.4	3.4	0.3899	175	27.00	25	22553.	7.0	7.0	0.7978
121	100.00	8	1650.	0.5	0.5	0.0584							
122	99.00	25	18488.	5.7	5.7	0.6540							
123	98.00	25	21094.	6.5	6.5	0.7462							
124	97.00	29	64200.	19.8	19.8	2.2710							
125	96.00	25	11926.	3.7	3.7	0.4219							
126	95.00	25	22272.	6.9	6.9	0.7878*							
127	93.00	29	838.	0.3	0.3	0.0296							
128	92.00	17	6420.	2.0	2.0	0.2271							
129	88.00	8	1476.	0.5	0.5	0.0522							
130	86.00	14	3551.	1.1	1.1	0.1256*							
131	85.00	21	50260.	15.5	15.5	1.7779							
132	84.00	25	8163.	2.5	2.5	0.2888							
133	83.00	35	116816.	36.1	36.1	4.1321							
134	82.00	29	17303.	5.3	5.3	0.6121							
135	81.00	35	35828.	11.1	11.1	1.2673							
136	80.00	25	3622.	1.1	1.1	0.1281							
137	78.00	25	5495.	1.7	1.7	0.1944							
138	77.00	25	5113.	1.6	1.6	0.1809							
139	76.00	10	3180.	1.0	1.0	0.1125							
140	73.00	17	3714.	1.1	1.1	0.1314							
141	72.00	17	9632.	3.0	3.0	0.3407							
142	71.00	35	187456.	57.9	57.9	6.6309							
143	70.00	25	14534.	4.5	4.5	0.5141							
144	69.00	35	161520.	49.9	49.9	5.7135*							
145	68.00	29	25701.	7.9	7.9	0.9091*							
146	67.00	29	3028.	0.9	0.9	0.1071							
147	66.00	25	1300.	0.4	0.4	0.0460							
148	65.00	25	11669.	3.6	3.6	0.4128							
149	64.00	14	5790.	1.8	1.8	0.2048							
150	63.00	21	3883.	1.2	1.2	0.1374							
151	61.00	14	5527.	1.7	1.7	0.1955							
152	58.00	21	10974.	3.4	3.4	0.3882*							
153	57.00	35	323520.	100.0	100.0	*11.44*							
154	56.00	29	101216.	31.3	31.3	3.5803							
155	55.00	35	187760.	58.0	58.0	6.6417*							
156	54.00	25	9756.	3.0	3.0	0.3451							
157	53.00	29	11387.	3.5	3.5	0.4028							
158	52.00	21	4013.	1.2	1.2	0.1420							
159	50.00	21	3321.	1.0	1.0	0.1175							
160	49.00	8	1159.	0.4	0.4	0.0410							
161	45.00	25	4152.	1.3	1.3	0.1469							
162	44.00	35	10095.	3.1	3.1	0.3571							
163	43.00	43	311104.	96.2	96.2	*11.00*							
164	42.00	35	59218.	18.3	18.3	2.0947							
165	41.00	35	206660.	63.9	63.9	7.3102							

AL16.1 [TIC=151838728, 188X=17897472] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	6	4873.	0.0	0.0	0.0032	56	195.00	10	17360.	0.1	0.1	0.0114
2	354.00	14	121056.	0.7	0.7	0.0797*	57	194.00	6	2414.	0.0	0.0	0.0016
3	353.00	25	1026832.	5.7	5.7	0.5763*	58	193.00	8	19070.	0.1	0.1	0.0126
4	352.00	35	4832768.	27.0	27.0	3.1828*	59	191.00	10	16131.	0.1	0.1	0.0106
5	351.00	10	19654.	0.1	0.1	0.0129*	60	185.00	10	19176.	0.1	0.1	0.0126
6	335.00	6	2235.	0.0	0.0	0.0015	61	184.00	17	312928.	1.7	1.7	0.2061
7	334.00	12	100696.	0.6	0.6	0.0663	62	183.00	21	484512.	2.7	2.7	0.3191*
8	333.00	17	372852.	2.1	2.1	0.2495	63	182.00	17	81464.	0.5	0.5	0.0537*
9	324.00	10	53702.	0.3	0.3	0.0354	64	181.00	17	88604.	0.5	0.5	0.0584*
10	323.00	14	293072.	1.6	1.6	0.1930	65	180.00	17	122200.	0.7	0.7	0.0805*
11	323.00	8	12657.	0.1	0.1	0.0083	66	179.00	12	55681.	0.3	0.3	0.0367*
12	310.00	17	239000.	1.3	1.3	0.1573*	67	178.00	6	1402.	0.0	0.0	0.0009
13	309.00	17	1387328.	7.8	7.8	0.9137	68	177.00	10	18413.	0.1	0.1	0.0121
14	297.00	8	6147.	0.0	0.0	0.0040	69	171.00	6	4832.	0.0	0.0	0.0032
15	296.00	12	84280.	0.5	0.5	0.0555	70	170.00	17	140012.	0.8	0.8	0.0922*
16	295.00	17	213768.	1.2	1.2	0.1408	71	169.00	29	1441408.	8.1	8.1	0.9493
17	283.00	10	2658.	0.0	0.0	0.0018	72	168.00	12	36361.	0.2	0.2	0.0239
18	282.00	10	33590.	0.2	0.2	0.0221	73	167.00	14	101036.	0.6	0.6	0.0665
19	281.00	17	190104.	1.1	1.1	0.1252	74	166.00	17	168640.	0.9	0.9	0.1111
20	272.00	8	1028.	0.0	0.0	0.0007	75	165.00	12	48290.	0.3	0.3	0.0318
21	271.00	8	1981.	0.0	0.0	0.0013	76	164.00	6	3080.	0.0	0.0	0.0020
22	269.00	10	5425.	0.0	0.0	0.0036	77	163.00	10	37920.	0.2	0.2	0.0250
23	268.00	14	126432.	0.7	0.7	0.0833	78	161.00	8	2019.	0.0	0.0	0.0013
24	267.00	17	838320.	4.7	4.7	0.5521*	79	157.00	12	56321.	0.3	0.3	0.0371
25	255.00	10	30545.	0.2	0.2	0.0201	80	156.00	25	897136.	5.0	5.0	0.5908*
26	254.00	21	396288.	2.2	2.2	0.2610*	81	155.00	43	8766976.	49.0	49.0	5.7739*
27	253.00	25	2049600.	11.5	11.5	1.3499*	82	154.00	12	75456.	0.4	0.4	0.0497*
28	252.00	10	12602.	0.1	0.1	0.0083	83	153.00	21	209644.	1.2	1.2	0.1381*
29	251.00	6	2005.	0.0	0.0	0.0013	84	152.00	17	160260.	0.9	0.9	0.1055
30	241.00	10	9324.	0.1	0.1	0.0061	85	151.00	10	35924.	0.2	0.2	0.0237
31	240.00	14	129392.	0.7	0.7	0.0852	86	150.00	8	7532.	0.0	0.0	0.0050
32	239.00	14	179184.	1.0	1.0	0.1180	87	149.00	17	129040.	0.7	0.7	0.0850*
33	235.00	8	18274.	0.1	0.1	0.0120	88	147.00	10	19034.	0.1	0.1	0.0125
34	234.00	14	81072.	0.5	0.5	0.0534	89	145.00	10	12109.	0.1	0.1	0.0080
35	226.00	12	67524.	0.4	0.4	0.0445	90	144.00	14	158932.	0.9	0.9	0.1047*
36	225.00	17	282736.	1.6	1.6	0.1862	91	143.00	29	3390720.	18.9	18.9	2.2331*
37	224.00	8	2682.	0.0	0.0	0.0018	92	142.00	43	12088832.	67.5	67.5	7.9616*
38	223.00	6	1835.	0.0	0.0	0.0012	93	141.00	25	666592.	3.7	3.7	0.4390
39	221.00	8	17353.	0.1	0.1	0.0114	94	140.00	17	124920.	0.7	0.7	0.0823*
40	213.00	8	13768.	0.1	0.1	0.0091	95	139.00	21	297584.	1.7	1.7	0.1960
41	212.00	21	378976.	2.1	2.1	0.2496*	96	138.00	14	95092.	0.5	0.5	0.0526
42	211.00	29	2985216.	16.7	16.7	1.9660*	97	137.00	14	78180.	0.4	0.4	0.0515
43	210.00	14	103792.	0.6	0.6	0.0684*	98	136.00	14	99612.	0.6	0.6	0.0656*
44	209.00	17	105612.	0.6	0.6	0.0696*	99	135.00	25	963856.	5.4	5.4	0.6348
45	208.00	21	542576.	3.0	3.0	0.3573*	100	134.00	6	791.	0.0	0.0	0.0005
46	207.00	17	146920.	0.8	0.8	0.0968	101	133.00	8	11471.	0.1	0.1	0.0076
47	205.00	10	1514.	0.0	0.0	0.0010	102	133.00	8	4741.	0.0	0.0	0.0031
48	204.00	6	905.	0.0	0.0	0.0006	103	131.00	8	6024.	0.0	0.0	0.0040
49	203.00	8	2602.	0.0	0.0	0.0006	104	129.00	14	58241.	0.3	0.3	0.0384*
50	202.00	6	936.	0.0	0.0	0.0017	105	128.00	29	1283136.	7.2	7.2	0.8451*
51	200.00	8	2997.	0.0	0.0	0.0006	106	127.00	21	178812.	1.0	1.0	0.1178*
52	199.00	12	50441.	0.3	0.3	0.0332	107	126.00	21	481312.	2.7	2.7	0.3170
53	198.00	21	798864.	4.5	4.5	0.5261	108	125.00	17	186504.	1.0	1.0	0.1228
54	197.00	21	983184.	5.5	5.5	0.6475	109	124.00	21	354032.	2.0	2.0	0.2332
55	196.00	8	7873.	0.0	0.0	0.0052	110	122.00	25	621424.	3.5	3.5	0.4093

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. CASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	121.00	17	160368.	0.9	0.9	0.1056	166	54.00	21	763232.	4.3	4.3	0.5027
112	119.00	10	16481.	0.1	0.1	0.0109	167	53.00	21	490464.	2.7	2.7	0.3230
113	118.00	10	11929.	0.1	0.1	0.0079*	168	52.00	12	19153.	0.1	0.1	0.0126*
114	115.00	8	3890.	0.0	0.0	0.0026	169	51.00	14	77972.	0.4	0.4	0.0514*
115	114.00	10	35145.	0.2	0.2	0.0231*	170	50.00	10	11029.	0.1	0.1	0.0073*
116	113.00	25	725888.	4.1	4.1	0.4781*	171	47.00	12	56792.	0.3	0.3	0.0374*
117	112.00	21	363072.	2.0	2.0	0.2391	172	45.00	17	95352.	0.5	0.5	0.0628*
118	111.00	25	1048768.	5.9	5.9	0.6907	173	44.00	35	707232.	4.0	4.0	0.4658*
119	110.00	21	309024.	1.7	1.7	0.2035	174	43.00	43	17897472.	100.0	100.0	*11.78*
120	109.00	21	333392.	1.9	1.9	0.2196*	175	42.00	35	2592384.	14.5	14.5	1.7073
121	108.00	10	30525.	0.2	0.2	0.0201	176	41.00	35	9839872.	55.0	55.0	6.4805
122	107.00	14	125852.	0.7	0.7	0.0829*	177	40.00	21	256516.	1.4	1.4	0.1689*
123	106.00	6	2138.	0.1	0.1	0.0014	178	39.00	29	1188672.	6.6	6.6	0.7829*
124	105.00	10	14505.	0.4	0.4	0.0096*	179	38.00	10	200406.	0.1	0.1	0.0134
125	100.00	12	76032.	0.4	0.4	0.0501*	180	37.00	10	6869.	0.0	0.0	0.0045*
126	99.00	21	977856.	5.5	5.5	0.6440	181	36.00	17	79020.	0.4	0.4	0.0520*
127	98.00	25	1265024.	7.1	7.1	0.8331							
128	97.00	25	2695488.	15.1	15.1	1.7752*							
129	96.00	25	658288.	3.7	3.7	0.4335*							
130	95.00	21	605024.	3.4	3.4	0.3985							
131	94.00	12	89484.	0.5	0.5	0.0589							
132	93.00	17	154420.	0.9	0.9	0.1017							
133	92.00	12	2872.	0.0	0.0	0.0019							
134	91.00	10	38697.	0.2	0.2	0.0255							
135	87.00	8	4486.	0.0	0.0	0.0030							
136	86.00	17	199176.	1.1	1.1	0.1312*							
137	85.00	25	3221952.	18.0	18.0	2.1220							
138	84.00	25	1627328.	9.1	9.1	1.0717							
139	83.00	35	5023232.	28.1	28.1	3.3083*							
140	82.00	21	752992.	4.2	4.2	0.4959*							
141	81.00	25	850864.	4.8	4.8	0.5604							
142	80.00	17	149800.	0.8	0.8	0.0987*							
143	79.00	17	203332.	1.1	1.1	0.1339*							
144	78.00	12	71444.	0.4	0.4	0.0471							
145	77.00	17	211892.	1.2	1.2	0.1396*							
146	75.00	8	4744.	0.0	0.0	0.0031							
147	74.00	10	45241.	0.3	0.3	0.0298							
148	73.00	14	100296.	0.6	0.6	0.0661							
149	72.00	17	271952.	1.5	1.5	0.1791*							
150	71.00	35	5701888.	31.9	31.9	3.7552*							
151	70.00	25	1322688.	7.4	7.4	0.8711							
152	69.00	35	598864.	33.5	33.5	3.9442							
153	68.00	25	966224.	5.4	5.4	0.6363							
154	67.00	21	999184.	5.6	5.6	0.6581							
155	66.00	12	51639.	0.3	0.3	0.0340*							
156	65.00	12	77204.	0.4	0.4	0.0508*							
157	64.00	14	83164.	0.5	0.5	0.0548*							
158	63.00	12	41076.	0.2	0.2	0.0271							
159	61.00	14	63260.	0.4	0.4	0.0417*							
160	60.00	8	13754.	0.1	0.1	0.0091*							
161	59.00	17	89084.	0.5	0.5	0.0587*							
162	58.00	25	560336.	3.1	3.1	0.3690							
163	57.00	35	12078336.	67.5	67.5	7.9547*							
164	56.00	29	2449984.	13.7	13.7	1.6135*							
165	55.00	35	10640128.	59.5	59.5	7.0075*							

ALP6.1 [TIC=1838#3984, 180X-22625280] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	138.00	14	140568.	0.6	0.6	0.0765	166	70.00	25	1702912.	7.5	7.5	0.9265
112	137.00	14	95524.	0.4	0.4	0.0520	167	69.00	35	7513344.	33.2	33.2	4.0877*
113	136.00	17	140464.	0.6	0.6	0.0764*	168	68.00	25	1229184.	5.4	5.4	0.6687
114	135.00	25	1055424.	4.7	4.7	0.5742	169	67.00	25	1290944.	5.7	5.7	0.7023
115	133.00	10	20627.	0.1	0.1	0.0112	170	66.00	12	72332.	0.3	0.3	0.0394*
116	131.00	8	6139.	0.0	0.0	0.0033	171	65.00	17	88304.	0.4	0.4	0.0480*
117	129.00	8	6180.	0.0	0.0	0.0034	172	64.00	14	85836.	0.4	0.4	0.0467
118	128.00	12	66776.	0.3	0.3	0.0363*	173	63.00	14	32552.	0.1	0.1	0.0177*
119	127.00	27	1466496.	6.5	6.5	0.7979	174	61.00	14	83768.	0.4	0.4	0.0456*
120	126.00	19	192228.	0.8	0.8	0.1046	175	60.00	10	16771.	0.1	0.1	0.0091
121	125.00	21	627440.	2.8	2.8	0.3414	176	59.00	14	93172.	0.4	0.4	0.0507*
122	124.00	17	218464.	1.0	1.0	0.1189*	177	58.00	25	791648.	3.5	3.5	0.4307*
123	123.00	25	425280.	1.9	1.9	0.2314*	178	57.00	43	15505408.	68.5	68.5	8.4358*
124	122.00	25	709824.	3.1	3.1	0.3862	179	56.00	29	3061888.	13.5	13.5	1.6658*
125	121.00	17	198864.	0.9	0.9	0.1082*	180	55.00	35	12967168.	57.3	57.3	7.0549*
126	120.00	6	3648.	0.0	0.0	0.0020	181	54.00	25	933568.	4.1	4.1	0.5079
127	119.00	12	24673.	0.1	0.1	0.0134*	182	53.00	21	582736.	2.6	2.6	0.3170
128	118.00	10	14137.	0.1	0.1	0.0077*	183	52.00	10	16145.	0.1	0.1	0.0088*
129	115.00	6	1162.	0.0	0.0	0.0006	184	51.00	17	73864.	0.3	0.3	0.0402*
130	114.00	12	56513.	0.2	0.2	0.0307*	185	50.00	8	22969.	0.1	0.1	0.0125*
131	113.00	29	869264.	3.8	3.8	0.4729	186	49.00	8	4535.	0.0	0.0	0.0025
132	112.00	21	398272.	1.8	1.8	0.2167	187	47.00	12	79452.	0.4	0.4	0.0432*
133	111.00	21	1337728.	5.9	5.9	0.7278	188	45.00	17	116612.	0.5	0.5	0.0634*
134	110.00	17	376464.	1.7	1.7	0.2048	189	44.00	35	870864.	3.8	3.8	0.4738*
135	109.00	21	398944.	1.8	1.8	0.2170	190	43.00	43	22625280.	100.0	100.0	*12.30*
136	108.00	14	55552.	0.2	0.2	0.0302*	191	42.00	35	3145024.	13.9	13.9	1.7111
137	107.00	17	160980.	0.7	0.7	0.0876*	192	41.00	35	11976448.	52.0	52.0	6.5159*
138	106.00	10	3908.	0.0	0.0	0.0021*	193	40.00	21	313472.	1.4	1.4	0.1705*
139	105.00	12	15672.	0.1	0.1	0.0085*	194	39.00	29	1372992.	6.1	6.1	0.7470*
140	100.00	12	95124.	0.4	0.4	0.0518	195	38.00	10	31088.	0.1	0.1	0.0169*
141	99.00	25	1200960.	5.3	5.3	0.6534	196	37.00	12	8525.	0.0	0.0	0.0046*
142	98.00	25	1581632.	7.0	7.0	0.8605	197	36.00	14	65094.	0.3	0.3	0.0354*
143	97.00	29	3329792.	14.7	14.7	0.8116*	198	35.00	6	1143.	0.0	0.0	0.0006
144	96.00	25	876016.	3.9	3.9	0.4766							
145	95.00	21	706272.	3.1	3.1	0.3843							
146	94.00	14	111516.	0.5	0.5	0.0607*							
147	93.00	17	169492.	0.7	0.7	0.0922							
148	92.00	12	3002.	0.0	0.0	0.0016							
149	91.00	14	58671.	0.3	0.3	0.0319*							
150	87.00	6	3325.	0.0	0.0	0.0018							
151	86.00	17	265136.	1.2	1.2	0.1442*							
152	85.00	29	4160448.	18.4	18.4	2.2635*							
153	84.00	25	1988480.	8.8	8.8	1.0818							
154	83.00	35	6162944.	27.2	27.2	3.3530*							
155	82.00	21	935472.	4.1	4.1	0.5090							
156	81.00	25	1023360.	4.5	4.5	0.5568							
157	80.00	21	218624.	1.0	1.0	0.1189*							
158	79.00	21	271920.	1.2	1.2	0.1479							
159	78.00	14	90784.	0.4	0.4	0.0494*							
160	77.00	17	258532.	1.1	1.1	0.1407							
161	75.00	8	7878.	0.0	0.0	0.0043							
162	74.00	12	38535.	0.2	0.2	0.0210							
163	73.00	17	141316.	0.6	0.6	0.0769*							
164	72.00	21	378672.	1.7	1.7	0.2060							
165	71.00	35	7532544.	33.3	33.3	4.0381							

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 6/24/98
 S3424-3424 [TIC-1918728, 188X-194628] EI

2,6,10,14-tetramethylpentadecanoic acid,
 2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	381.00	8	1011.	0.5	0.5	0.0527	56	223.00	21	7066.	3.6	3.6	0.3683
2	382.00	10	6848.	3.5	3.5	0.3569	57	222.00	25	46808.	24.1	24.1	2.4395
3	374.00	8	1827.	0.9	0.9	0.0952	58	220.00	21	5367.	2.8	2.8	0.2797
4	365.00	10	2270.	1.2	1.2	0.1183	59	219.00	17	310.	0.2	0.2	0.0162
5	362.00	10	474.	0.2	0.2	0.0247	60	218.00	17	1986.	1.0	1.0	0.1035
6	361.00	17	212.	0.1	0.1	0.0110	61	217.00	12	256.	0.1	0.1	0.0133
7	360.00	6	3954.	2.0	2.0	0.2051	62	216.00	10	1028.	0.5	0.5	0.0536
8	356.00	8	3195.	1.6	1.6	0.1665*	63	213.00	8	1666.	0.9	0.9	0.0868
9	349.00	6	1474.	0.8	0.8	0.0768	64	211.00	17	986.	0.5	0.5	0.0514
10	346.00	12	1910.	1.0	1.0	0.0995	65	210.00	10	2463.	1.3	1.3	0.1284
11	344.00	14	2658.	1.4	1.4	0.1385	66	209.00	21	4514.	2.3	2.3	0.2353
12	343.00	10	1883.	1.0	1.0	0.0981	67	206.00	17	3193.	1.6	1.6	0.1664
13	340.00	6	874.	0.4	0.4	0.0456	68	205.00	25	5082.	2.6	2.6	0.2649
14	337.00	10	1331.	0.7	0.7	0.0694	69	204.00	21	3145.	1.6	1.6	0.1639
15	334.00	8	743.	0.4	0.4	0.0387	70	202.00	10	167.	0.1	0.1	0.0087
16	331.00	12	36.	0.0	0.0	0.0019	71	200.00	8	1828.	0.9	0.9	0.0953
17	330.00	10	871.	0.4	0.4	0.0454	72	199.00	8	1539.	0.8	0.8	0.0802
18	329.00	10	2216.	1.1	1.1	0.1155	73	198.00	21	7005.	3.6	3.6	0.3651
19	322.00	8	1406.	0.7	0.7	0.0733	74	197.00	21	11633.	6.0	6.0	0.6063
20	319.00	14	3319.	1.7	1.7	0.1730	75	196.00	17	1158.	0.6	0.6	0.0604
21	318.00	10	835.	0.4	0.4	0.0435	76	195.00	21	12595.	6.5	6.5	0.6564
22	315.00	8	1401.	0.7	0.7	0.0730	77	192.00	14	1075.	0.6	0.6	0.0560
23	309.00	8	1625.	0.8	0.8	0.0847	78	187.00	14	1271.	0.7	0.7	0.0662
24	306.00	8	1996.	1.0	1.0	0.1040	79	184.00	8	1086.	0.6	0.6	0.0566
25	303.00	12	292.	0.2	0.2	0.0152	80	183.00	17	1590.	0.8	0.8	0.0829
26	301.00	6	1406.	0.7	0.7	0.0733	81	180.00	12	697.	0.4	0.4	0.0363
27	298.00	6	1027.	0.5	0.5	0.0535	82	179.00	17	8182.	4.2	4.2	0.4264
28	295.00	17	958.	0.5	0.5	0.0499	83	178.00	17	2213.	1.1	1.1	0.1153
29	291.00	17	912.	0.5	0.5	0.0475	84	177.00	21	7952.	4.1	4.1	0.4144
30	289.00	10	35.	0.0	0.0	0.0018	85	176.00	12	4019.	2.1	2.1	0.2095
31	288.00	6	1493.	0.8	0.8	0.0778	86	175.00	17	1556.	0.8	0.8	0.0811
32	281.00	12	3020.	1.6	1.6	0.1574	87	171.00	12	1494.	0.8	0.8	0.0779
33	276.00	14	4030.	2.1	2.1	0.2100	88	170.00	17	5536.	2.8	2.8	0.2885
34	275.00	14	2614.	1.3	1.3	0.1362	89	169.00	29	28008.	14.4	14.4	1.4597*
35	274.00	10	2726.	1.4	1.4	0.1421	90	168.00	14	2459.	1.3	1.3	0.1282
36	267.00	17	2908.	1.5	1.5	0.1516	91	167.00	21	6189.	3.2	3.2	0.3226
37	266.00	8	851.	0.4	0.4	0.0444	92	165.00	21	2143.	1.1	1.1	0.1117
38	265.00	14	27.	0.0	0.0	0.0014	93	164.00	17	2478.	1.3	1.3	0.1291
39	264.00	10	2704.	1.4	1.4	0.1409*	94	163.00	21	3960.	2.0	2.0	0.2064
40	260.00	8	1199.	0.6	0.6	0.0625	95	160.00	12	3175.	1.6	1.6	0.1655
41	259.00	8	3456.	1.8	1.8	0.1801*	96	158.00	17	1254.	0.6	0.6	0.0654
42	257.00	8	1830.	0.9	0.9	0.0954	97	157.00	21	10217.	5.2	5.2	0.5325*
43	251.00	8	133.	0.1	0.1	0.0069	98	156.00	29	189976.	97.6	97.6	9.9012
44	250.00	17	2307.	1.2	1.2	0.1202	99	155.00	29	3335.	1.7	1.7	0.1738
45	249.00	14	2101.	1.1	1.1	0.1095*	100	153.00	25	3391.	1.7	1.7	0.1767
46	247.00	14	5031.	2.6	2.6	0.2622*	101	152.00	21	3715.	1.9	1.9	0.1936
47	246.00	10	4570.	2.3	2.3	0.2382*	102	151.00	25	1945.	1.0	1.0	0.1014
48	239.00	10	127.	0.1	0.1	0.0066	103	150.00	14	1176.	0.6	0.6	0.0613
49	238.00	10	1826.	0.9	0.9	0.0952	104	149.00	29	4307.	2.3	2.3	0.2286
50	235.00	21	4325.	2.2	2.2	0.2254	105	148.00	12	1623.	0.8	0.8	0.0846
51	235.00	21	1763.	0.9	0.9	0.0919	106	147.00	21	2766.	1.4	1.4	0.1442
52	233.00	21	4580.	2.4	2.4	0.2387	107	146.00	10	676.	0.3	0.3	0.0352
53	231.00	14	1803.	1.0	1.0	0.0981	108	145.00	21	4989.	2.6	2.6	0.2600
54	225.00	21	15410.	7.9	7.9	0.8031	109	143.00	17	276.	0.1	0.1	0.0144
55	224.00	14	2024.	1.0	1.0	0.1055	110	141.00	21	16021.	8.2	8.2	0.8350*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	139.00	25	20720.	10.6	10.6	1.0799	166	41.00	35	115488.	59.3	59.3	6.0190
112	138.00	21	8397.	4.3	4.3	0.4376	167	40.00	21	857.	0.4	0.4	0.0447
113	137.00	21	14938.	7.7	7.7	0.7785	168	39.00	35	12852.	6.6	6.6	0.6698
114	136.00	25	3556.	1.8	1.8	0.1853	169	38.00	17	530.	0.3	0.3	0.0276
115	130.00	17	2799.	1.4	1.4	0.1459	170	36.00	6	631.	0.3	0.3	0.0329
116	129.00	21	245.	0.1	0.1	0.0128	171	32.00	8	1640.	0.8	0.8	0.0855
117	127.00	25	24658.	12.7	12.7	1.2851	172	30.00	14	1540.	0.8	0.8	0.0803*
118	126.00	21	6883.	3.5	3.5	0.3587	173	29.00	43	25288.	13.0	13.0	1.3180
119	125.00	29	19754.	10.2	10.2	1.0295	174	28.00	35	4357.	2.2	2.2	0.2271
120	124.00	25	6928.	3.6	3.6	0.3611*	175	27.00	25	6576.	3.4	3.4	0.3427
121	123.00	29	7132.	3.7	3.7	0.3717							
122	120.00	21	3431.	1.8	1.8	0.1788							
123	119.00	21	3385.	1.7	1.7	0.1764							
124	117.00	21	3931.	2.0	2.0	0.2049							
125	116.00	14	773.	0.4	0.4	0.0403							
126	115.00	17	2468.	1.3	1.3	0.1286							
127	113.00	25	17433.	9.0	9.0	0.9086							
128	111.00	25	21519.	11.1	11.1	1.1215							
129	110.00	21	8536.	4.4	4.4	0.4449							
130	108.00	21	3205.	1.6	1.6	0.1670							
131	106.00	21	1594.	0.8	0.8	0.0831							
132	105.00	17	7992.	4.1	4.1	0.4165							
133	104.00	8	3146.	1.6	1.6	0.1640							
134	103.00	21	589.	0.3	0.3	0.0307							
135	102.00	14	4488.	2.3	2.3	0.2339							
136	99.00	21	6620.	3.4	3.4	0.3450							
137	97.00	35	89516.	46.0	46.0	4.6654							
138	91.00	25	3635.	1.9	1.9	0.1894							
139	89.00	10	5230.	2.7	2.7	0.2726*							
140	86.00	10	3145.	1.6	1.6	0.1639							
141	85.00	25	54214.	27.9	27.9	2.8255							
142	83.00	35	20372.	10.5	10.5	1.0617							
143	81.00	35	4604.	2.4	2.4	0.2400							
144	80.00	25	4524.	2.3	2.3	0.2358							
145	79.00	29	5420.	2.8	2.8	0.2825							
146	77.00	21	584.	0.3	0.3	0.0304							
147	75.00	12	2292.	1.2	1.2	0.1195							
148	72.00	25	12110.	6.2	6.2	0.6311*							
149	71.00	29	133172.	68.4	68.4	6.9407							
150	70.00	29	18618.	9.6	9.6	0.9703							
151	69.00	35	79560.	40.9	40.9	4.1465							
152	65.00	25	945.	0.5	0.5	0.0493*							
153	64.00	25	4620.	2.4	2.4	0.2400							
154	63.00	8	715.	0.4	0.4	0.0373*							
155	59.00	17	2387.	1.2	1.2	0.1244							
156	58.00	21	12023.	6.2	6.2	0.6266							
157	57.00	35	194620.	100.0	100.0	10.14							
158	56.00	29	45927.	23.6	23.6	2.3936							
159	55.00	35	70600.	36.3	36.3	3.6800							
160	53.00	25	311.	0.2	0.2	0.0162							
161	52.00	12	1034.	0.5	0.5	0.0539							
162	45.00	25	6704.	3.4	3.4	0.3494							
163	44.00	35	4575.	2.4	2.4	0.2384							
164	43.00	35	176372.	90.6	90.6	9.1922							
165	42.00	35	13465.	6.9	6.9	0.7020							

PAL6.1 [TIC-173381768, 188X-28953888] EI

Nonadecanoic acid,
2,2,2-Trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_{17}\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	430.00	8	1545.	0.0	0.0	0.0009	56	227.00	8	5478.	0.7	0.0	0.0032
2	429.00	8	4428.	0.0	0.0	0.0026	57	226.00	14	138876.	0.7	0.7	0.0001
3	383.00	10	21425.	0.1	0.1	0.0124	58	225.00	17	409408.	2.0	2.0	0.2362
4	382.00	17	165732.	0.8	0.8	0.0956*	59	223.00	10	10431.	0.0	0.0	0.0060
5	381.00	25	1386560.	6.6	6.6	0.8001*	60	222.00	8	4034.	0.0	0.0	0.0023
6	380.00	35	5816832.	27.8	27.8	3.3565*	61	221.00	8	19546.	0.1	0.1	0.0113
7	379.00	12	13241.	0.1	0.1	0.0076*	62	219.00	6	5227.	0.0	0.0	0.0030
8	378.00	14	2354.	0.0	0.0	0.0014	63	219.00	10	33518.	0.2	0.2	0.0193
9	363.00	12	19970.	0.1	0.1	0.0115	64	212.00	17	425248.	2.0	2.0	0.2454
10	362.00	12	106760.	0.8	0.8	0.0616	65	211.00	25	2856256.	13.6	13.6	1.6481*
11	361.00	17	378480.	1.8	1.8	0.2184*	66	210.00	14	58673.	0.3	0.3	0.0339*
12	356.00	6	1529.	0.0	0.0	0.0009	67	209.00	17	91424.	0.4	0.4	0.0528*
13	355.00	8	29321.	0.1	0.1	0.0169	68	208.00	17	133800.	0.6	0.6	0.0772*
14	352.00	8	48101.	0.2	0.2	0.0278	69	207.00	17	411024.	2.0	2.0	0.2372
15	351.00	12	205948.	1.0	1.0	0.1188	70	200.00	8	2666.	0.0	0.0	0.0015
16	342.00	6	1338.	0.0	0.0	0.0008	71	199.00	10	70684.	0.3	0.3	0.0408
17	341.00	6	6042.	0.0	0.0	0.0035	72	198.00	21	907376.	4.3	4.3	0.5236
18	340.00	6	2796.	0.0	0.0	0.0016	73	197.00	25	920720.	4.4	4.4	0.5313
19	339.00	10	18846.	0.1	0.1	0.109	74	196.00	8	30741.	0.1	0.1	0.0177
20	338.00	17	233072.	1.1	1.1	0.1345*	75	195.00	12	58352.	0.3	0.3	0.0337*
21	337.00	17	1233024.	5.9	5.9	0.7115	76	194.00	14	129228.	0.6	0.6	0.0746*
22	326.00	6	1336.	0.0	0.0	0.0008	77	193.00	12	46844.	0.2	0.2	0.0270*
23	325.00	12	11471.	0.1	0.1	0.0065	78	191.00	14	66752.	0.3	0.3	0.0385*
24	324.00	10	83640.	0.4	0.4	0.0483	79	188.00	8	2038.	0.0	0.0	0.0012
25	323.00	17	261880.	1.2	1.2	0.0242	80	187.00	6	1076.	0.1	0.1	0.0105
26	310.00	10	41853.	0.2	0.2	0.0965	81	185.00	8	18252.	0.1	1.4	0.1684
27	309.00	12	167156.	0.8	0.8	0.0565	82	184.00	17	291920.	1.4	3.3	0.3944
28	297.00	6	2483.	0.3	0.3	0.0396	83	183.00	25	683424.	3.3	3.3	0.0289*
29	296.00	12	68620.	0.3	0.3	0.0396	84	182.00	14	50052.	0.2	0.2	0.0467*
30	295.00	17	352048.	1.7	1.7	0.2031	85	181.00	17	80944.	0.4	0.4	0.0914*
31	283.00	12	42936.	0.2	0.2	0.0248	86	180.00	17	158420.	0.8	0.8	0.0232
32	282.00	21	372304.	1.8	1.8	0.2148*	87	179.00	10	40292.	0.2	0.2	0.0023
33	281.00	25	1666304.	8.0	8.0	0.9615	88	178.00	6	4008.	0.0	0.0	0.0256*
34	280.00	10	34088.	0.2	0.2	0.0197	89	177.00	12	44361.	0.2	0.2	0.0019
35	269.00	17	13170.	0.1	0.1	0.0076	90	171.00	8	3372.	0.0	0.0	0.1113
36	268.00	14	160680.	0.8	0.8	0.0927	91	170.00	17	192840.	0.9	0.9	0.9569
37	267.00	17	654432.	3.1	3.1	0.3776	92	169.00	29	1658304.	7.9	7.9	0.0408*
38	265.00	6	971.	0.0	0.0	0.0006	93	168.00	14	70660.	0.3	0.3	0.0754*
39	264.00	8	7989.	0.0	0.0	0.0046	94	167.00	17	130688.	0.6	0.6	0.0567*
40	263.00	14	33074.	0.2	0.2	0.0191*	95	166.00	14	98196.	0.5	0.5	0.0172*
41	262.00	12	65506.	0.3	0.3	0.0378	96	165.00	12	29830.	0.1	0.1	0.0089
42	255.00	10	12143.	0.1	0.1	0.0070	97	164.00	10	15432.	0.1	0.1	0.0311
43	254.00	14	168316.	0.8	0.8	0.0971	98	163.00	12	53976.	0.3	0.3	0.0009
44	253.00	17	460848.	2.2	2.2	0.2659	99	161.00	6	1502.	0.0	0.0	0.0003
45	252.00	8	4576.	0.0	0.0	0.0026*	100	160.00	6	505.	0.0	0.0	0.0000
46	251.00	8	3760.	0.0	0.0	0.0022	101	157.00	12	59509.	0.3	0.3	0.0343
47	249.00	6	901.	0.0	0.0	0.0005	102	156.00	25	1006048.	4.8	4.8	0.5805*
48	246.00	6	937.	0.0	0.0	0.0005	103	155.00	35	8752640.	41.8	41.8	5.0505*
49	241.00	8	4711.	0.0	0.0	0.0027	104	154.00	14	87644.	0.4	0.4	0.0506
50	240.00	17	171304.	0.8	0.8	0.0988	105	153.00	21	257332.	1.2	1.2	0.1485*
51	239.00	21	403904.	1.9	1.9	0.2331*	106	152.00	17	121204.	0.6	0.6	0.0699*
52	238.00	14	82796.	0.4	0.4	0.0478	107	151.00	10	37489.	0.2	0.2	0.0216
53	237.00	14	153924.	0.7	0.7	0.0888*	108	150.00	8	14846.	0.1	0.1	0.0086
54	236.00	17	403936.	1.9	1.9	0.2331*	109	149.00	17	141324.	0.7	0.7	0.0815*
55	235.00	8	2101.	0.0	0.0	0.0012	110	148.00	10	2793.	0.0	0.0	0.0016

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
166	83.00	35	5731840.	27.4	27.4	3.3074*
167	82.00	21	953088.	4.5	4.5	0.5500
168	81.00	25	967232.	4.6	4.6	0.5581
169	80.00	21	212572.	1.0	1.0	0.1227*
170	79.00	17	249036.	1.2	1.2	0.1437*
171	78.00	12	61375.	0.3	0.3	0.0354
172	77.00	17	222876.	1.1	1.1	0.1286*
173	75.00	8	13690.	0.1	0.1	0.0079
174	74.00	12	58030.	0.3	0.3	0.0335*
175	73.00	17	157708.	0.8	0.8	0.0910
176	72.00	21	344512.	1.6	1.6	0.1988
177	71.00	35	7097088.	33.9	33.9	4.0952*
178	69.00	25	1646848.	7.9	7.9	0.9503*
179	68.00	35	6964224.	33.2	33.2	4.0186
180	67.00	21	1198528.	5.7	5.7	0.6916
181	66.00	10	1151232.	5.5	5.5	0.6643
182	65.00	14	44063.	0.2	0.2	0.0254*
183	64.00	12	69864.	0.3	0.3	0.0403*
184	63.00	10	58136.	0.3	0.3	0.0335*
185	62.00	8	35355.	0.2	0.2	0.0204
186	61.00	10	3404.	0.0	0.0	0.0020
187	59.00	12	55310.	0.3	0.3	0.0319
188	58.00	14	13253.	0.1	0.1	0.0076*
189	57.00	25	732528.	3.5	3.5	0.0434*
190	56.00	43	15166464.	72.4	72.4	8.7515*
191	55.00	29	2992960.	14.3	14.3	1.7270*
192	54.00	35	11933440.	57.0	57.0	6.8859*
193	53.00	21	852480.	4.1	4.1	0.4919
194	52.00	21	502848.	2.4	2.4	0.2902
195	51.00	12	28730.	0.1	0.1	0.0160*
196	50.00	14	72176.	0.3	0.3	0.0416*
197	49.00	10	15950.	0.1	0.1	0.0092*
198	48.00	14	44806.	0.2	0.2	0.0259*
199	47.00	14	90492.	0.4	0.4	0.0522
200	45.00	35	810112.	3.9	3.9	0.4675
201	44.00	43	20953088.	100.0	100.0	*12.09*
202	43.00	35	2751936.	13.1	13.1	1.5879
203	42.00	35	10453248.	49.9	49.9	6.0318
204	41.00	21	255724.	1.2	1.2	0.1476*
205	39.00	25	1152512.	5.5	5.5	0.6650
206	38.00	8	26032.	0.1	0.1	0.0150*
207	37.00	8	3403.	0.0	0.0	0.0020
208	36.00	14	56893.	0.3	0.3	0.0328*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	147.00	12	23143.	0.1	0.1	0.0134
112	145.00	10	3593.	0.0	0.0	0.0021
113	144.00	17	182536.	0.9	0.9	0.1053
114	143.00	25	4023808.	19.2	19.2	2.3219*
115	142.00	43	12106240.	57.8	57.8	6.9856*
116	141.00	25	685248.	3.3	3.3	0.3954*
117	140.00	17	154856.	0.7	0.7	0.0894*
118	139.00	21	381600.	1.8	1.8	0.2202
119	138.00	14	127360.	0.6	0.6	0.0735*
120	137.00	14	97404.	0.5	0.5	0.0562*
121	136.00	14	94124.	0.4	0.4	0.0543*
122	135.00	25	924320.	4.4	4.4	0.5334*
123	134.00	8	5392.	0.0	0.0	0.0031
124	133.00	12	51978.	0.2	0.2	0.0300
125	131.00	8	16191.	0.1	0.1	0.0093
126	129.00	10	3362.	0.0	0.0	0.0019
127	128.00	14	64561.	0.3	0.3	0.0373*
128	127.00	29	1270144.	6.1	6.1	0.7329
129	126.00	21	176232.	0.8	0.8	0.1017*
130	125.00	21	686608.	3.3	3.3	0.3962
131	124.00	17	224644.	1.1	1.1	0.1296
132	123.00	25	377552.	1.8	1.8	0.2179
133	122.00	25	625712.	3.0	3.0	0.3611
134	121.00	17	181648.	0.9	0.9	0.1048*
135	120.00	14	5136.	0.0	0.0	0.0030
136	119.00	25	33927.	0.2	0.2	0.0196*
137	118.00	25	30970.	0.1	0.1	0.0179*
138	117.00	8	5749.	0.0	0.0	0.0033
139	115.00	8	8983.	0.0	0.0	0.0052
140	114.00	12	42232.	0.2	0.2	0.0244*
141	113.00	25	823552.	3.9	3.9	0.4752
142	112.00	21	421744.	2.0	2.0	0.2434
143	111.00	25	1340544.	6.4	6.4	0.7735
144	110.00	21	355952.	1.7	1.7	0.2054*
145	109.00	21	416688.	2.0	2.0	0.2404
146	108.00	12	58975.	0.3	0.3	0.0340*
147	107.00	17	139580.	0.7	0.7	0.0805*
148	106.00	12	3524.	0.0	0.0	0.0020*
149	105.00	8	17197.	0.1	0.1	0.0099*
150	104.00	6	1769.	0.0	0.0	0.0010
151	103.00	8	1003.	0.0	0.0	0.0006
152	101.00	8	4048.	0.0	0.0	0.0023
153	100.00	17	94288.	0.4	0.4	0.0544*
154	99.00	25	1135936.	5.4	5.4	0.6555
155	98.00	25	1493520.	7.1	7.1	0.8560
156	97.00	25	3276544.	15.6	15.6	1.8907*
157	96.00	25	832736.	4.0	4.0	0.4805
158	95.00	21	731968.	3.5	3.5	0.4224
159	94.00	14	116544.	0.6	0.6	0.0672*
160	93.00	17	170884.	0.8	0.8	0.0986*
161	91.00	10	49711.	0.2	0.2	0.0287
162	87.00	8	3636.	0.0	0.0	0.0021
163	86.00	17	252232.	1.2	1.2	0.1455
164	85.00	29	4131008.	19.7	19.7	2.3837
165	84.00	25	1981760.	9.5	9.5	1.1435*

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 5/24/98
 S3643.3643 [TIC-9854976, 188X-1287424] EI

3,7,11,15-tetramethylhexadecanoic acid,
 2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	395.00	14	7750.	0.6	0.6	0.0786	56	284.00	14	3179.	0.3	0.3	0.0323
2	394.00	14	24671.	2.0	2.0	0.2503	57	283.00	14	4168.	0.3	0.3	0.0423
3	393.00	6	1026.	0.1	0.1	0.0104	58	282.00	8	3425.	0.3	0.3	0.0348
4	390.00	6	829.	0.1	0.1	0.0084	59	281.00	17	6015.	0.5	0.5	0.0610
5	386.00	8	1516.	0.1	0.1	0.0154	60	280.00	17	4000.	0.3	0.3	0.0406
6	384.00	10	2722.	0.2	0.2	0.0276	61	279.00	12	2591.	0.2	0.2	0.0263
7	380.00	8	2135.	0.2	0.2	0.0217	62	277.00	17	9794.	0.8	0.8	0.0994
8	379.00	12	5095.	0.4	0.4	0.0517	63	276.00	21	28059.	2.3	2.3	0.0166
9	378.00	12	2861.	0.2	0.2	0.0290	64	275.00	12	1632.	0.1	0.1	0.0166
10	377.00	17	9572.	0.8	0.8	0.0971	65	268.00	10	3372.	0.3	0.3	0.0342
11	376.00	21	24531.	2.0	2.0	0.2489	66	267.00	14	4937.	0.4	0.4	0.0501
12	375.00	17	10789.	0.9	0.9	0.1087	67	266.00	12	3417.	0.3	0.3	0.0347
13	374.00	14	2512.	0.2	0.2	0.0255	68	265.00	17	7122.	0.6	0.6	0.0723
14	372.00	10	338.	0.0	0.0	0.0034	69	264.00	21	4834.	0.4	0.4	0.0491
15	371.00	6	1051.	0.1	0.1	0.0107	70	263.00	17	4223.	0.3	0.3	0.0429
16	370.00	8	1638.	0.1	0.1	0.0166	71	261.00	17	4188.	0.3	0.3	0.0425
17	369.00	8	1015.	0.1	0.1	0.0103	72	259.00	10	1027.	0.1	0.1	0.0104*
18	367.00	12	1556.	0.1	0.1	0.0158	73	258.00	10	1500.	0.1	0.1	0.0152
19	366.00	12	5825.	0.5	0.5	0.0591	74	254.00	12	6576.	0.5	0.5	0.0667*
20	365.00	12	4879.	0.4	0.4	0.0495	75	253.00	17	12623.	1.0	1.0	0.1281
21	364.00	10	1287.	0.1	0.1	0.0131	76	252.00	17	8508.	0.7	0.7	0.0863
22	362.00	10	1584.	0.1	0.1	0.0161	77	251.00	17	8474.	0.7	0.7	0.0860
23	358.00	8	508.	0.0	0.0	0.0052	78	250.00	21	47968.	4.0	4.0	0.4867*
24	357.00	8	802.	0.1	0.1	0.0081	79	249.00	17	3262.	0.3	0.3	0.0331
25	356.00	10	2638.	0.2	0.2	0.0268	80	247.00	17	3267.	0.3	0.3	0.0332
26	355.00	8	89.	0.0	0.0	0.0009	81	246.00	10	700.	0.1	0.1	0.0071
27	351.00	12	5363.	0.4	0.4	0.0544	82	245.00	17	473.	0.0	0.0	0.0048
28	345.00	12	500.	0.0	0.0	0.0051	83	244.00	10	2930.	0.2	0.2	0.0297
29	344.00	6	144.	0.0	0.0	0.0015	84	243.00	6	772.	0.1	0.1	0.0078
30	343.00	10	675.	0.1	0.1	0.0068	85	241.00	12	2210.	0.2	0.2	0.0224
31	342.00	8	200.	0.0	0.0	0.0020	86	240.00	12	8658.	0.7	0.7	0.0879*
32	338.00	10	3204.	0.3	0.3	0.0325	87	239.00	25	67552.	5.6	5.6	0.6855
33	337.00	12	4419.	0.4	0.4	0.0448	88	238.00	10	297.	0.0	0.0	0.0030
34	333.00	10	3169.	0.3	0.3	0.0322	89	237.00	14	5442.	0.5	0.5	0.0552
35	332.00	6	968.	0.1	0.1	0.0098	90	236.00	17	876.	0.1	0.1	0.0089
36	329.00	10	1461.	0.1	0.1	0.0148	91	235.00	17	4657.	0.4	0.4	0.0473
37	328.00	8	1053.	0.1	0.1	0.0107	92	234.00	21	6186.	0.5	0.5	0.0628
38	323.00	14	3157.	0.3	0.3	0.0320	93	231.00	8	313.	0.0	0.0	0.0032*
39	318.00	10	1373.	0.1	0.1	0.0139	94	230.00	10	1622.	0.1	0.1	0.0165
40	315.00	8	1498.	0.1	0.1	0.0152	95	228.00	8	599.	0.0	0.0	0.0061
41	311.00	10	3346.	0.3	0.3	0.0340	96	227.00	12	962.	0.1	0.1	0.0098
42	310.00	14	7451.	0.6	0.6	0.0756	97	225.00	17	6975.	0.6	0.6	0.0708
43	309.00	29	24837.	2.1	2.1	0.2520	98	222.00	17	6114.	0.5	0.5	0.0620
44	308.00	6	1132.	0.1	0.1	0.0115	99	222.00	21	6660.	0.6	0.6	0.0676
45	305.00	14	778.	0.1	0.1	0.0079	100	221.00	17	4326.	0.4	0.4	0.0439
46	303.00	14	2277.	0.2	0.2	0.0231	101	219.00	17	2529.	0.2	0.2	0.0257
47	302.00	6	1473.	0.1	0.1	0.0149	102	217.00	14	2743.	0.2	0.2	0.0278
48	301.00	10	3835.	0.3	0.3	0.0389	103	214.00	8	1341.	0.1	0.1	0.0136
49	296.00	17	5203.	0.4	0.4	0.0528	104	213.00	12	2852.	0.2	0.2	0.0289*
50	295.00	17	14653.	1.2	1.2	0.1487	105	212.00	17	13444.	1.1	1.1	0.1364
51	294.00	14	8725.	0.7	0.7	0.0885	106	211.00	17	26439.	2.2	2.2	0.2683
52	291.00	10	1333.	0.1	0.1	0.0135	107	210.00	17	4539.	0.4	0.4	0.0461
53	290.00	6	1628.	0.1	0.1	0.0165	108	209.00	21	25655.	2.1	2.1	0.2603
54	289.00	8	784.	0.1	0.1	0.0080	109	208.00	10	2329.	0.2	0.2	0.0236
55	288.00	8	1722.	0.1	0.1	0.0175	110	205.00	17	2121.	0.2	0.2	0.0215

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	204.00	17	2621.	0.2	0.2	0.0266	166	127.00	35	111924.	9.3	9.3	1.1357
112	199.00	14	3307.	0.3	0.3	0.0336	167	126.00	25	29365.	2.4	2.4	0.2980
113	198.00	21	6808.	0.6	0.6	0.0691	168	125.00	29	58564.	4.9	4.9	0.5943
114	197.00	25	21535.	1.8	1.8	0.2185	169	124.00	21	10617.	0.9	0.9	0.1077
115	196.00	21	6633.	0.5	0.5	0.0673	170	123.00	25	15089.	1.2	1.2	0.1531
116	195.00	21	8182.	0.7	0.7	0.0830	171	122.00	29	10979.	0.9	0.9	0.1114
117	194.00	21	12420.	1.0	1.0	0.1260	172	121.00	21	14062.	1.2	1.2	0.1427
118	193.00	21	9967.	0.8	0.8	0.1011	173	119.00	25	1476.	0.1	0.1	0.0150
119	191.00	21	11439.	0.9	0.9	0.1161	174	117.00	17	427.	0.0	0.0	0.0043
120	189.00	17	718.	0.1	0.1	0.0073	175	114.00	17	11675.	1.0	1.0	0.1185*
121	187.00	10	5154.	0.4	0.4	0.0523*	176	113.00	35	85116.	7.0	7.0	0.8637
122	186.00	10	957.	0.1	0.1	0.0097	177	112.00	35	70712.	5.9	5.9	0.7175
123	184.00	35	2758.	0.2	0.2	0.0280	178	111.00	35	165148.	13.7	13.7	1.6758
124	183.00	29	38757.	3.2	3.2	0.3933	179	110.00	25	31815.	2.6	2.6	0.3228
125	182.00	21	8866.	0.7	0.7	0.0900	180	109.00	35	10857.	0.9	0.9	0.1102
126	181.00	21	13247.	1.1	1.1	0.1344	181	106.00	17	6235.	0.5	0.5	0.0633*
127	180.00	21	22080.	1.8	1.8	0.2240	182	103.00	14	3626.	0.3	0.3	0.0368
128	179.00	17	1181.	0.1	0.1	0.0120	183	101.00	14	504.	0.0	0.0	0.0051
129	178.00	17	4426.	0.4	0.4	0.0450	184	100.00	12	3616.	0.3	0.3	0.0367
130	176.00	14	3246.	0.3	0.3	0.0329	185	99.00	25	78300.	6.5	6.5	0.7945
131	175.00	21	7771.	0.6	0.6	0.0789	186	98.00	25	45433.	3.8	3.8	0.4610*
132	170.00	21	22076.	1.8	1.8	0.2240	187	97.00	35	261672.	21.7	21.7	2.6552
133	169.00	35	314256.	26.0	26.0	3.1888*	188	96.00	29	47311.	3.9	3.9	0.4801
134	168.00	25	4736.	0.4	0.4	0.0481	189	95.00	35	12865.	1.1	1.1	0.1305
135	167.00	29	45294.	3.8	3.8	0.4596	190	92.00	17	3185.	0.3	0.3	0.0323
136	166.00	17	7336.	0.6	0.6	0.0744	191	88.00	8	954.	0.1	0.1	0.0097
137	165.00	25	5755.	0.5	0.5	0.0584	192	87.00	10	4008.	0.3	0.3	0.0407
138	164.00	14	4879.	0.4	0.4	0.0495	193	86.00	17	16707.	1.4	1.4	0.1695
139	163.00	21	9657.	0.8	0.8	0.0980	194	85.00	35	220484.	18.3	18.3	2.2373
140	162.00	21	7327.	0.6	0.6	0.0743	195	84.00	25	50876.	4.2	4.2	0.5162
141	161.00	21	1566.	0.1	0.1	0.0159	196	83.00	35	239924.	19.9	19.9	2.4345
142	159.00	17	416.	0.0	0.0	0.0042	197	82.00	29	18699.	1.5	1.5	0.1897
143	157.00	21	758.	0.1	0.1	0.0077	198	81.00	35	47374.	3.9	3.9	0.4807*
144	155.00	29	35770.	3.0	3.0	0.3630*	199	80.00	29	986.	0.1	0.1	0.0100
145	154.00	21	9974.	0.8	0.8	0.1012	200	78.00	17	1587.	0.1	0.1	0.0161
146	153.00	25	33407.	2.8	2.8	0.3390	201	77.00	25	12816.	1.1	1.1	0.1300
147	152.00	21	6647.	0.6	0.6	0.0674	202	75.00	17	3426.	0.3	0.3	0.0348
148	151.00	21	4008.	0.3	0.3	0.0407	203	73.00	14	6548.	0.5	0.5	0.0664*
149	150.00	17	13033.	1.1	1.1	0.1322	204	72.00	25	20887.	1.7	1.7	0.2119
150	149.00	29	47109.	3.9	3.9	0.4780	205	71.00	51	641728.	53.1	53.1	6.5117
151	148.00	17	2680.	0.2	0.2	0.0272	206	70.00	35	128560.	10.6	10.6	1.3045*
152	147.00	17	2054.	0.2	0.2	0.0208*	207	69.00	43	502096.	41.6	41.6	5.0948
153	144.00	14	3326.	0.3	0.3	0.0337	208	68.00	25	24522.	2.0	2.0	0.2488
154	143.00	21	21138.	1.8	1.8	0.2145	209	67.00	29	36212.	3.0	3.0	0.3674
155	142.00	25	94728.	7.8	7.8	0.9612*	210	65.00	21	6916.	0.6	0.6	0.0702
156	141.00	35	81124.	6.7	6.7	0.8232	211	64.00	21	8384.	0.7	0.7	0.0851*
157	140.00	25	21193.	1.8	1.8	0.2150	212	63.00	14	1237.	0.1	0.1	0.0126
158	139.00	29	101584.	8.4	8.4	1.0308	213	62.00	6	1835.	0.2	0.2	0.0186
159	138.00	17	15397.	1.3	1.3	0.1562	214	61.00	17	10209.	0.8	0.8	0.1036
160	137.00	17	10766.	0.9	0.9	0.1092	215	59.00	17	1927.	0.2	0.2	0.0196*
161	136.00	21	956.	0.1	0.1	0.0097	216	58.00	35	42149.	3.5	3.5	0.4277
162	135.00	25	12139.	1.0	1.0	0.1232	217	57.00	51	1101440.	91.2	91.2	*1.17*
163	133.00	21	555.	0.0	0.0	0.0056	218	56.00	35	308600.	25.6	25.6	3.1315*
164	130.00	10	2303.	0.2	0.2	0.0234*	219	55.00	43	675696.	56.0	56.0	6.8564*
165	128.00	21	3406.	0.3	0.3	0.0346	220	54.00	25	35648.	3.0	3.0	0.3638

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
221	53.00	29	40260.	J.3	3.3	0.4085
222	52.00	14	5116.	0.4	0.4	0.0519
223	51.00	17	6511.	0.5	0.5	0.0661
224	50.00	17	2225.	0.2	0.2	0.0226
225	48.00	6	416.	0.0	0.0	0.0042
226	47.00	14	6083.	0.5	0.5	0.0617*
227	45.00	21	15832.	1.3	1.3	0.1606
228	44.00	43	49289.	4.1	4.1	0.5001*
229	43.00	51	1207424.	100.0	100.0	*12.25*
230	42.00	35	192100.	15.9	15.9	1.9493*
231	41.00	35	676672.	56.0	56.0	6.8663*
232	40.00	25	25127.	2.1	2.1	0.2550*
233	39.00	25	98060.	8.1	8.1	0.9950*
234	38.00	14	1924.	0.2	0.2	0.0195*
235	36.00	12	5383.	0.4	0.4	0.0546*
236	33.00	29	15607.	1.3	1.3	0.1584*
237	32.00	21	4830.	0.4	0.4	0.0490
238	31.00	17	4770.	0.4	0.4	0.0484
239	30.00	12	1599.	0.1	0.1	0.0162
240	29.00	43	292384.	24.2	24.2	2.9669*
241	28.00	35	48512.	4.0	4.0	0.4923
242	27.00	35	126280.	10.5	10.5	1.2814*

GAL6.1 [TIC=165621768, 188X-19833856] EI

Eicosanoic acid,
2,2,2-trifluoroethyl ester
 $\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	503.00	6	1037.	0.0	0.0	0.0006	56	252.00	14	82852.	0.4	0.4	0.0500*
2	429.00	8	1574.	0.0	0.0	0.0010	57	251.00	14	139832.	0.7	0.7	0.0844*
3	401.00	8	1175.	0.0	0.0	0.0007	58	250.00	17	348720.	1.8	1.8	0.2106
4	398.00	8	1846.	0.0	0.0	0.0011	59	249.00	8	5396.	0.0	0.0	0.0033
5	397.00	8	19451.	0.1	0.1	0.0117	60	248.00	6	2579.	0.0	0.0	0.0016
6	396.00	17	201372.	1.0	1.0	0.1216*	61	243.00	8	3934.	0.0	0.0	0.0024
7	395.00	21	1556096.	7.8	7.8	0.9395*	62	241.00	10	11623.	0.1	0.1	0.0070
8	394.00	35	6076672.	30.6	30.6	3.6690*	63	240.00	17	146500.	0.7	0.7	0.0885
9	393.00	12	24591.	0.1	0.1	0.0148*	64	239.00	17	294944.	1.5	1.5	0.1781
10	392.00	12	2752.	0.0	0.0	0.0017	65	238.00	6	2463.	0.0	0.0	0.0015
11	378.00	6	1111.	0.0	0.0	0.0007	66	237.00	10	3856.	0.0	0.0	0.0023
12	377.00	8	20018.	0.1	0.1	0.0121	67	236.00	8	1885.	0.0	0.0	0.0011
13	376.00	12	153792.	0.8	0.8	0.0929*	68	233.00	8	6060.	0.0	0.0	0.0037
14	375.00	14	319344.	1.6	1.6	0.1928	69	227.00	8	4950.	0.0	0.0	0.0030
15	367.00	8	10116.	0.1	0.1	0.0051	70	226.00	14	116248.	0.6	0.6	0.0702
16	366.00	10	44649.	0.2	0.2	0.0270	71	225.00	17	277344.	1.4	1.4	0.1675
17	365.00	14	203980.	1.0	1.0	0.1232	72	224.00	10	40881.	0.2	0.2	0.0247*
18	357.00	8	1615.	0.0	0.0	0.0010	73	223.00	10	19161.	0.1	0.1	0.0116
19	356.00	6	2150.	0.0	0.0	0.0013	74	222.00	8	21867.	0.1	0.1	0.0132
20	355.00	8	22002.	0.1	0.1	0.0133	75	221.00	14	55564.	0.3	0.3	0.0335*
21	353.00	8	26151.	0.1	0.1	0.0158	76	220.00	10	1130.	0.0	0.0	0.0007
22	352.00	14	242472.	1.2	1.2	0.1464	77	219.00	10	3773.	0.0	0.0	0.0023
23	351.00	21	1188096.	6.0	6.0	0.7174	78	213.00	10	24529.	0.1	0.1	0.0148
24	339.00	10	7505.	0.0	0.0	0.0045	79	212.00	17	388464.	2.0	2.0	0.2345
25	338.00	10	45447.	0.2	0.2	0.0280	80	211.00	25	2821696.	14.2	14.2	1.7037
26	337.00	12	162488.	0.8	0.8	0.0981	81	210.00	8	21795.	0.1	0.1	0.0132
27	325.00	6	10744.	0.1	0.1	0.0065	82	209.00	21	151756.	0.8	0.8	0.0916
28	324.00	10	28406.	0.1	0.1	0.0172	83	208.00	25	258468.	1.3	1.3	0.1561*
29	323.00	12	160852.	0.8	0.8	0.0971	84	207.00	17	726160.	3.7	3.7	0.4384
30	313.00	6	1523.	0.0	0.0	0.0009	85	206.00	6	938.	0.0	0.0	0.0006
31	311.00	10	4165.	0.0	0.0	0.0025	86	201.00	8	2065.	0.0	0.0	0.0012
32	310.00	12	85468.	0.4	0.4	0.0516	87	200.00	8	2194.	0.0	0.0	0.0013
33	309.00	14	387072.	2.0	2.0	0.2337	88	199.00	12	80368.	0.4	0.4	0.0485
34	297.00	10	52652.	0.3	0.3	0.0318	89	198.00	21	936160.	4.7	4.7	0.5652*
35	296.00	21	453056.	2.3	2.3	0.2735*	90	197.00	25	944656.	4.8	4.8	0.5704
36	295.00	21	1237760.	6.2	6.2	0.7473*	91	196.00	10	43255.	0.2	0.2	0.0261*
37	294.00	10	21165.	0.1	0.1	0.0128	92	195.00	14	65616.	0.3	0.3	0.0396*
38	293.00	10	5443.	0.0	0.0	0.0033	93	194.00	14	91784.	0.5	0.5	0.0554
39	290.00	6	1075.	0.0	0.0	0.0006	94	193.00	12	57009.	0.3	0.3	0.0344*
40	283.00	10	41866.	0.2	0.2	0.0253*	95	192.00	8	8174.	0.0	0.0	0.0049
41	282.00	17	145168.	0.7	0.7	0.0877	96	191.00	14	98768.	0.5	0.5	0.0596
42	281.00	17	290160.	1.5	1.5	0.1752	97	185.00	8	14303.	0.1	0.1	0.0086
43	278.00	8	9205.	0.0	0.0	0.0056	98	184.00	17	299552.	1.5	1.5	0.1809
44	277.00	10	32199.	0.2	0.2	0.0194*	99	183.00	25	651424.	3.3	3.3	0.3933
45	276.00	12	75840.	0.4	0.4	0.0458	100	182.00	14	58319.	0.3	0.3	0.0352*
46	271.00	6	969.	0.0	0.0	0.0006	101	181.00	17	114884.	0.6	0.6	0.0694*
47	269.00	8	6867.	0.0	0.0	0.0041	102	180.00	17	117080.	0.6	0.6	0.0707
48	268.00	14	125476.	0.6	0.6	0.0758	103	179.00	10	35330.	0.2	0.2	0.0213
49	267.00	21	642112.	3.2	3.2	0.0877	104	178.00	12	5215.	0.0	0.0	0.0031
50	266.00	12	5731.	0.0	0.0	0.0035*	105	177.00	8	51972.	0.3	0.3	0.0314*
51	265.00	10	18977.	0.1	0.1	0.0115*	106	176.00	6	2666.	0.0	0.0	0.0016
52	260.00	6	953.	0.0	0.0	0.0006	107	174.00	6	1507.	0.0	0.0	0.0009
53	255.00	8	9707.	0.0	0.0	0.0059	108	171.00	8	1419.	0.0	0.0	0.0009
54	254.00	17	214656.	1.1	1.1	0.1296	109	170.00	17	179860.	0.9	0.9	0.1086*
55	253.00	25	625424.	3.2	3.2	0.3776*	110	169.00	25	1505664.	7.6	7.6	0.5091

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	168.00	14	72736.	0.4	0.4	0.0439	166	105.00	10	18616.	0.1	0.1	0.0112*
112	167.00	17	136320.	0.7	0.7	0.0823*	167	104.00	6	1776.	0.0	0.0	0.0011
113	166.00	14	91520.	0.5	0.5	0.0553*	168	103.00	8	1869.	0.1	0.1	0.0063
114	165.00	12	48529.	0.2	0.2	0.0293*	169	101.00	8	92568.	0.0	0.0	0.0011
115	164.00	8	17029.	0.1	0.1	0.0103	170	100.00	17	1103424.	0.5	0.5	0.0559*
116	163.00	17	79320.	0.4	0.4	0.0479*	171	99.00	21	1496896.	5.6	5.6	0.6662
117	161.00	8	2213.	0.0	0.0	0.0013	172	98.00	25	3263616.	7.5	7.5	0.9038*
118	157.00	10	56133.	0.3	0.3	0.0339*	173	97.00	29	870336.	16.5	16.5	1.9705*
119	156.00	25	919792.	4.6	4.6	0.5554*	174	96.00	25	104312.	4.4	4.4	0.5255
120	155.00	35	8249600.	41.6	41.6	4.9810*	175	95.00	21	170336.	3.6	3.6	0.4289
121	154.00	14	90576.	0.5	0.5	0.0547	176	94.00	17	162436.	0.5	0.5	0.0630*
122	153.00	21	279216.	1.4	1.4	0.1686	177	93.00	17	3331.	0.8	0.8	0.0981
123	152.00	17	124712.	0.6	0.6	0.0753*	178	92.00	8	56208.	0.0	0.0	0.0020
124	151.00	10	44319.	0.2	0.2	0.0268	179	91.00	12	2374.	0.3	0.3	0.0339
125	150.00	10	17651.	0.1	0.1	0.0107	180	88.00	8	16904.	0.0	0.0	0.0014
126	149.00	21	176808.	0.9	0.9	0.1068*	181	87.00	8	268128.	0.1	0.1	0.0102*
127	148.00	8	5588.	0.0	0.0	0.0034	182	86.00	21	3988736.	1.4	1.4	0.1619*
128	147.00	12	49838.	0.3	0.3	0.0301*	183	85.00	29	1788096.	20.1	20.1	2.4083
129	146.00	6	1331.	0.0	0.0	0.0008	184	84.00	25	5262336.	9.0	9.0	1.0796
130	145.00	8	16265.	0.1	0.1	0.0098	185	83.00	35	874096.	26.5	26.5	3.1773
131	144.00	17	193344.	1.0	1.0	0.1167	186	82.00	21	899120.	4.4	4.4	0.5278
132	143.00	29	3971904.	20.0	20.0	2.3982*	187	81.00	21	169508.	4.5	4.5	0.5429
133	142.00	35	11014144.	55.5	55.5	6.6502*	188	80.00	17	244228.	0.9	0.9	0.1023
134	141.00	29	643024.	3.2	3.2	0.3882	189	79.00	17	54532.	1.2	1.2	0.1475*
135	140.00	17	159852.	0.8	0.8	0.0965*	190	78.00	14	183380.	0.3	0.3	0.0329
136	139.00	21	456272.	2.3	2.3	0.2755	191	77.00	17	16898.	0.9	0.9	0.1107*
137	138.00	17	122460.	0.6	0.6	0.0739*	192	75.00	10	42380.	0.1	0.1	0.0102*
138	137.00	14	105008.	0.5	0.5	0.0634	193	74.00	12	215572.	0.2	0.2	0.0256*
139	136.00	17	110080.	0.6	0.6	0.0665*	194	73.00	21	365040.	1.1	1.1	0.1302*
140	135.00	25	862432.	4.3	4.3	0.5207	195	72.00	21	6964224.	1.8	1.8	0.2204*
141	134.00	10	4483.	0.0	0.0	0.0027	196	71.00	29	1592384.	35.1	35.1	4.2049
142	133.00	14	67528.	0.3	0.3	0.0408	197	70.00	25	6569216.	8.0	8.0	0.9615*
143	131.00	8	10080.	0.1	0.1	0.0061	198	69.00	35	1129408.	33.1	33.1	3.9664*
144	130.00	6	1587.	0.0	0.0	0.0010	199	68.00	21	47611.	5.7	5.7	0.6819
145	128.00	12	62537.	0.3	0.3	0.0378*	200	67.00	21	50397.	5.6	5.6	0.6745*
146	127.00	29	1133824.	5.7	5.7	0.6846	201	66.00	10	52151.	0.2	0.2	0.0287
147	126.00	17	199876.	1.0	1.0	0.1207	202	65.00	10	25985.	0.3	0.3	0.0304
148	125.00	21	692432.	3.5	3.5	0.4181	203	64.00	14	1109.	0.3	0.3	0.0315
149	124.00	17	204260.	1.0	1.0	0.1233	204	63.00	10	59331.	0.1	0.1	0.0157
150	123.00	21	362576.	1.8	1.8	0.2189*	205	62.00	6	11487.	0.0	0.0	0.0007
151	122.00	21	549024.	2.8	2.8	0.3315	206	61.00	14	69316.	0.3	0.3	0.0358*
152	121.00	17	190504.	1.0	1.0	0.1150	207	60.00	10	11487.	0.1	0.1	0.0069
153	120.00	8	2680.	0.0	0.0	0.0016	208	59.00	12	69316.	0.3	0.3	0.0419*
154	119.00	10	50621.	0.3	0.3	0.0306*	209	58.00	25	14383872.	3.5	3.5	0.4210
155	118.00	12	12789.	0.1	0.1	0.0077*	210	57.00	43	2814656.	72.5	72.5	8.6848*
156	115.00	8	8572.	0.0	0.0	0.0052	211	56.00	29	10913536.	14.2	14.2	1.6994
157	114.00	12	58385.	0.3	0.3	0.0353*	212	55.00	35	827056.	55.0	55.0	6.5894*
158	113.00	29	774176.	3.9	3.9	0.4674*	213	54.00	21	434752.	4.2	4.2	0.4994
159	112.00	21	411952.	2.1	2.1	0.2487	214	53.00	21	7390.	2.2	2.2	0.2625*
160	111.00	25	1342208.	6.8	6.8	0.8104	215	52.00	8	86600.	0.0	0.0	0.0045
161	110.00	21	357952.	1.8	1.8	0.2161	216	51.00	14	21477.	0.4	0.4	0.0523*
162	109.00	21	378928.	1.9	1.9	0.2288	217	50.00	10	4378.	0.1	0.1	0.0130
163	108.00	10	54375.	0.3	0.3	0.0328	218	49.00	8	38236.	0.0	0.0	0.0026
164	107.00	17	144008.	0.7	0.7	0.0869	219	47.00	14	77936.	0.2	0.2	0.0231*
165	106.00	21	6273.	0.0	0.0	0.0038*	220	45.00	14		0.4	0.4	0.0471*

PAGE	5					
PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	44.00	35	750416.	3.8	3.8	0.4531*
222	43.00	43	19833856.	100.0	100.0	*11.97*
223	42.00	35	2451328.	12.4	12.4	1.4801
224	41.00	35	9392128.	47.4	47.4	5.6708
225	40.00	21	245396.	1.2	1.2	0.1482*
226	39.00	25	981280.	4.9	4.9	0.5925
227	38.00	12	30347.	0.2	0.2	0.0183*
228	37.00	6	1751.	0.0	0.0	0.0011
229	36.00	17	64295.	0.3	0.3	0.0388*

LCO 2415, ACID, FR. 6, ETHYL, . 35 UL. INJ AFTER DILUTING, 5/24/98
S4249.4249 [TIC=619856, 1892-58712] EI

Heneicosanoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	489.00	8	882.	1.5	1.5	0.1423	56	197.00	17	3013.	5.1	5.1	0.4861
2	425.00	8	531.	0.9	0.9	0.0857	57	196.00	6	1552.	2.6	2.6	0.2504
3	410.00	10	1887.	3.2	3.2	0.3044	58	191.00	21	917.	1.6	1.6	0.1479
4	409.00	14	6584.	11.2	11.2	1.0622	59	187.00	14	2193.	3.7	3.7	0.3538
5	408.00	17	21090.	35.9	35.9	3.4024	60	185.00	8	1858.	3.2	3.2	0.2997
6	394.00	10	467.	0.8	0.8	0.0753	61	184.00	12	1323.	2.3	2.3	0.2134
7	389.00	14	3172.	5.4	5.4	0.5117	62	179.00	8	3881.	6.6	6.6	0.6261*
8	367.00	8	1949.	3.3	3.3	0.3144	63	178.00	17	2857.	4.9	4.9	0.4609
9	366.00	12	1966.	3.3	3.3	0.3172	64	177.00	21	385.	0.7	0.7	0.0621
10	365.00	14	5100.	8.7	8.7	0.8228	65	171.00	6	2510.	4.3	4.3	0.4049
11	356.00	8	1516.	2.6	2.6	0.2446	66	170.00	10	542.	0.9	0.9	0.0874
12	355.00	10	1253.	2.1	2.1	0.2021	67	169.00	25	3419.	5.8	5.8	0.5516
13	353.00	6	1288.	2.2	2.2	0.2078	68	168.00	6	353.	0.6	0.6	0.0569*
14	349.00	6	1626.	2.8	2.8	0.2623	69	167.00	17	4252.	7.2	7.2	0.6860*
15	344.00	6	790.	1.3	1.3	0.1483	70	166.00	8	1865.	3.2	3.2	0.3009
16	343.00	6	919.	1.6	1.6	0.1789	71	165.00	29	3028.	5.2	5.2	0.4885
17	337.00	6	1109.	1.9	1.9	0.1789	72	159.00	12	666.	1.1	1.1	0.1074*
18	332.00	6	1209.	2.1	2.1	0.1950	73	156.00	10	6048.	10.3	10.3	0.9757*
19	327.00	8	1445.	2.5	2.5	0.2331	74	155.00	21	25511.	43.5	43.5	0.9757*
20	325.00	8	299.	0.5	0.5	0.0482	75	154.00	6	2976.	5.1	5.1	0.4801*
21	323.00	8	518.	0.9	0.9	0.0836	76	148.00	10	570.	1.0	1.0	0.0920
22	311.00	8	1973.	3.4	3.4	0.3183	77	147.00	21	4687.	8.0	8.0	0.7561
23	310.00	8	1801.	3.2	3.2	0.3035	78	146.00	8	1888.	3.2	3.2	0.3046
24	309.00	17	1072.	1.8	1.8	0.1729	79	143.00	21	23280.	39.7	39.7	3.7557
25	306.00	10	6553.	11.2	11.2	1.0572	80	142.00	25	43692.	74.4	74.4	7.0487
26	300.00	6	1737.	3.0	3.0	0.2802	81	140.00	6	943.	1.6	1.6	0.1521
27	296.00	8	1155.	2.4	2.4	0.1863	82	136.00	12	2421.	4.1	4.1	0.3906
28	295.00	8	1392.	2.4	2.4	0.2246	83	135.00	25	959.	1.6	1.6	0.1547
29	293.00	8	1954.	3.3	3.3	0.3152	84	131.00	10	3.	0.0	0.0	0.0005
30	292.00	6	378.	0.6	0.6	0.0610	85	129.00	12	1722.	2.9	2.9	0.2778
31	288.00	6	717.	1.2	1.2	0.1157	86	128.00	10	1606.	2.7	2.7	0.2591*
32	284.00	6	2149.	3.7	3.7	0.3457	87	127.00	8	1214.	2.1	2.1	0.1959
33	284.00	6	1090.	1.9	1.9	0.1758	88	124.00	12	825.	1.4	1.4	0.1331
34	277.00	8	745.	1.3	1.3	0.1204	89	122.00	21	3839.	6.5	6.5	0.6193
35	267.00	6	556.	0.9	0.9	0.0897	90	116.00	10	322.	0.5	0.5	0.0519
36	264.00	8	3250.	11.3	11.3	1.0736	91	112.00	8	776.	1.3	1.3	0.1252
37	263.00	8	841.	5.5	5.5	0.5243*	92	111.00	17	2698.	4.6	4.6	0.4353
38	256.00	6	714.	1.4	1.4	0.1357	93	111.00	21	2808.	4.8	4.8	0.4530*
39	254.00	10	2528.	1.2	1.2	0.1152	94	105.00	21	2032.	3.5	3.5	0.3278
40	252.00	6	862.	4.3	4.3	0.4078	95	104.00	8	1893.	3.2	3.2	0.3054
41	247.00	6	383.	1.5	1.5	0.1391	96	102.00	6	870.	1.5	1.5	0.1404
42	240.00	12	941.	0.7	0.7	0.0618	97	99.00	8	2780.	4.7	4.7	0.4485*
43	239.00	8	1170.	1.6	1.6	0.1518*	98	98.00	12	7398.	12.6	12.6	1.1935*
44	237.00	10	2371.	2.0	2.0	0.1888	99	97.00	21	4261.	7.3	7.3	0.6874
45	219.00	8	1950.	4.0	4.0	0.3825	100	97.00	29	10514.	17.9	17.9	1.6962
46	217.00	6	976.	3.3	3.3	0.3146	101	95.00	21	1000.	1.7	1.7	0.1613
47	213.00	10	3318.	1.7	1.7	0.1575	102	93.00	17	995.	1.7	1.7	0.1605
48	212.00	14	3295.	5.7	5.7	0.5353*	103	89.00	10	1899.	3.2	3.2	0.3064
49	211.00	21	15954.	5.6	5.6	0.5316	104	87.00	10	1306.	2.2	2.2	0.2107
50	210.00	6	1239.	27.2	27.2	2.5738	105	85.00	29	12969.	22.1	22.1	2.0923
51	203.00	12	3095.	2.1	2.1	0.1999	106	84.00	25	7078.	12.1	12.1	1.1419
52	203.00	12	108.	5.3	5.3	0.4993	107	83.00	35	12162.	20.7	20.7	1.9621
53	199.00	8	2558.	0.2	0.2	0.0174	108	82.00	14	4660.	7.9	7.9	0.7518*
54	198.00	12	4554.	4.4	4.4	0.4127	109	78.00	8	1115.	1.9	1.9	0.1799
55		12		7.8	7.8	0.7347*	110	75.00	10	864.	1.5	1.5	0.1394

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	73.00	25	402.	0.7	0.7	0.0649
112	72.00	8	1869.	3.2	3.2	0.3015
113	71.00	29	24159.	41.1	41.1	3.8975
114	70.00	25	1787.	3.0	3.0	0.2883*
115	69.00	35	10123.	17.2	17.2	1.6331
116	68.00	12	9015.	15.4	15.4	1.4544*
117	66.00	12	844.	1.4	1.4	0.1362
118	61.00	8	1913.	3.3	3.3	0.3086
119	60.00	17	4060.	6.9	6.9	0.6550
120	59.00	12	4713.	8.0	8.0	0.7603*
121	58.00	6	901.	1.5	1.5	0.1454
122	57.00	35	37744.	64.3	64.3	6.0892
123	56.00	25	4495.	7.7	7.7	0.7252
124	55.00	29	16301.	27.8	27.8	2.6298
125	54.00	14	7277.	12.4	12.4	1.1740*
126	53.00	21	4711.	8.0	8.0	0.7600
127	43.00	35	58712.	100.0	100.0	9.4719
128	42.00	14	4698.	8.0	8.0	0.7579*
129	41.00	29	24340.	41.5	41.5	3.9267
130	39.00	17	4336.	7.4	7.4	0.6995*
131	36.00	10	3031.	5.2	5.2	0.4890
132	32.00	10	5125.	8.7	8.7	0.8268*
133	29.00	35	13186.	22.5	22.5	2.1273
134	27.00	25	3212.	5.5	5.5	0.5182

BY3PK.1 [TIC-1352488, 100X-2703552] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	840.	0.0	0.0	0.0014	56	85.00	14	58756.	0.4	0.4	0.0844
2	231.00	6	1014.	0.0	0.0	0.0017	57	84.00	17	99096.	0.8	0.8	0.1647*
3	198.00	8	2527.	0.0	0.0	0.0042	58	83.00	25	1643840.	13.9	13.9	2.7328*
4	197.00	17	115556.	1.0	1.0	0.1921	59	82.00	10	9304.	0.1	0.1	0.0155*
5	196.00	25	1009504.	8.5	8.5	1.6782	60	81.00	17	143932.	1.2	1.2	0.2393*
6	195.00	17	174356.	1.5	1.5	0.2899	61	80.00	12	21013.	0.2	0.2	0.0349
7	182.00	6	1068.	0.0	0.0	0.0018	62	79.00	21	190636.	1.6	1.6	0.3169*
8	181.00	17	109740.	0.9	0.9	0.1824*	63	77.00	12	26949.	0.2	0.2	0.0448*
9	179.00	8	3354.	0.0	0.0	0.0056	64	73.00	17	30507.	0.3	0.3	0.0507*
10	178.00	8	9105.	0.1	0.1	0.0151	65	72.00	14	12915.	0.1	0.1	0.0215
11	177.00	14	62543.	0.5	0.5	0.1040	66	71.00	12	17710.	0.1	0.1	0.0294
12	176.00	8	3798.	0.0	0.0	0.0063	67	70.00	25	456240.	3.9	3.9	0.7585
13	175.00	10	37532.	0.3	0.3	0.0064	68	69.00	43	9393664.	79.5	79.5	*15.61*
14	169.00	14	96980.	0.8	0.8	0.1612*	69	68.00	35	2258240.	19.1	19.1	3.7542*
15	168.00	25	1439360.	12.2	12.2	2.3928*	70	67.00	35	2383552.	20.2	20.2	3.9625*
16	167.00	14	74296.	0.6	0.6	0.1235*	71	66.00	25	193228.	1.6	1.6	0.3212*
17	161.00	6	2405.	0.0	0.0	0.0040	72	65.00	21	346080.	2.9	2.9	0.5753*
18	157.00	17	49660.	0.4	0.4	0.0826*	73	64.00	21	243492.	2.1	2.1	0.4048*
19	156.00	25	563440.	4.8	4.8	0.09367*	74	63.00	21	182940.	1.5	1.5	0.3041*
20	155.00	51	11822080.	0.2	0.2	*19.65*	75	62.00	8	10041.	0.1	0.1	0.0167
21	154.00	17	21022.	0.6	0.6	0.0349*	76	61.00	17	65548.	0.6	0.6	0.1090*
22	153.00	17	70744.	0.1	0.1	0.1176*	77	59.00	14	33761.	0.3	0.3	0.0561*
23	149.00	8	13834.	0.1	0.1	0.0230*	78	57.00	21	91844.	0.8	0.8	0.1527*
24	148.00	21	353568.	3.0	3.0	0.5078	79	56.00	17	143616.	1.2	1.2	0.2388*
25	143.00	8	5295.	0.0	0.0	0.0088	80	55.00	35	3706112.	31.3	31.3	6.1612*
26	142.00	17	85432.	0.7	0.7	0.1420*	81	54.00	21	150692.	1.3	1.3	0.2505
27	141.00	12	30242.	0.3	0.3	0.0503*	82	53.00	25	587056.	5.0	5.0	0.9759
28	140.00	8	8644.	0.1	0.1	0.0144	83	52.00	17	58478.	0.5	0.5	0.0972*
29	139.00	12	23730.	0.2	0.2	0.0394*	84	51.00	21	252764.	2.1	2.1	0.4202
30	136.00	14	53862.	0.5	0.5	0.0895*	85	50.00	17	252764.	0.8	0.8	0.1577
31	135.00	25	1372928.	11.6	11.6	2.2824	86	49.00	12	12988.	0.1	0.1	0.0216*
32	131.00	10	31186.	0.3	0.3	0.0518	87	47.00	14	94856.	0.2	0.2	0.0425*
33	130.00	6	694.	0.0	0.0	0.0012	88	45.00	21	119488.	1.0	1.0	0.1986*
34	127.00	12	43623.	0.4	0.4	0.0725	89	44.00	35	113832.	1.0	1.0	0.1892*
35	126.00	14	14747.	0.1	0.1	0.0245*	90	43.00	35	335712.	2.8	2.8	0.5581
36	123.00	6	3261.	0.0	0.0	0.0054	91	42.00	35	1799936.	15.2	15.2	*14.62*
37	122.00	8	5954.	0.1	0.1	0.0099	92	41.00	43	8794880.	74.4	74.4	1.5543*
38	119.00	12	27414.	0.2	0.2	0.0456*	93	40.00	35	934928.	7.9	7.9	6.1415*
39	118.00	21	37723.	0.3	0.3	0.0627*	94	39.00	35	3694272.	31.2	31.2	0.4854
40	117.00	17	20133.	0.2	0.2	0.0335*	95	38.00	25	291968.	2.5	2.5	0.1145*
41	113.00	17	97980.	0.8	0.8	0.1629	96	37.00	17	68892.	0.6	0.6	0.0550*
42	111.00	8	2404.	0.0	0.0	0.0046	97	36.00	10	33072.	0.3	0.3	
43	110.00	6	5268.	0.0	0.0	0.0088							
44	109.00	21	501520.	4.2	4.2	0.0837							
45	103.00	12	36003.	0.3	0.3	0.0599							
46	102.00	14	4172.	0.0	0.0	0.0069							
47	100.00	12	37736.	0.3	0.3	0.0627*							
48	99.00	14	75080.	0.6	0.6	0.1248							
49	98.00	17	91536.	0.8	0.8	0.1522*							
50	97.00	25	1879616.	15.9	15.9	3.1247							
51	96.00	21	251936.	2.1	2.1	0.4188							
52	95.00	21	230136.	0.0	0.0	0.3826							
53	93.00	9	2759.	0.0	0.0	0.0046							
54	91.00	10	6097.	0.1	0.1	0.0101							
55	86.00	6	2331.	0.0	0.0	0.0039							

804PA.Y [TIC=100159488, 100X=16854016] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	1554.	0.0	0.0	0.0016	56	109.00	25	1140928.	6.8	5.8	1.1391
2	269.00	8	1813.	0.0	0.0	0.0018	57	103.00	17	4652.	0.0	0.0	0.0046
3	219.00	8	9817.	0.1	0.1	0.0098	58	100.00	8	23489.	0.1	0.1	0.0235
4	212.00	8	8644.	0.1	0.1	0.0086	59	99.00	10	41262.	0.2	0.2	0.0412
5	211.00	17	265152.	1.6	1.6	0.2647*	60	97.00	10	10210.	0.1	0.1	0.0102
6	210.00	29	2823424.	16.8	16.8	2.8189*	61	95.00	17	82536.	0.5	0.5	0.0824*
7	209.00	17	134512.	0.8	0.8	0.1343	62	94.00	10	17254.	0.1	0.1	0.0172
8	196.00	8	15341.	0.1	0.1	0.0153	63	93.00	21	382912.	2.3	2.3	0.3823
9	195.00	17	367200.	2.2	2.2	0.3666	64	92.00	14	67609.	0.4	0.4	0.0675
10	193.00	6	2951.	0.0	0.0	0.0029	65	91.00	12	50655.	0.3	0.3	0.0505
11	192.00	8	22771.	0.1	0.1	0.0227	66	85.00	17	52413.	0.3	0.3	0.0523
12	191.00	14	68204.	0.4	0.4	0.0681	67	84.00	25	652352.	3.9	3.9	0.6513
13	190.00	6	1837.	0.0	0.0	0.0018	68	83.00	43	12941568.	76.8	76.8	*12.92*
14	189.00	10	8914.	0.1	0.1	0.0089	69	82.00	29	2493696.	14.8	14.8	2.4897*
15	182.00	17	155716.	0.9	0.9	0.1555	70	81.00	29	2747584.	16.3	16.3	2.7432*
16	181.00	25	1170048.	6.9	6.9	1.1682	71	80.00	21	183448.	1.1	1.1	0.1832*
17	179.00	6	1519.	0.0	0.0	0.0015	72	79.00	25	809296.	4.8	4.8	0.8080
18	170.00	10	25478.	0.2	0.2	0.0254	73	78.00	17	113568.	0.7	0.7	0.1134*
19	169.00	21	641632.	3.8	3.8	0.6406	74	77.00	25	401280.	2.4	2.4	0.4006*
20	168.00	21	505136.	0.5	0.5	0.0543	75	74.00	8	4442.	0.0	0.0	0.0044
21	167.00	14	86836.	0.5	0.5	0.0867	76	73.00	12	26139.	0.2	0.2	0.0261
22	166.00	8	2719.	0.1	0.1	0.0027	77	71.00	14	35008.	0.2	0.2	0.0350*
23	162.00	10	17742.	0.1	0.1	0.0177	78	70.00	12	70092.	0.4	0.4	0.0700*
24	161.00	17	135260.	0.8	0.8	0.1350	79	69.00	35	2486216.	14.8	14.8	0.0700*
25	157.00	8	13893.	0.1	0.1	0.0139	80	68.00	35	6362368.	37.7	37.7	6.3522*
26	156.00	21	323632.	1.9	1.9	0.3231	81	67.00	29	2566912.	15.2	15.2	2.5628*
27	155.00	35	6382592.	37.9	37.9	6.3724*	82	66.00	21	257000.	1.5	1.5	0.2566*
28	154.00	10	24937.	0.1	0.1	0.0249*	83	65.00	17	271248.	1.6	1.6	0.2708
29	153.00	17	110476.	0.7	0.7	0.1103	84	64.00	21	284480.	1.7	1.7	0.2840*
30	149.00	10	44007.	0.3	0.3	0.0439	85	63.00	21	215128.	1.3	1.3	0.2148*
31	148.00	14	70340.	0.4	0.4	0.0702	86	62.00	8	6777.	0.0	0.0	0.0608
32	144.00	8	3827.	0.0	0.0	0.0038	87	61.00	17	112668.	0.7	0.7	0.1125*
33	143.00	21	343728.	2.0	2.0	0.3432	88	59.00	17	71268.	0.4	0.4	0.0712*
34	142.00	21	1090496.	6.5	6.5	1.0688	89	58.00	8	1552.	0.0	0.0	0.0015
35	141.00	8	2602.	0.0	0.0	0.0026	90	57.00	25	353888.	2.1	2.1	0.3533*
36	140.00	12	76428.	0.5	0.5	0.0763	91	56.00	35	5578496.	33.1	33.1	5.5696*
37	139.00	17	103500.	0.6	0.6	0.1033	92	55.00	51	16854016.	100.0	100.0	*16.82*
38	137.00	10	7481.	0.0	0.0	0.0075	93	54.00	29	1759488.	10.4	10.4	1.7567
39	136.00	12	56585.	0.3	0.3	0.0565*	94	53.00	29	1755264.	10.4	10.4	1.7525
40	135.00	25	1110016.	6.6	6.6	1.1082	95	52.00	21	255936.	1.5	1.5	0.2555*
41	131.00	14	62951.	0.4	0.4	0.0638	96	51.00	25	563552.	3.3	3.3	0.5627*
42	129.00	10	27653.	0.2	0.2	0.0276	97	50.00	21	225776.	1.3	1.3	0.2254*
43	128.00	6	8191.	0.0	0.0	0.0082	98	49.00	10	12934.	0.1	0.1	0.0129
44	127.00	21	432240.	2.6	2.6	0.4316	99	47.00	10	22720.	0.0	0.0	0.0027*
45	126.00	8	2218.	0.0	0.0	0.0022	100	46.00	8	4696.	0.0	0.0	0.0047
46	123.00	10	35364.	0.2	0.2	0.0353	101	45.00	21	153054.	0.9	0.9	0.1528*
47	122.00	14	85260.	0.5	0.5	0.0851	102	44.00	21	157648.	0.9	0.9	0.1574*
48	119.00	12	65408.	0.4	0.4	0.0653*	103	43.00	35	1252416.	7.4	7.4	1.2504
49	118.00	12	7857.	0.0	0.0	0.0078*	104	42.00	35	1134464.	6.7	6.7	1.1327
50	117.00	10	7427.	0.0	0.0	0.0074	105	41.00	35	8991232.	53.3	53.3	8.9769*
51	114.00	6	1199.	0.0	0.0	0.0012	106	40.00	35	737664.	4.4	4.4	0.7365*
52	113.00	17	165696.	1.0	1.0	0.1654	107	39.00	35	4323584.	25.7	25.7	4.3167*
53	112.00	14	86284.	0.5	0.5	0.0861	108	38.00	21	199536.	1.2	1.2	0.1992*
54	111.00	25	1540288.	9.1	9.1	1.5378	109	37.00	10	40081.	0.2	0.2	0.0400*
55	110.00	25	1854976.	11.0	11.0	1.8520*	110	36.00	29	162752.	1.0	1.0	0.1625*

8Y4AV.1 [TIC-9:467776, 188X-21177344] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	226.00	6	2043.	0.0	0.0	0.0022	56	96.00	25	882224.	4.2	4.2	0.9645
2	225.00	17	195268.	0.9	0.5	0.2135	57	95.00	25	876000.	4.1	4.1	0.9577*
3	224.00	25	1477888.	7.0	7.0	1.6157	58	94.00	12	13734.	0.1	0.1	0.0150*
4	223.00	6	675.	0.0	0.0	0.0007	59	93.00	17	90824.	0.4	0.4	0.0993*
5	211.00	6	2519.	0.0	0.0	0.0028	60	92.00	10	7192.	0.0	0.0	0.0079
6	210.00	14	58234.	0.3	0.3	0.0637	61	91.00	17	120788.	0.6	0.6	0.1321
7	209.00	21	662384.	3.1	3.1	0.7242	62	85.00	10	8695.	0.0	0.0	0.0095
8	196.00	8	10168.	0.0	0.0	0.0111	63	84.00	12	34951.	0.2	0.2	0.0382*
9	195.00	17	189524.	0.9	0.9	0.2072	64	83.00	35	2262912.	10.7	10.7	0.4740*
10	189.00	14	50224.	0.2	0.2	0.0549	65	82.00	25	623024.	2.9	2.9	0.6811
11	183.00	12	36681.	0.2	0.2	0.0401*	66	81.00	29	2016064.	9.5	9.5	2.2004*
12	182.00	17	121868.	0.6	0.6	0.1332	67	80.00	21	117264.	0.6	0.6	0.1282
13	181.00	10	47253.	0.2	0.2	0.0517	68	79.00	25	484864.	2.3	2.3	0.5301
14	179.00	8	2537.	0.0	0.0	0.0028	69	78.00	17	65411.	0.3	0.3	0.0715
15	175.00	8	633.	0.0	0.0	0.0007	70	77.00	21	358240.	1.7	1.7	0.3917
16	171.00	10	11291.	0.1	0.1	0.0123	71	75.00	6	2071.	0.0	0.0	0.0023
17	170.00	21	319120.	1.5	1.5	0.3489	72	74.00	6	1340.	0.0	0.0	0.0015
18	169.00	35	5311232.	25.1	25.1	5.8067*	73	73.00	10	16445.	0.1	0.1	0.0180
19	168.00	12	36851.	0.2	0.2	0.0403*	74	71.00	12	54363.	0.3	0.3	0.0594
20	167.00	17	59916.	0.3	0.3	0.0655*	75	70.00	29	523984.	2.5	2.5	0.5729*
21	162.00	6	1282.	0.0	0.0	0.0014	76	69.00	25	4086208.	19.3	19.3	4.4674*
22	161.00	8	2742.	0.0	0.0	0.0030	77	68.00	31	660016.	3.1	3.1	0.7216*
23	157.00	12	22939.	0.1	0.1	0.0251*	78	67.00	25	1651200.	7.8	7.8	1.8052
24	156.00	25	717200.	3.4	3.4	0.7841	79	66.00	29	130992.	0.6	0.6	0.1432*
25	155.00	17	179852.	0.8	0.8	0.1966	80	65.00	21	313984.	1.5	1.5	0.3433
26	154.00	10	25557.	0.1	0.1	0.0229	81	64.00	21	219020.	1.0	1.0	0.2395
27	153.00	14	61266.	0.3	0.3	0.0670*	82	63.00	21	175304.	0.8	0.8	0.0036
28	150.00	12	32258.	0.2	0.2	0.0353	83	62.00	8	3263.	0.0	0.0	0.0036
29	149.00	21	731552.	3.5	3.5	0.7998	84	61.00	14	76512.	0.4	0.4	0.0836*
30	143.00	10	8776.	0.0	0.0	0.0096	85	59.00	17	71968.	0.3	0.3	0.0787*
31	142.00	8	19125.	0.1	0.1	0.0209	86	58.00	8	2180.	0.0	0.0	0.0024
32	141.00	17	148708.	0.7	0.7	0.1625	87	57.00	29	335936.	1.8	1.8	0.4219
33	140.00	8	10705.	0.1	0.1	0.0117	88	56.00	35	3279360.	15.5	15.5	3.5853
34	139.00	17	98964.	0.4	0.4	0.0994	89	55.00	71	21177344.	100.0	100.0	*23.15*
35	137.00	6	2771.	0.0	0.0	0.0030	90	54.00	25	797440.	3.8	3.8	0.8718
36	136.00	17	75756.	0.4	0.4	0.0828*	91	53.00	35	1611712.	7.6	7.6	1.7621
37	135.00	17	89384.	0.4	0.4	0.0977*	92	52.00	21	202632.	1.0	1.0	0.2215*
38	131.00	10	13151.	0.1	0.1	0.0144	93	51.00	25	402000.	1.9	1.9	0.4395
39	127.00	21	290016.	1.4	1.4	0.3171	94	50.00	21	115264.	0.5	0.5	0.1260*
40	126.00	12	26740.	0.1	0.1	0.0292*	95	49.00	17	15823.	0.1	0.1	0.0173*
41	125.00	21	282128.	1.3	1.3	0.3084	96	47.00	17	65159.	0.3	0.3	0.0712
42	124.00	21	325424.	1.5	1.5	0.3558	97	45.00	25	189380.	0.9	0.9	0.2070*
43	123.00	25	686336.	3.2	3.2	0.7504	98	44.00	21	99480.	0.5	0.5	0.1088*
44	122.00	8	2488.	0.0	0.0	0.0027	99	43.00	35	1613248.	7.6	7.6	1.7637
45	119.00	10	15656.	0.1	0.1	0.0171	100	42.00	29	590560.	2.8	2.8	0.6456*
46	113.00	17	114976.	0.5	0.5	0.1257	101	41.00	35	6104576.	28.8	28.8	6.6740*
47	110.00	6	2284.	0.0	0.0	0.0025	102	40.00	29	599600.	2.8	2.8	0.6555*
48	109.00	25	208308.	1.0	1.0	0.2277	103	39.00	35	3241664.	15.3	15.3	3.5441
49	108.00	6	2989.	0.0	0.0	0.0033	104	38.00	21	128856.	0.6	0.6	0.1409*
50	107.00	17	83324.	0.4	0.4	0.0911*	105	37.00	10	11091.	0.1	0.1	0.0121
51	105.00	8	3769.	0.0	0.0	0.0041	106	36.00	17	54038.	0.3	0.3	0.0591*
52	100.00	14	4292.	0.0	0.0	0.0047*							
53	99.00	14	52933.	0.2	0.2	0.0579*							
54	98.00	29	1498240.	7.1	7.1	1.6380*							
55	97.00	59	20400128.	96.3	96.3	*22.30*							

BH8AV.1 [TIC=143253504, 100%-233390008] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	246.00	10	3552.	0.0	0.0	0.0025	56	106.00	8	6778.	0.0	0.0	0.0047
2	239.00	10	20843.	0.1	0.1	0.00145	57	105.00	17	76424.	0.3	0.3	0.0533*
3	238.00	10	69692.	0.3	0.3	0.00486	58	104.00	14	13662.	0.1	0.1	0.0095*
4	221.00	10	2003.	0.0	0.0	0.00014	59	103.00	10	9667.	0.0	0.0	0.0067*
5	220.00	14	158312.	0.7	0.7	0.1105*	60	102.00	8	7205.	0.0	0.0	0.0050
6	219.00	8	16297.	0.1	0.1	0.00114	61	99.00	10	58169.	0.2	0.2	0.0406
7	210.00	10	99044.	0.4	0.4	0.00691	62	98.00	25	1529536.	6.6	6.6	1.0677*
8	209.00	21	616560.	2.6	2.6	0.4304	63	97.00	51	21502976.	92.1	92.1	*15.01*
9	196.00	8	1490.	0.0	0.0	0.0010	64	96.00	35	234080.	10.9	10.9	1.7689*
10	191.00	8	8074.	0.0	0.0	0.0056	65	95.00	29	2265984.	9.7	9.7	1.5818*
11	189.00	8	6183.	0.0	0.0	0.0043	66	94.00	25	1351936.	5.8	5.8	0.9437
12	182.00	6	3059.	0.0	0.0	0.0021	67	93.00	25	713280.	3.1	3.1	0.4979
13	181.00	8	23634.	0.1	0.1	0.0165*	68	92.00	17	161004.	0.7	0.7	0.1124*
14	178.00	10	26077.	0.1	0.1	0.00182	69	91.00	25	511296.	2.2	2.2	0.3569
15	169.00	10	22822.	0.1	0.1	0.0159*	70	90.00	6	2042.	0.0	0.0	0.0014
16	167.00	8	11397.	0.0	0.0	0.0080	71	89.00	8	2744.	0.0	0.0	0.0019
17	166.00	6	1310.	0.0	0.0	0.0009	72	85.00	10	18214.	0.1	0.1	0.0127
18	165.00	8	4193.	0.0	0.0	0.0029	73	84.00	29	586256.	2.5	2.5	0.4092
19	161.00	8	2344.	0.0	0.0	0.0016	74	83.00	43	10682880.	45.8	45.8	7.4573*
20	158.00	6	1162.	0.0	0.0	0.0008	75	82.00	25	912240.	3.9	3.9	0.6368
21	157.00	10	42348.	0.2	0.2	0.0296	76	81.00	35	4284160.	18.4	18.4	2.9906
22	156.00	21	896192.	3.8	3.8	0.6256	77	80.00	25	429552.	1.8	1.8	0.2999
23	155.00	29	4007232.	17.2	17.2	2.7973*	78	79.00	25	1516864.	6.5	6.5	1.0589
24	154.00	8	5281.	0.0	0.0	0.0037	79	78.00	21	217536.	0.9	0.9	0.1519*
25	153.00	21	283104.	1.2	1.2	0.1976*	80	77.00	25	792688.	3.4	3.4	0.5533*
26	152.00	12	7624.	0.0	0.0	0.0053	81	76.00	8	2980.	0.0	0.0	0.0021
27	151.00	6	1981.	0.0	0.0	0.0014	82	75.00	8	8434.	0.0	0.0	0.0059
28	144.00	10	17947.	0.1	0.1	0.0125	83	74.00	12	76928.	0.3	0.3	0.0537
29	143.00	21	586240.	2.5	2.5	0.4092	84	73.00	8	27186.	0.1	0.1	0.0190
30	142.00	29	4104896.	17.6	17.6	2.8655*	85	71.00	12	63204.	0.3	0.3	0.0441*
31	141.00	12	35398.	0.2	0.2	0.0247	86	70.00	17	166508.	0.7	0.7	0.1162*
32	140.00	17	225744.	1.0	1.0	0.1576	87	69.00	35	3001536.	12.9	12.9	2.0953*
33	139.00	25	1715264.	7.3	7.3	1.1974	88	68.00	35	2343232.	10.0	10.0	1.6357*
34	138.00	21	776896.	3.3	3.3	0.5423	89	67.00	35	5242880.	22.5	22.5	3.6599*
35	137.00	17	183624.	0.8	0.8	0.1282	90	66.00	25	404096.	1.7	1.7	0.2821*
36	136.00	17	268352.	1.1	1.1	0.1873	91	65.00	25	553376.	2.4	2.4	0.3863*
37	135.00	21	792400.	3.4	3.4	0.5531	92	64.00	21	323728.	1.4	1.4	0.2260*
38	131.00	8	11753.	0.1	0.1	0.0082	93	63.00	21	268528.	1.2	1.2	0.1874*
39	128.00	10	2438.	0.0	0.0	0.0017	94	62.00	12	14006.	0.1	0.1	0.0098
40	127.00	21	370240.	1.6	1.6	0.2585*	95	61.00	17	191572.	0.8	0.8	0.1337*
41	126.00	6	1430.	0.0	0.0	0.0010	96	60.00	8	3512.	0.0	0.0	0.0025
42	123.00	17	185280.	0.8	0.8	0.1293*	97	59.00	14	60405.	0.3	0.3	0.0422*
43	122.00	25	767696.	3.3	3.3	0.5359	98	58.00	10	38616.	0.2	0.2	0.0270*
44	121.00	25	2550272.	10.9	10.9	1.7803*	99	57.00	29	1005424.	4.3	4.3	0.7018
45	120.00	21	787744.	3.4	3.4	0.5499	100	56.00	35	1944448.	8.3	8.3	1.3573
46	119.00	17	168508.	0.7	0.7	0.1176*	101	55.00	43	23339008.	100.0	100.0	*16.29*
47	118.00	10	6769.	0.0	0.0	0.0047*	102	54.00	35	2864256.	12.3	12.3	1.9994
48	117.00	6	3160.	0.0	0.0	0.0022	103	53.00	29	2360320.	10.1	10.1	1.6477
49	115.00	6	1189.	0.0	0.0	0.0008	104	52.00	21	306864.	1.3	1.3	0.2142*
50	113.00	17	148000.	0.6	0.6	0.1033*	105	51.00	25	655296.	2.8	2.8	0.4574*
51	111.00	14	101740.	0.4	0.4	0.0710	106	50.00	17	224076.	1.0	1.0	0.1564*
52	110.00	21	499904.	2.1	2.1	0.3490	107	49.00	17	24992.	0.1	0.1	0.0174*
53	109.00	25	565488.	2.4	2.4	0.3947	108	48.00	12	21886.	0.1	0.1	0.0153
54	108.00	8	7496.	0.0	0.0	0.0052	109	47.00	12	82236.	0.4	0.4	0.0574*
55	107.00	10	24661.	0.1	0.1	0.0172	110	46.00	8	9450.	0.0	0.0	0.0066

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	45.00	17	188556.	0.8	0.8	0.1316*
112	44.00	25	316496.	1.4	1.4	0.2209*
113	43.00	35	3373632.	14.5	14.5	2.3550
114	42.00	35	2603648.	11.2	11.2	1.8175
115	41.00	35	13193984.	56.5	56.5	9.2102*
116	40.00	29	903888.	3.9	3.9	0.6310*
117	39.00	35	5239296.	22.4	22.4	3.6574*
118	38.00	17	151824.	0.7	0.7	0.1060*
119	37.00	12	35767.	0.2	0.2	0.0250*
120	36.00	21	162936.	0.7	0.7	0.1137*
121	35.00	10	14340.	0.1	0.1	0.0100

8XAV9.1 [TIC-89911296, 160X-9089536] EI

9-octadecenoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	366.00	12	6798.	0.1	0.1	0.0076	56	198.00	10	22151.	0.2	0.2	0.0246
2	365.00	10	29188.	0.3	0.3	0.0325	57	197.00	17	109384.	1.2	1.2	0.1217*
3	364.00	14	205476.	2.3	2.3	0.2285	58	196.00	17	150932.	1.7	1.7	0.1679
4	357.00	6	928.	0.0	0.0	0.0010	59	195.00	17	103448.	1.1	1.1	0.1151
5	355.00	10	16345.	0.2	0.2	0.0182	60	194.00	14	70576.	0.8	0.8	0.0785*
6	347.00	12	14060.	0.2	0.2	0.0156	61	193.00	17	96048.	1.1	1.1	0.1068*
7	346.00	12	38727.	0.4	0.4	0.0431	62	192.00	8	5518.	0.1	0.1	0.0061
8	345.00	12	67144.	0.7	0.7	0.0747	63	191.00	10	26896.	0.3	0.3	0.0299
9	341.00	10	11080.	0.1	0.1	0.0123	64	190.00	8	2283.	0.0	0.0	0.0025
10	336.00	6	1060.	0.0	0.0	0.0012	65	189.00	10	6863.	0.1	0.1	0.0076
11	321.00	10	8410.	0.1	0.1	0.0094	66	184.00	8	6679.	0.1	0.1	0.0074
12	308.00	6	836.	0.0	0.0	0.0009	67	183.00	17	205988.	2.3	2.3	0.2291
13	307.00	8	2484.	0.0	0.0	0.0028	68	182.00	17	131672.	1.4	1.4	0.1464*
14	294.00	8	3013.	0.0	0.0	0.0034	69	181.00	17	102340.	1.1	1.1	0.1138*
15	293.00	10	6785.	0.1	0.1	0.0075	70	180.00	21	220344.	2.4	2.4	0.2451
16	292.00	6	1395.	0.0	0.0	0.0016	71	179.00	17	135412.	1.5	1.5	0.1506
17	283.00	10	8166.	0.1	0.1	0.0091*	72	178.00	8	5036.	0.1	0.1	0.0056
18	282.00	8	19002.	0.2	0.2	0.0211	73	177.00	8	20523.	0.2	0.2	0.0228
19	281.00	17	82184.	0.9	0.9	0.0914	74	176.00	8	1842.	0.0	0.0	0.0020
20	280.00	6	1981.	0.0	0.0	0.0022	75	175.00	10	31738.	0.3	0.3	0.0353*
21	279.00	10	12411.	0.1	0.1	0.0138	76	170.00	8	6777.	0.1	0.1	0.0075
22	269.00	8	1157.	0.0	0.0	0.0013	77	169.00	21	178984.	2.0	2.0	0.1991
23	268.00	6	1375.	0.0	0.0	0.0015	78	168.00	12	35400.	0.4	0.4	0.0394
24	267.00	12	35950.	0.4	0.4	0.0400*	79	167.00	21	169208.	1.9	1.9	0.1882
25	266.00	17	90040.	1.1	1.1	0.1090*	80	166.00	17	172304.	1.9	1.9	0.1916
26	265.00	21	579008.	6.4	6.4	0.6440*	81	165.00	17	193092.	2.1	2.1	0.2148*
27	264.00	17	318432.	3.5	3.5	0.3542	82	164.00	12	29999.	0.3	0.3	0.0334*
28	263.00	10	3236.	0.0	0.0	0.0036	83	163.00	12	56048.	0.6	0.6	0.0623*
29	254.00	6	1566.	0.0	0.0	0.0017	84	162.00	10	12015.	0.1	0.1	0.0134*
30	253.00	8	3342.	0.0	0.0	0.0037	85	161.00	14	75352.	0.8	0.8	0.0838*
31	252.00	8	4588.	0.1	0.1	0.0051	86	156.00	10	16073.	0.2	0.2	0.0179*
32	251.00	10	39091.	0.4	0.4	0.0435	87	155.00	21	398352.	4.4	4.4	0.4431
33	250.00	6	1958.	0.0	0.0	0.0022	88	154.00	17	91544.	1.0	1.0	0.1018*
34	247.00	12	39005.	0.4	0.4	0.0434	89	153.00	25	368400.	4.1	4.1	0.4097
35	246.00	10	34859.	0.4	0.4	0.0388	90	152.00	21	260800.	2.9	2.9	0.2901
36	239.00	10	23136.	0.3	0.3	0.0257	91	151.00	21	284352.	3.1	3.1	0.3163
37	238.00	8	13987.	0.2	0.2	0.0156	92	150.00	10	32650.	0.4	0.4	0.0363
38	237.00	14	58916.	0.6	0.6	0.0655*	93	149.00	17	95080.	1.0	1.0	0.1057*
39	236.00	10	29357.	0.3	0.3	0.0327*	94	148.00	14	64441.	0.7	0.7	0.0717*
40	235.00	8	5066.	0.1	0.1	0.0056	95	147.00	17	148920.	1.6	1.6	0.1656
41	233.00	6	1172.	0.0	0.0	0.0013	96	143.00	10	38476.	0.4	0.4	0.0428*
42	225.00	10	43690.	0.5	0.5	0.0486	97	142.00	21	392736.	4.3	4.3	0.4368
43	224.00	10	8987.	0.1	0.1	0.0100	98	141.00	17	171268.	1.9	1.9	0.1905
44	223.00	17	93256.	1.0	1.0	0.1037*	99	140.00	21	235080.	2.6	2.6	0.2615
45	222.00	17	345792.	3.8	3.8	0.3846	100	139.00	25	431120.	4.7	4.7	0.4795
46	221.00	17	77464.	0.9	0.9	0.0862*	101	138.00	21	377520.	4.2	4.2	0.4199
47	220.00	17	201424.	2.2	2.2	0.2240	102	137.00	21	329504.	3.6	3.6	0.3665
48	212.00	8	2928.	0.0	0.0	0.0033	103	136.00	17	86552.	1.0	1.0	0.0963*
49	211.00	17	85128.	0.9	0.9	0.0947	104	135.00	25	320768.	3.5	3.5	0.3568*
50	210.00	12	36879.	0.4	0.4	0.0410*	105	134.00	17	104480.	1.1	1.1	0.1162*
51	209.00	17	209620.	2.3	2.3	0.2331	106	133.00	21	179128.	2.0	2.0	0.1992
52	208.00	17	95492.	1.1	1.1	0.1062*	107	131.00	12	8966.	0.1	0.1	0.0105*
53	207.00	21	318096.	3.5	3.5	0.3538	108	128.00	8	7006.	0.1	0.1	0.0078
54	205.00	6	2478.	0.0	0.0	0.0028	109	127.00	25	374624.	4.1	4.1	0.4167
55	203.00	8	3257.	0.0	0.0	0.0035	110	126.00	21	257604.	2.8	2.8	0.2865

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	125.00	25	693440.	7.6	7.6	0.7712
112	124.00	21	587760.	6.5	6.5	0.6537
113	123.00	25	595296.	6.5	6.5	0.6621
114	122.00	21	176848.	1.9	1.9	0.1967*
115	121.00	21	194992.	2.1	2.1	0.2169*
116	120.00	8	27490.	0.3	0.3	0.0306*
117	119.00	21	167144.	1.8	1.8	0.1859*
118	114.00	8	2032.	0.0	0.0	0.0023
119	113.00	21	157976.	1.7	1.7	0.1757*
120	112.00	25	501008.	5.5	5.5	0.5572
121	111.00	25	1571776.	17.3	17.3	1.7481
122	110.00	25	1029392.	11.3	11.3	1.1449
123	109.00	25	718960.	7.9	7.9	0.7996
124	108.00	17	136396.	1.5	1.5	0.1517*
125	107.00	21	173068.	1.9	1.9	0.1925
126	105.00	10	12201.	0.1	0.1	0.0136
127	105.00	14	72960.	0.8	0.8	0.0811*
128	103.00	8	2850.	0.0	0.0	0.0032
129	99.00	21	173416.	1.9	1.9	0.1929
130	98.00	25	1350784.	14.9	14.9	1.5024
131	97.00	29	3511360.	38.6	38.6	3.9054
132	96.00	29	2262144.	24.9	24.9	2.5160
133	95.00	25	1259264.	13.9	13.9	1.4006
134	94.00	21	201740.	2.2	2.2	0.2244*
135	93.00	21	220340.	2.4	2.4	0.2451*
136	92.00	10	15364.	0.2	0.2	0.0171
137	91.00	21	144100.	1.6	1.6	0.1603*
138	86.00	12	7794.	0.1	0.1	0.0087*
139	85.00	25	656912.	7.2	7.2	0.7306
140	84.00	29	2380400.	26.2	26.2	2.6476
141	83.00	35	5711104.	62.8	62.8	6.3519
142	82.00	29	1842304.	20.3	20.3	2.0490
143	81.00	25	2073920.	22.8	22.8	2.3066
144	80.00	21	237644.	2.6	2.6	0.2643*
145	79.00	25	489056.	5.4	5.4	0.5439*
146	78.00	10	54132.	0.6	0.6	0.0502*
147	77.00	21	172740.	1.9	1.9	0.1921*
148	74.00	8	2496.	0.0	0.0	0.0028
149	73.00	14	84424.	0.9	0.9	0.0939*
150	72.00	12	47619.	0.5	0.5	0.0530*
151	71.00	25	1246272.	13.7	13.7	1.3861
152	70.00	29	2923520.	32.2	32.2	3.2516
153	69.00	35	6452224.	71.0	71.0	7.1762
154	68.00	29	2196800.	24.2	24.2	2.4433
155	67.00	25	2570752.	28.3	28.3	2.8592
156	66.00	17	137540.	1.5	1.5	0.1530*
157	65.00	21	155600.	1.7	1.7	0.1731*
158	64.00	10	20012.	0.2	0.2	0.0231*
159	63.00	12	13646.	0.2	0.2	0.0152
160	61.00	10	41331.	0.5	0.5	0.0460*
161	59.00	8	10401.	0.1	0.1	0.0116
162	58.00	17	133080.	1.5	1.5	0.1480*
163	57.00	35	3660032.	40.3	40.3	4.0707*
164	56.00	35	3452352.	38.0	38.0	3.8397
165	55.00	35	9089536.	100.0	100.0	*10.10*

EXAV4.1 [TIC-72994816, 188X=25464832] EI

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	219.00	8	1413.	0.0	0.0	0.0019	56	52.00	29	434928.	1.7	1.7	0.5958*
2	206.00	12	41464.	0.2	0.2	0.0568*	57	51.00	35	8325376.	32.7	32.7	*11.40*
3	205.00	25	607040.	2.4	2.4	0.0316*	58	50.00	35	3414336.	13.4	13.4	4.6775*
4	204.00	43	6739456.	26.5	26.5	9.2328*	59	49.00	25	228344.	0.9	0.9	0.3128*
5	203.00	17	182424.	0.7	0.7	0.2499*	60	48.00	10	4244.	0.0	0.0	0.0058
6	186.00	8	12777.	0.1	0.1	0.0175	61	45.00	12	64865.	0.3	0.3	0.0089*
7	185.00	17	240964.	0.9	0.9	0.3301	62	44.00	17	96648.	0.4	0.4	0.1324*
8	181.00	12	7994.	0.0	0.0	0.0110	63	40.00	10	8960.	0.0	0.0	0.0123
9	169.00	8	10737.	0.0	0.0	0.0147	64	39.00	25	599728.	2.4	2.4	0.8216
10	160.00	6	3712.	0.0	0.0	0.0051	65	38.00	35	530752.	2.1	2.1	0.7271*
11	159.00	8	16918.	0.1	0.1	0.0232	66	37.00	21	173968.	0.7	0.7	0.2383*
12	155.00	6	2330.	0.0	0.0	0.0032	67	36.00	21	166900.	0.7	0.7	0.2286*
13	140.00	12	21156.	0.1	0.1	0.0290	68	35.00	17	4621.	0.0	0.0	0.0063*
14	136.00	8	6981.	0.0	0.0	0.0096							
15	135.00	10	23923.	0.1	0.1	0.0328							
16	131.00	8	11187.	0.0	0.0	0.0153							
17	127.00	6	3077.	0.0	0.0	0.0042							
18	123.00	8	2605.	0.0	0.0	0.0036							
19	121.00	8	1191.	0.0	0.0	0.0016							
20	120.00	12	50114.	0.2	0.2	0.0687							
21	119.00	17	136888.	0.5	0.5	0.1875*							
22	109.00	8	12736.	0.1	0.1	0.0174							
23	108.00	6	964.	0.0	0.0	0.0013							
24	107.00	17	101440.	0.4	0.4	0.1390*							
25	106.00	25	1827648.	7.2	7.2	2.5038*							
26	105.00	71	25464832.	100.0	100.0	*34.88*							
27	104.00	21	138364.	0.5	0.5	0.1896*							
28	103.00	10	15850.	0.1	0.1	0.0217*							
29	100.00	6	1251.	0.0	0.0	0.0017							
30	95.00	8	13763.	0.1	0.1	0.0189							
31	93.00	6	1811.	0.0	0.0	0.0025							
32	92.00	17	120416.	0.5	0.5	0.1650*							
33	91.00	21	253180.	1.0	1.0	0.3468							
34	83.00	21	553264.	2.2	2.2	0.7579							
35	81.00	6	2023.	0.0	0.0	0.0028							
36	79.00	10	22100.	0.1	0.1	0.0303*							
37	78.00	25	1067072.	4.2	4.2	1.4618							
38	77.00	51	16240896.	63.8	63.8	*22.24*							
39	76.00	25	10600864.	4.2	4.2	1.4533*							
40	75.00	25	686384.	2.7	2.7	0.9403							
41	74.00	25	935696.	3.7	3.7	1.2819*							
42	73.00	21	151484.	0.6	0.6	0.2075*							
43	72.00	10	2981.	0.0	0.0	0.0041							
44	70.00	10	2734.	0.0	0.0	0.0037							
45	69.00	25	1163136.	4.6	4.6	1.5935							
46	67.00	6	3977.	0.0	0.0	0.0054							
47	65.00	17	91564.	0.4	0.4	0.1254*							
48	64.00	21	341984.	1.3	1.3	0.4685							
49	63.00	21	213020.	0.8	0.8	0.2918							
50	62.00	17	103432.	0.4	0.4	0.1417*							
51	61.00	12	36696.	0.1	0.1	0.0503*							
52	57.00	10	8786.	0.0	0.0	0.0120							
53	56.00	17	32895.	0.1	0.1	0.0451*							
54	54.00	10	6845.	0.0	0.0	0.0094							
55	53.00	17	138700.	0.5	0.5	0.1900*							

806PA.1 [TIC-84643849, 188X-14585988] EI

2-methylbenzoic acid,
2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	1971.	0.0	0.0	0.0023	2792.	0.0	0.0	0.0033
2	231.00	8	3220.	0.0	0.0	0.0038	2339.	0.0	0.0	0.0028
3	220.00	12	54276.	0.4	0.4	0.0641	64179.	0.4	0.4	0.0758*
4	219.00	25	707216.	4.8	4.8	0.8355*	1134400.	7.8	7.8	1.3402
5	218.00	43	6873088.	47.1	47.1	8.1200*	334096.	2.3	2.3	0.3947*
6	217.00	21	253816.	1.7	1.7	0.2999	1502400.	10.3	10.3	1.7750*
7	203.00	17	191376.	1.3	1.3	0.2261	166988.	1.1	1.1	0.1973
8	200.00	10	35627.	0.2	0.2	0.0421*	210068.	1.4	1.4	0.2482*
9	199.00	17	320496.	2.2	2.2	0.3786	232058.	1.6	1.6	0.2742*
10	181.00	6	19462.	0.1	0.1	0.0230	25932.	0.2	0.2	0.0306
11	173.00	12	41486.	0.3	0.3	0.0490	37267.	0.3	0.3	0.0440*
12	172.00	16	1045.	0.0	0.0	0.0012	7267.	7.4	7.4	1.2769*
13	169.00	12	54134.	0.4	0.4	0.0640	100832.	0.1	0.1	0.0107*
14	155.00	8	22093.	0.2	0.2	0.0261*	9038.	0.1	0.1	0.0115*
15	154.00	8	10564.	0.1	0.1	0.0125	314054.	2.2	2.2	0.3710
16	153.00	8	1445.	0.0	0.0	0.0017	5921536.	40.6	40.6	6.9958*
17	150.00	10	2036.	0.0	0.0	0.0024	1036512.	7.1	7.1	1.2246*
18	149.00	10	9374.	0.1	0.1	0.0111	2600640.	17.8	17.8	3.0725
19	147.00	8	4630.	0.0	0.0	0.0055	819600.	5.6	5.6	0.9683
20	142.00	8	2442.	0.0	0.0	0.0029	225884.	1.5	1.5	0.2669*
21	137.00	12	44717.	0.3	0.3	0.0528	4733.	0.0	0.0	0.0056
22	136.00	17	130588.	0.9	0.9	0.1543	414016.	2.8	2.8	0.4891*
23	135.00	25	1695936.	11.6	11.6	2.0036*	19877.	0.0	0.0	0.0018
24	134.00	12	52802.	0.4	0.4	0.0624	1488.	0.0	0.0	0.0235
25	133.00	17	197568.	1.4	1.4	0.2334	273872.	1.9	1.9	0.3236*
26	131.00	12	37593.	0.3	0.3	0.0449*	346528.	2.4	2.4	0.4094
27	127.00	8	3166.	0.0	0.0	0.0037	1728832.	11.9	11.9	2.0425
28	123.00	8	4516.	0.0	0.0	0.0053	854368.	5.9	5.9	1.0094*
29	121.00	12	54648.	0.4	0.4	0.0646*	52039.	0.4	0.4	0.0615*
30	120.00	25	1147584.	7.9	7.9	1.3558*	1987.	0.0	0.0	0.0023
31	119.00	59	14585088.	100.0	100.0	*17.23*	3773.	0.0	0.0	0.0045
32	118.00	51	10872832.	74.5	74.5	*12.84*	5014.	9.0	9.0	0.0059
33	117.00	6	3768.	0.0	0.0	0.0045	443232.	3.0	3.0	0.5236*
34	116.00	8	2694.	0.0	0.0	0.0032	147444.	1.0	1.0	0.1742*
35	110.00	8	4397.	0.0	0.0	0.0052	82580.	0.6	0.6	0.0976*
36	109.00	17	119228.	0.8	0.8	0.1409*	11482.	0.1	0.1	0.0135
37	107.00	21	174852.	1.2	1.2	0.2066*	637424.	4.4	4.4	0.7531
38	106.00	12	70728.	0.5	0.5	0.0836*	297248.	2.0	2.0	0.3512*
39	105.00	25	484016.	3.3	3.3	0.5718	3220416.	22.1	22.1	3.8047
40	104.00	8	3951.	0.0	0.0	0.0047	496336.	3.4	3.4	0.5864*
41	103.00	6	4153.	0.0	0.0	0.0049	135560.	0.9	0.9	0.1602*
42	99.00	6	4349.	0.0	0.0	0.0051	71488.	0.5	0.5	0.0844*
43	98.00	6	1719.	0.0	0.0	0.0020	5037.	0.0	0.0	0.0060*
44	95.00	8	1290.	0.0	0.0	0.0015				
45	93.00	10	23670.	0.2	0.2	0.0280				
46	92.00	25	960896.	6.6	6.6	0.0280				
47	91.00	43	12979968.	89.0	89.0	*15.33*				
48	90.00	35	4022272.	27.6	27.6	4.7520*				
49	89.00	35	2390976.	16.4	16.4	2.8247*				
50	88.00	17	85328.	0.6	0.6	0.1008*				
51	87.00	17	119844.	0.8	0.8	0.1416				
52	86.00	17	130080.	0.9	0.9	0.1537*				
53	85.00	12	37968.	0.3	0.3	0.0449				
54	84.00	10	5396.	0.0	0.0	0.0064				
55	83.00	21	591856.	4.1	4.1	0.6992				

0XAV6.1 [TIC-92410848, 155X-28418888] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	231.00	8	3753.	0.0	0.0	0.0041	56	73.00	10	34350.	0.1	0.1	0.0372*
2	220.00	12	54067.	0.2	0.2	0.0585	57	70.00	17	42846.	0.2	0.2	0.0464*
3	219.00	21	957968.	3.4	3.4	1.0366*	58	69.00	43	1128512.	4.0	4.0	1.2311*
4	218.00	43	9428224.	33.2	33.2	*10.20*	59	66.00	21	328720.	1.2	1.2	0.3557*
5	217.00	25	423872.	1.5	1.5	0.4586*	60	55.00	43	6835456.	24.1	24.1	7.3962*
6	216.00	10	15541.	0.1	0.1	0.0168*	61	64.00	29	972128.	3.4	3.4	1.0519*
7	204.00	6	2803.	0.0	0.0	0.0030	62	63.00	29	2833280.	10.0	10.0	3.0657*
8	203.00	17	161228.	0.6	0.6	0.1745	63	62.00	25	938064.	3.3	3.3	1.0150*
9	199.00	12	26105.	0.1	0.1	0.0282	64	61.00	21	242248.	0.9	0.9	0.2621
10	193.00	17	406464.	1.4	1.4	0.4398	65	59.00	25	358384.	1.3	1.3	0.3878*
11	189.00	12	2866.	0.0	0.0	0.0031	66	57.00	6	1459.	0.0	0.0	0.0016
12	173.00	14	6944.	0.2	0.2	0.0757	67	55.00	8	4651.	0.0	0.0	0.0050
13	169.00	8	21950.	0.1	0.1	0.0238	68	53.00	21	217648.	0.8	0.8	0.2355*
14	155.00	5	5847.	0.0	0.0	0.0063	69	52.00	25	410960.	1.4	1.4	0.4447
15	154.00	10	6018.	0.0	0.0	0.0065	70	51.00	29	1611456.	5.7	5.7	1.7437
16	151.00	8	1873.	0.0	0.0	0.0020	71	50.00	29	1104256.	3.9	3.9	1.1948
17	150.00	8	21078.	0.1	0.1	0.0228	72	49.00	14	64873.	0.2	0.2	0.0702*
18	149.00	12	84520.	0.3	0.3	0.0915	73	47.00	8	3844.	0.0	0.0	0.0042
19	137.00	6	1668.	0.0	0.0	0.0018	74	46.00	14	19352.	0.1	0.1	0.0209*
20	136.00	8	4840.	0.0	0.0	0.0052	75	45.00	43	528128.	1.9	1.9	0.5715*
21	135.00	17	155404.	0.5	0.5	0.1488	76	44.00	25	214528.	0.8	0.8	0.2321*
22	134.00	14	51292.	0.2	0.2	0.0555*	77	43.00	17	89060.	0.3	0.3	0.0964*
23	133.00	14	124912.	0.4	0.4	0.1352	78	42.00	14	17600.	0.1	0.1	0.0190*
24	131.00	10	6358.	0.0	0.0	0.0069	79	41.00	25	764720.	2.7	2.7	0.8275
25	127.00	6	1436.	0.0	0.0	0.0016	80	40.00	21	249564.	0.9	0.9	0.2700*
26	125.00	8	2537.	0.0	0.0	0.0027	81	39.00	35	3491328.	12.3	12.3	3.7778
27	123.00	8	7494.	0.0	0.0	0.0081	82	38.00	29	578096.	2.0	2.0	0.6255*
28	121.00	17	137520.	0.5	0.5	0.1488	83	37.00	21	134164.	0.5	0.5	0.1452*
29	120.00	29	2380992.	8.4	8.4	2.5763*	84	36.00	21	176732.	0.6	0.6	0.1912*
30	119.00	71	28410000.	100.0	100.0	*30.74*	85	35.00	10	12684.	0.0	0.0	0.0137*
31	118.00	35	385248.	1.4	1.4	0.4159*							
32	117.00	10	15853.	0.1	0.1	0.0172							
33	109.00	10	24223.	0.1	0.1	0.0262							
34	107.00	14	34229.	0.1	0.1	0.0370*							
35	106.00	14	86812.	0.3	0.3	0.0939*							
36	105.00	21	33400.	1.2	1.2	0.3618							
37	99.00	8	3003.	0.0	0.0	0.0032							
38	93.00	12	43649.	0.2	0.2	0.0472*							
39	92.00	25	1331776.	4.7	4.7	1.4410*							
40	91.00	51	17114112.	60.2	60.2	*18.51*							
41	90.00	29	1689792.	5.9	5.9	1.8284*							
42	89.00	35	2400000.	8.4	8.4	2.5969*							
43	88.00	17	109952.	0.4	0.4	0.1190*							
44	87.00	17	165116.	0.6	0.6	0.1787*							
45	86.00	17	135164.	0.5	0.5	0.1463							
46	85.00	12	56529.	0.2	0.2	0.0612*							
47	84.00	8	5943.	0.0	0.0	0.0064							
48	83.00	21	684416.	2.4	2.4	0.7406							
49	81.00	6	392.	0.0	0.0	0.0004							
50	79.00	14	83648.	0.3	0.3	0.0905*							
51	78.00	17	200548.	0.7	0.7	0.2170*							
52	77.00	21	405472.	1.4	1.4	0.4387							
53	76.00	21	178148.	0.6	0.6	0.1928*							
54	75.00	21	266560.	1.0	1.0	0.3101*							
55	74.00	21	253504.	0.9	0.9	0.2743*							

FV3AV.1 [TIC-59129856, 188X-19358528] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	221.00	8	2032.	0.0	0.0	0.0034
2	220.00	14	26144.	0.1	0.1	0.0442*
3	219.00	29	480736.	2.5	2.5	0.8130*
4	218.00	43	4656896.	24.1	24.1	7.8757*
5	217.00	29	187076.	1.0	1.0	0.3164*
6	216.00	10	5194.	0.0	0.0	0.0088*
7	209.00	6	675.	0.0	0.0	0.0011
8	204.00	8	2089.	0.0	0.0	0.0035
9	203.00	14	33897.	0.2	0.2	0.0573*
10	200.00	14	25228.	0.1	0.1	0.0427
11	199.00	25	287568.	1.5	1.5	0.4863*
12	190.00	8	7112.	0.0	0.0	0.0120
13	189.00	17	107144.	0.6	0.6	0.1812
14	174.00	6	2825.	0.0	0.0	0.0048
15	173.00	12	24644.	0.1	0.1	0.0417
16	172.00	8	1953.	0.0	0.0	0.0033
17	169.00	8	12323.	0.1	0.1	0.0208
18	159.00	8	1496.	0.0	0.0	0.0025
19	155.00	6	1100.	0.0	0.0	0.0019
20	154.00	10	14103.	0.1	0.1	0.0239
21	153.00	10	2519.	0.0	0.0	0.0043
22	151.00	12	3213.	0.0	0.0	0.0054
23	150.00	10	6355.	0.0	0.0	0.0107
24	149.00	10	26035.	0.1	0.1	0.0440
25	137.00	8	1221.	0.0	0.0	0.0021
26	135.00	12	33604.	0.2	0.2	0.0568*
27	134.00	10	14066.	0.1	0.1	0.0238
28	133.00	17	81028.	0.4	0.4	0.1370
29	131.00	10	19116.	0.1	0.1	0.0323*
30	123.00	8	11413.	0.1	0.1	0.0193
31	122.00	8	3634.	0.0	0.0	0.0061
32	121.00	21	103424.	0.5	0.5	0.1749*
33	120.00	35	1538816.	8.0	8.0	2.6024*
34	119.00	71	19350528.	100.0	100.0	*32.72*
35	118.00	43	247756.	1.3	1.3	0.4190*
36	117.00	12	11735.	0.1	0.1	0.0198*
37	116.00	6	1772.	0.0	0.0	0.0030
38	109.00	10	26742.	0.1	0.1	0.0452*
39	108.00	8	5736.	0.0	0.0	0.0097
40	107.00	21	128796.	0.7	0.7	0.2178*
41	106.00	14	32986.	0.2	0.2	0.0558*
42	105.00	25	212280.	1.1	1.1	0.3590*
43	104.00	8	8383.	0.0	0.0	0.0142
44	100.00	8	5056.	0.0	0.0	0.0086
45	99.00	8	1666.	0.0	0.0	0.0028
46	98.00	10	2240.	0.0	0.0	0.0038
47	97.00	6	2520.	0.0	0.0	0.0043
48	95.00	6	5223.	0.0	0.0	0.0088
49	93.00	8	16660.	0.1	0.1	0.0282
50	92.00	35	696320.	3.6	3.6	1.1776
51	91.00	51	9823744.	50.8	50.8	*16.61*
52	90.00	35	1054656.	5.5	5.5	1.7836*
53	89.00	35	1590528.	8.2	8.2	2.6899*
54	88.00	21	83088.	0.4	0.4	0.1405*
55	87.00	21	138192.	0.7	0.7	0.2337*

BH6AV.1 [TIC=189842432, 188X=54624256] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	220.00	10	65780.	0.1	0.1	0.0599	56	74.00	17	214892.	0.4	0.4	0.1956*
2	219.00	21	863840.	1.6	1.6	0.7864*	57	73.00	10	14893.	0.0	0.0	0.0136
3	218.00	35	8460544.	15.5	15.5	7.7024*	58	69.00	25	1242304.	2.3	2.3	1.1310
4	217.00	10	23579.	0.0	0.0	0.0215*	59	66.00	21	430752.	0.8	0.8	0.3922
5	216.00	6	1226.	0.0	0.0	0.0011	60	65.00	35	7918080.	14.5	14.5	7.2086*
6	200.00	8	8309.	0.0	0.0	0.0076	61	64.00	25	1276672.	2.3	2.3	1.1623
7	199.00	14	218648.	0.4	0.4	0.1991	62	63.00	35	3256128.	6.0	6.0	2.9644*
8	198.00	6	1459.	0.0	0.0	0.0013	63	62.00	25	996000.	1.8	1.8	0.9068*
9	190.00	8	6279.	0.0	0.0	0.0057	64	61.00	21	388992.	0.7	0.7	0.3541*
10	189.00	10	39530.	0.1	0.1	0.0360	65	60.00	10	33626.	0.1	0.1	0.0306*
11	181.00	6	1492.	0.0	0.0	0.0014	66	59.00	12	53378.	0.1	0.1	0.0486*
12	177.00	6	1401.	0.0	0.0	0.0013	67	55.00	10	5761.	0.0	0.0	0.0052
13	176.00	10	92412.	0.2	0.2	0.0841	68	53.00	17	137988.	0.3	0.3	0.1256*
14	169.00	8	21501.	0.0	0.0	0.0196	69	52.00	25	625808.	1.1	1.1	0.5697
15	159.00	10	18642.	0.0	0.0	0.0170	70	51.00	35	2580800.	4.7	4.7	2.3495
16	153.00	6	2265.	0.0	0.0	0.0021	71	50.00	29	1282112.	2.3	2.3	1.1672
17	150.00	8	1852.	0.0	0.0	0.0017	72	49.00	14	102764.	0.2	0.2	0.0936*
18	135.00	10	67836.	0.1	0.1	0.0618	73	47.00	10	7866.	0.0	0.0	0.0072*
19	133.00	6	1786.	0.0	0.0	0.0016	74	46.00	17	71504.	0.1	0.1	0.0651*
20	131.00	10	28709.	0.1	0.1	0.0261	75	45.00	35	1110208.	2.0	2.0	1.0107*
21	127.00	10	18154.	0.0	0.0	0.0165	76	44.00	25	445440.	0.8	0.8	0.4055*
22	123.00	8	2204.	0.0	0.0	0.0020	77	43.00	12	72568.	0.1	0.1	0.0661*
23	120.00	10	49671.	0.1	0.1	0.0452	78	42.00	17	163352.	0.3	0.3	0.1487*
24	119.00	25	875808.	1.6	1.6	0.7973	79	41.00	25	950880.	1.7	1.7	0.8657*
25	118.00	21	794336.	1.5	1.5	0.7232	80	40.00	21	343760.	0.6	0.6	0.3130*
26	110.00	8	2057.	0.0	0.0	0.0019	81	39.00	35	4575744.	8.4	8.4	4.1657
27	109.00	14	80960.	0.1	0.1	0.0737*	82	38.00	29	822512.	1.5	1.5	0.7488*
28	107.00	14	149424.	0.3	0.3	0.1360*	83	37.00	17	219988.	0.4	0.4	0.2003*
29	106.00	12	106388.	0.2	0.2	0.0969*	84	36.00	17	117796.	0.2	0.2	0.1072*
30	105.00	17	245364.	0.4	0.4	0.2234*	85	35.00	12	12963.	0.0	0.0	0.0118*
31	103.00	8	6897.	0.0	0.0	0.0063							
32	102.00	6	2549.	0.0	0.0	0.0023							
33	100.00	8	2103.	0.0	0.0	0.0019							
34	99.00	6	2014.	0.0	0.0	0.0018							
35	98.00	10	2576.	0.0	0.0	0.0023							
36	96.00	8	3619.	0.0	0.0	0.0033							
37	95.00	6	1420.	0.0	0.0	0.0013							
38	93.00	17	116676.	0.2	0.2	0.1062							
39	92.00	29	4026432.	7.4	7.4	3.6656*							
40	91.00	87	54624256.	100.0	100.0	*49.72*							
41	90.00	35	2076736.	3.8	3.8	1.8907*							
42	89.00	35	2884096.	5.3	5.3	2.6257*							
43	88.00	14	74056.	0.1	0.1	0.0674*							
44	87.00	17	134724.	0.2	0.2	0.1227							
45	86.00	14	133864.	0.2	0.2	0.1219*							
46	85.00	14	45742.	0.1	0.1	0.0416*							
47	84.00	10	29630.	0.1	0.1	0.0270							
48	83.00	25	2255040.	4.1	4.1	2.0530							
49	81.00	8	10417.	0.0	0.0	0.0095							
50	80.00	10	19662.	0.0	0.0	0.0179							
51	79.00	21	353312.	0.6	0.6	0.3217*							
52	78.00	21	384800.	0.7	0.7	0.3503							
53	77.00	25	599744.	1.1	1.1	0.5460							
54	76.00	17	149412.	0.3	0.3	0.1360							
55	75.00	17	176104.	0.3	0.3	0.1603*							

8XAV7.1 [TIC-85888192, 188X-12829952] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	246.00	10	7752.	0.1	0.1	0.0091*	56	88.00	10	16528.	0.1	0.1	0.0194
2	234.00	12	58956.	0.5	0.5	0.0694	57	87.00	17	98444.	0.8	0.8	0.1158
3	233.00	21	726816.	6.0	6.0	0.8551*	58	86.00	12	36487.	0.3	0.3	0.0429
4	232.00	35	6782464.	56.4	56.4	7.9794*	59	85.00	8	7970.	0.1	0.1	0.0094
5	231.00	25	305312.	2.5	2.5	0.3592*	60	84.00	8	6180.	0.1	0.1	0.0073
6	230.00	10	9901.	0.1	0.1	0.0116	61	83.00	43	699456.	5.8	5.8	0.8229*
7	218.00	10	13043.	0.1	0.1	0.0153	62	82.00	12	28712.	0.2	0.2	0.0338*
8	217.00	17	330880.	2.8	2.8	0.3893	63	81.00	8	11448.	0.1	0.1	0.0135
9	214.00	12	39462.	0.3	0.3	0.0464	64	80.00	21	191500.	1.6	1.6	0.2253*
10	213.00	21	426896.	3.5	3.5	0.5022	65	79.00	35	3163648.	26.3	26.3	3.7219*
11	189.00	12	24186.	0.2	0.2	0.0285	66	78.00	29	2395328.	19.9	19.9	2.8180*
12	187.00	14	68844.	0.6	0.6	0.0810	67	77.00	35	5841152.	48.6	48.6	6.8719*
13	181.00	6	4914.	0.0	0.0	0.0058	68	76.00	25	366864.	3.0	3.0	0.4316*
14	173.00	10	12818.	0.1	0.1	0.0151	69	75.00	29	372592.	3.1	3.1	0.4383*
15	169.00	8	13656.	0.1	0.1	0.0161	70	74.00	21	277744.	2.3	2.3	0.3268
16	168.00	8	4871.	0.0	0.0	0.0057	71	73.00	21	14067.	0.1	0.1	0.0165*
17	161.00	8	4435.	0.0	0.0	0.0052	72	69.00	21	651392.	5.4	5.4	0.7663
18	153.00	6	1129.	0.0	0.0	0.0013	73	67.00	10	37377.	0.3	0.3	0.0440*
19	151.00	12	34729.	0.3	0.3	0.0409	74	66.00	35	958112.	7.9	7.9	1.1178*
20	150.00	17	163540.	1.4	1.4	0.1924*	75	65.00	35	1117632.	9.3	9.3	1.3149*
21	149.00	25	1858176.	15.4	15.4	2.1861	76	64.00	25	534096.	4.4	4.4	0.6283*
22	148.00	12	56536.	0.5	0.5	0.0665*	77	63.00	25	1413056.	11.7	11.7	1.6624
23	147.00	17	133420.	1.1	1.1	0.1570*	78	62.00	25	385776.	3.2	3.2	0.4539*
24	137.00	10	9700.	0.1	0.1	0.0115	79	61.00	17	89536.	0.7	0.7	0.1053*
25	135.00	14	90544.	0.8	0.8	0.1065*	80	60.00	12	9820.	0.1	0.1	0.0116*
26	134.00	25	1013024.	8.4	8.4	1.1918*	81	59.00	21	185580.	1.5	1.5	0.2183*
27	133.00	51	12029952.	100.0	100.0	*12.65*	82	57.00	6	598.	0.0	0.0	0.0007
28	132.00	51	10760968.	89.5	89.5	*14.15*	83	55.00	12	51290.	0.4	0.4	0.0603*
29	131.00	17	164272.	1.4	1.4	0.1933*	84	54.00	10	30388.	0.3	0.3	0.0358
30	129.00	8	3781.	0.0	0.0	0.0044	85	53.00	25	863952.	7.2	7.2	1.0164
31	123.00	12	49883.	0.4	0.4	0.0587	86	52.00	29	700640.	5.8	5.8	0.8243*
32	122.00	10	2765.	0.0	0.0	0.0033	87	51.00	43	2918912.	24.3	24.3	3.4340*
33	121.00	17	188464.	1.6	1.6	0.02217	88	50.00	25	916464.	7.6	7.6	1.0782
34	120.00	12	49867.	0.4	0.4	0.0587*	89	49.00	12	43561.	0.4	0.4	0.0512*
35	119.00	21	451472.	3.8	3.8	0.5311	90	45.00	17	111076.	0.9	0.9	0.1307
36	118.00	17	119468.	1.0	1.0	0.1406*	91	44.00	17	171224.	0.8	0.8	0.1109
37	117.00	8	6592.	0.1	0.1	0.0078	92	43.00	21	171224.	1.4	1.4	0.2014*
38	109.00	10	32812.	0.3	0.3	0.0386	93	42.00	8	3845.	0.0	0.0	0.0045
39	107.00	10	25483.	0.2	0.2	0.0300	94	41.00	21	261960.	2.2	2.2	0.3082*
40	106.00	25	764928.	6.4	6.4	0.8999*	95	40.00	21	164024.	1.4	1.4	0.1930
41	105.00	43	9690800.	80.6	80.6	*11.40*	96	39.00	29	1886016.	15.7	15.7	2.2188
42	104.00	35	4354560.	36.2	36.2	5.1230*	97	38.00	29	328016.	2.7	2.7	0.3859*
43	103.00	35	3208448.	26.7	26.7	3.7746*	98	37.00	12	37488.	0.3	0.3	0.0441*
44	102.00	25	521520.	4.3	4.3	0.6136*	99	36.00	21	176812.	1.5	1.5	0.2080*
45	101.00	17	117684.	1.0	1.0	0.1385*	100	35.00	8	3167.	0.0	0.0	0.0037
46	99.00	12	10382.	0.1	0.1	0.0122							
47	98.00	14	17476.	0.1	0.1	0.0206							
48	97.00	8	6969.	0.1	0.1	0.0082							
49	95.00	6	1115.	0.0	0.0	0.0013							
50	94.00	6	3261.	0.0	0.0	0.0038							
51	93.00	21	317472.	2.6	2.6	0.1510*							
52	92.00	17	128392.	1.1	1.1	0.1510*							
53	91.00	25	1318912.	11.0	11.0	1.5517							
54	90.00	21	266752.	2.2	2.2	0.3138							
55	89.00	25	522576.	4.3	4.3	0.6148							

807PA.1 [TIC-82255872, 188X-12686592] EI

2,6-dimethylbenzoic acid
2,2,2-trifluoroethyl ester

BY6AV.1 [TIC-88318464, 188X-18995288] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	234.00	12	39768.	0.4	0.4	0.0495	56	97.00	6	2262.	0.0	0.0	0.0028
2	233.00	21	512496.	4.7	4.7	0.6381*	57	95.00	12	4462.	0.0	0.0	0.0056
3	232.00	43	4492800.	40.9	40.9	5.5937*	58	94.00	8	2541.	0.0	0.0	0.0032
4	231.00	17	114560.	1.0	1.0	0.1426*	59	93.00	17	58583.	0.5	0.5	0.0729*
5	219.00	8	2174.	0.0	0.0	0.0027	60	92.00	21	175536.	1.6	1.6	0.2185
6	218.00	17	164728.	1.5	1.5	0.2051	61	91.00	29	1796736.	16.3	16.3	0.2370*
7	217.00	25	1510784.	13.7	13.7	1.8810*	62	90.00	25	858080.	7.8	7.8	1.0683
8	216.00	10	6467.	0.1	0.1	0.0081	63	89.00	29	1078976.	9.8	9.8	1.3434*
9	215.00	17	72416.	0.7	0.7	0.0902	64	88.00	10	23693.	0.2	0.2	0.0295
10	214.00	10	42753.	0.4	0.4	0.0532	65	87.00	17	82860.	0.8	0.8	0.1032*
11	213.00	21	414176.	3.8	3.8	0.5157	66	86.00	14	28821.	0.3	0.3	0.0359*
12	203.00	10	49834.	0.5	0.5	0.0620	67	85.00	6	1856.	0.0	0.0	0.0023
13	189.00	10	12733.	0.1	0.1	0.0159	68	84.00	12	7140.	0.1	0.1	0.0089*
14	187.00	10	8906.	0.1	0.1	0.0111	69	83.00	29	810064.	7.4	7.4	1.0086*
15	185.00	6	2698.	0.0	0.0	0.0034	70	82.00	14	40760.	0.4	0.4	0.0507*
16	181.00	8	3641.	0.0	0.0	0.0045	71	81.00	17	42500.	0.4	0.4	0.0529*
17	169.00	8	12228.	0.1	0.1	0.0152	72	80.00	25	174280.	1.6	1.6	0.2170*
18	159.00	8	7048.	0.1	0.1	0.0088	73	79.00	25	2458432.	22.4	22.4	3.0609
19	155.00	8	4886.	0.7	0.7	0.0937*	74	78.00	29	1835200.	16.7	16.7	2.2849
20	150.00	14	75232.	0.2	0.2	0.0061	75	77.00	35	5492224.	50.0	50.0	6.8381*
21	149.00	21	874400.	8.0	8.0	1.0887	76	76.00	25	590352.	5.4	5.4	0.7350*
22	148.00	8	17966.	0.2	0.2	0.0224	77	75.00	35	534352.	4.9	4.9	0.6653*
23	147.00	17	77848.	0.7	0.7	0.0965	78	74.00	25	400944.	3.6	3.6	0.4992*
24	139.00	8	3489.	0.0	0.0	0.0043	79	73.00	14	45111.	0.4	0.4	0.0562*
25	138.00	10	17659.	0.2	0.2	0.0220	80	69.00	25	547440.	5.0	5.0	0.6816
26	137.00	21	307600.	2.8	2.8	0.3830	81	66.00	25	255484.	2.3	2.3	0.3181*
27	136.00	17	60828.	0.6	0.6	0.0757*	82	65.00	35	814592.	7.4	7.4	1.0142*
28	135.00	21	761056.	6.9	6.9	0.9475	83	64.00	25	561472.	5.1	5.1	0.6991*
29	134.00	25	638944.	5.8	5.8	0.7955*	84	63.00	25	1374272.	12.5	12.5	1.7110
30	133.00	51	7280896.	56.2	56.2	9.0650*	85	62.00	25	331456.	3.0	3.0	0.4127
31	132.00	59	10995200.	100.0	100.0	*13.68*	86	61.00	17	124720.	1.1	1.1	0.1553
32	131.00	51	6563584.	59.7	59.7	8.1719*	87	60.00	8	6887.	0.1	0.1	0.0086
33	130.00	35	148300.	1.3	1.3	0.1846*	88	59.00	25	269008.	2.4	2.4	0.3349*
34	129.00	6	35368.	0.3	0.3	0.0440	89	57.00	6	8661.	0.1	0.1	0.0108
35	127.00	8	7884.	0.1	0.1	0.0098	90	55.00	25	272896.	2.5	2.5	0.3398
36	121.00	8	11727.	0.1	0.1	0.0146	91	54.00	6	2497.	0.0	0.0	0.0031
37	120.00	12	40735.	0.4	0.4	0.0507	92	53.00	29	402784.	3.7	3.7	0.5015
38	119.00	25	298288.	2.7	2.7	0.3714	93	52.00	25	513184.	4.7	4.7	0.6389
39	118.00	17	158572.	1.4	1.4	0.1974*	94	51.00	35	2678400.	24.4	24.4	3.3347*
40	117.00	10	9706.	0.1	0.1	0.0121	95	50.00	25	1066304.	9.7	9.7	1.3276*
41	116.00	12	25184.	0.2	0.2	0.0314	96	49.00	14	47568.	0.4	0.4	0.0592*
42	115.00	25	284384.	2.6	2.6	0.3541*	97	48.00	6	1054.	0.0	0.0	0.0013
43	113.00	10	3124.	0.1	0.1	0.0039	98	45.00	25	234732.	2.1	2.1	0.2923*
44	110.00	10	12146.	0.1	0.1	0.0151	99	44.00	21	90632.	0.8	0.8	0.1128*
45	109.00	21	465424.	4.2	4.2	0.5795	100	43.00	25	252212.	2.3	2.3	0.3140*
46	107.00	12	33020.	0.3	0.3	0.0411*	101	41.00	21	126600.	1.2	1.2	0.1576*
47	106.00	25	407440.	3.7	3.7	0.5073	102	40.00	29	169384.	1.5	1.5	0.2109*
48	105.00	43	4824064.	43.9	43.9	6.0062*	103	39.00	25	1343168.	12.2	12.2	1.6723
49	104.00	35	4250368.	38.7	38.7	5.2919*	104	38.00	25	259744.	2.4	2.4	0.3234
50	103.00	35	4902144.	44.6	44.6	6.1034*	105	37.00	17	47077.	0.4	0.4	0.0566*
51	102.00	25	585520.	5.3	5.3	0.7290*	106	36.00	14	35716.	0.3	0.3	0.0445*
52	101.00	29	210144.	1.9	1.9	0.2616*							
53	100.00	6	1731.	0.0	0.0	0.0022							
54	99.00	10	50812.	0.5	0.5	0.0633*							
55	98.00	10	21591.	0.2	0.2	0.0269							

FVAHV.1 [TIC-60430336, 100X=28F44208] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	234.00	12	34947.	0.1	0.1	0.0578*	56	87.00	14	46720.	0.2	0.2	0.0773*
2	233.00	25	464064.	1.7	1.7	0.7679*	57	86.00	10	18243.	0.1	0.1	0.0302*
3	232.00	35	4216320.	15.0	15.0	6.9772*	58	85.00	10	5681.	0.0	0.0	0.0094
4	231.00	17	70768.	0.3	0.3	0.1171*	59	84.00	8	15643.	0.1	0.1	0.0259*
5	230.00	12	6817.	0.0	0.0	0.0113*	60	83.00	35	1081472.	3.9	3.9	1.7896*
6	214.00	10	10100.	0.0	0.0	0.0167	61	82.00	8	1383.	0.0	0.0	0.0023
7	213.00	17	169848.	0.6	0.6	0.2811	62	81.00	8	8157.	0.0	0.0	0.0135
8	203.00	14	40640.	0.1	0.1	0.0673	63	80.00	21	153624.	0.5	0.5	0.2542*
9	202.00	8	1238.	0.0	0.0	0.0020	64	79.00	35	2232832.	8.0	8.0	3.6949*
10	190.00	12	22483.	0.1	0.1	0.0372	65	78.00	35	1727104.	6.2	6.2	2.8580*
11	189.00	21	130364.	0.5	0.5	0.2157	66	77.00	35	3424384.	12.2	12.2	5.6667*
12	187.00	10	2570.	0.0	0.0	0.0043	67	76.00	25	224400.	0.8	0.8	0.3713*
13	181.00	6	1446.	0.0	0.0	0.0024	68	75.00	25	198956.	0.7	0.7	0.3292*
14	173.00	8	4709.	0.0	0.0	0.0078*	69	74.00	25	191476.	0.7	0.7	0.3169*
15	169.00	10	5110.	0.0	0.0	0.0085	70	73.00	10	13816.	0.0	0.0	0.0229*
16	167.00	8	1783.	0.0	0.0	0.0030	71	69.00	29	424720.	1.5	1.5	0.7028*
17	163.00	6	946.	0.0	0.0	0.0016	72	67.00	6	2316.	0.0	0.0	0.0038
18	149.00	14	57667.	0.2	0.2	0.0954*	73	66.00	35	171224.	0.6	0.6	0.2833*
19	148.00	8	1104.	0.0	0.0	0.0018	74	65.00	29	611680.	2.2	2.2	1.0122
20	147.00	10	18311.	0.1	0.1	0.0303*	75	64.00	29	317792.	1.1	1.1	0.5259*
21	137.00	6	1959.	0.0	0.0	0.0032	76	63.00	35	902880.	3.2	3.2	1.4941*
22	133.00	8	5889.	0.0	0.0	0.0097	77	62.00	25	255804.	0.9	0.9	0.4233
23	134.00	21	143876.	0.5	0.5	0.2381*	78	61.00	17	78224.	0.3	0.3	0.1294*
24	132.00	25	242896.	0.9	0.9	0.4019*	79	60.00	17	22992.	0.1	0.1	0.0380*
25	131.00	17	78360.	0.3	0.3	0.1297*	80	59.00	17	28741.	0.1	0.1	0.0476*
26	127.00	10	6093.	0.0	0.0	0.0101	81	58.00	10	7269.	0.0	0.0	0.0146*
27	123.00	10	15531.	0.1	0.1	0.0257*	82	57.00	8	8036.	0.0	0.0	0.0120*
28	122.00	10	3170.	0.0	0.0	0.0052	83	56.00	12	9346.	0.0	0.0	0.0155*
29	121.00	17	56659.	0.2	0.2	0.0938*	84	55.00	8	8100.	0.0	0.0	0.0134
30	120.00	12	30134.	0.1	0.1	0.0499*	85	54.00	17	24700.	0.1	0.1	0.0409*
31	119.00	21	148072.	0.5	0.5	0.2450*	86	53.00	35	572352.	2.0	2.0	0.9471*
32	118.00	10	4011.	0.0	0.0	0.0066	87	52.00	59	1136000.	4.1	4.1	1.8799*
33	117.00	6	1409.	0.0	0.0	0.0023	88	51.00	51	1942400.	6.9	6.9	3.2143*
34	115.00	6	2009.	0.0	0.0	0.0033	89	50.00	35	649968.	2.3	2.3	1.0756*
35	109.00	6	2311.	0.0	0.0	0.0038	90	49.00	12	27901.	0.1	0.1	0.0462*
36	108.00	8	2631.	0.0	0.0	0.0044	91	48.00	12	7981.	0.0	0.0	0.0132*
37	107.00	21	117028.	0.4	0.4	0.1937*	92	47.00	12	11911.	0.0	0.0	0.0197*
38	106.00	35	2299328.	8.2	8.2	3.8049*	93	45.00	14	33052.	0.1	0.1	0.0547*
39	105.00	71	28044288.	100.0	100.0	46.40*	94	44.00	21	113544.	0.4	0.4	0.1879*
40	104.00	59	1584256.	5.6	5.6	2.6216*	95	43.00	12	6666.	0.0	0.0	0.1160*
41	103.00	43	1966080.	7.0	7.0	3.2535*	96	42.00	17	70076.	0.2	0.2	0.1160*
42	102.00	35	306288.	1.1	1.1	0.5068*	97	41.00	21	161720.	0.5	0.5	0.2676*
43	101.00	35	139860.	0.5	0.5	0.2314*	98	40.00	25	149584.	0.5	0.5	0.2475*
44	100.00	8	7570.	0.0	0.0	0.0125	99	39.00	25	1342592.	4.8	4.8	2.2217*
45	99.00	6	767.	0.0	0.0	0.0013	100	38.00	25	216264.	0.8	0.8	0.3579*
46	98.00	8	7635.	0.0	0.0	0.0126	101	37.00	14	39584.	0.1	0.1	0.0655*
47	97.00	6	1752.	0.0	0.0	0.0029	102	36.00	25	122716.	0.4	0.4	0.2031*
48	96.00	8	1304.	0.0	0.0	0.0022	103	35.00	10	14093.	0.1	0.1	0.0233*
49	95.00	6	1312.	0.0	0.0	0.0022							
50	93.00	21	86788.	0.3	0.3	0.1436*							
51	92.00	17	72628.	0.3	0.3	0.1202*							
52	91.00	29	503664.	1.8	1.8	0.8335*							
53	90.00	21	133721.	0.5	0.5	0.2213*							
54	89.00	25	310320.	1.1	1.1	0.5135*							
55	88.00	8	2170.	0.0	0.0	0.0036							

087AV.1 [TIC-97148928, 158X-38519296] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	248.00	8	27616.	0.1	0.1	0.0284	56	98.00	6	7205.	0.0	0.0	0.0074
2	247.00	17	440496.	1.4	1.4	0.4534*	57	97.00	17	27974.	0.1	0.1	0.0288*
3	246.00	35	3768064.	12.3	12.3	3.8786*	58	93.00	12	58617.	0.2	0.2	0.0603*
4	231.00	8	12113.	0.0	0.0	0.0125	59	92.00	25	2189760.	7.2	100.0	*31.41*
5	227.00	14	113592.	0.4	0.4	0.1169	60	91.00	59	30519296.	100.0	0.0	1.5531*
6	219.00	10	41035.	0.1	0.1	0.0422	61	90.00	25	1508864.	4.9	4.9	0.0412*
7	218.00	17	332544.	1.1	1.1	0.3423	62	89.00	25	1350528.	4.4	4.4	0.0968*
8	217.00	17	273040.	0.9	0.9	0.2811	63	88.00	10	40042.	0.1	0.1	0.0435*
9	198.00	8	19383.	0.1	0.1	0.0200	64	87.00	14	93992.	0.3	0.3	0.0032
10	191.00	8	1448.	0.0	0.0	0.0015	65	86.00	10	42269.	0.1	0.1	0.0034
11	190.00	14	133580.	0.4	0.4	0.1375	66	85.00	8	3296.	0.0	0.0	0.00372
12	189.00	25	1670720.	5.5	5.5	1.7198	67	84.00	10	36119.	0.1	0.1	0.00372
13	185.00	12	102792.	0.3	0.3	0.1058*	68	83.00	29	2480512.	8.1	8.1	0.0117*
14	181.00	8	1732.	0.0	0.0	0.0018	69	81.00	12	11366.	0.0	0.0	0.0892*
15	176.00	8	3105.	0.0	0.0	0.0032	70	80.00	12	86664.	0.3	0.3	0.0892*
16	169.00	8	7183.	0.0	0.0	0.0074	71	79.00	25	1301824.	4.3	4.3	1.3400
17	159.00	10	331.	0.0	0.0	0.0034	72	78.00	25	1715520.	5.6	5.6	1.7659*
18	155.00	8	2391.	0.0	0.0	0.0025	73	77.00	23	2540736.	8.3	8.3	2.6153
19	153.00	8	3601.	0.0	0.0	0.0037	74	76.00	21	305888.	1.0	1.0	0.3149*
20	147.00	10	41082.	0.1	0.1	0.0423	75	75.00	17	233872.	0.8	0.8	0.2407*
21	146.00	14	126640.	0.4	0.4	0.1304*	76	74.00	17	193508.	0.6	0.6	0.1992*
22	145.00	8	1146.	0.0	0.0	0.0012	77	73.00	8	12909.	0.0	0.0	0.0133
23	144.00	6	1712.	0.0	0.0	0.0018	78	70.00	43	221616.	0.7	0.7	0.2281*
24	142.00	8	3476.	0.0	0.0	0.0036	79	69.00	35	703536.	2.5	2.5	0.7242*
25	141.00	8	14833.	0.0	0.0	0.0153	80	68.00	8	6951.	0.0	0.0	0.0072
26	135.00	14	99272.	0.3	0.3	0.1022	81	67.00	6	3483.	0.0	0.0	0.0036
27	134.00	8	30039.	0.1	0.1	0.0309	82	66.00	14	94256.	0.3	0.3	0.0970*
28	133.00	12	40684.	0.1	0.1	0.0419*	83	65.00	25	1540608.	5.0	5.0	1.5858*
29	132.00	8	6116.	0.0	0.0	0.0063	84	64.00	25	575024.	1.9	1.9	0.5919
30	131.00	17	180292.	0.6	0.6	0.1856*	85	63.00	29	1393920.	4.6	4.6	1.4348
31	129.00	8	1314.	0.0	0.0	0.0014	86	62.00	21	338832.	1.1	1.1	0.3488*
32	129.00	8	1609.	0.0	0.0	0.0017	87	61.00	12	80340.	0.3	0.3	0.0827
33	128.00	8	5138.	0.0	0.0	0.0053	88	60.00	8	1469.	0.0	0.0	0.0015
34	127.00	14	95904.	0.3	0.3	0.0987	89	59.00	12	45537.	0.1	0.1	0.0469*
35	121.00	14	62044.	0.2	0.2	0.0639*	90	58.00	17	69376.	0.2	0.2	0.0714*
36	120.00	29	1569600.	5.1	5.1	1.6157*	91	57.00	17	127092.	0.4	0.4	0.1308*
37	119.00	51	17602560.	57.7	57.7	*18.11*	92	56.00	6	2335.	0.0	0.0	0.0024
38	118.00	25	1548544.	5.1	5.1	1.5940*	93	55.00	14	113696.	0.4	0.4	0.1170*
39	117.00	29	1563648.	5.1	5.1	1.6095*	94	54.00	8	2142.	0.0	0.0	0.0022
40	116.00	21	355536.	1.2	1.2	0.3660*	95	53.00	21	222992.	0.7	0.7	0.2295*
41	115.00	25	1510720.	5.0	5.0	1.5551*	96	52.00	25	508384.	1.7	1.7	0.5232
42	114.00	12	11742.	0.0	0.0	0.0121*	97	51.00	29	2193472.	7.2	7.2	2.2578
43	113.00	10	23159.	0.1	0.1	0.0238*	98	50.00	25	695008.	2.3	2.3	0.7154*
44	111.00	8	1178.	0.0	0.0	0.0012	99	49.00	6	12394.	0.0	0.0	0.0128
45	110.00	8	23885.	0.1	0.1	0.0246	100	47.00	8	12302.	0.0	0.0	0.0127
46	109.00	25	693168.	2.3	2.3	0.7135	101	46.00	6	1023.	0.0	0.0	0.0011
47	108.00	6	2578.	0.0	0.0	0.0027	102	45.00	17	151536.	0.5	0.5	0.1560*
48	107.00	17	256328.	0.8	0.8	0.2639*	103	44.00	17	194936.	0.6	0.6	0.2007*
49	106.00	14	124792.	0.4	0.4	0.4285	104	43.00	12	59628.	0.2	0.2	0.0614*
50	105.00	21	720640.	2.4	2.4	0.7418	105	42.00	12	78336.	0.3	0.3	0.0806*
51	104.00	25	1467520.	4.8	4.8	1.5106*	106	41.00	29	3128960.	10.3	10.3	3.2208
52	103.00	25	1439296.	4.7	4.7	1.4815	107	40.00	17	181956.	0.6	0.6	0.1873*
53	102.00	17	337744.	1.1	1.1	0.3477*	108	39.00	29	2280320.	7.5	7.5	2.3472
54	101.00	12	63206.	0.2	0.2	0.0651*	109	38.00	25	250484.	0.8	0.8	0.2578*
55	100.00	6	1532.	0.0	0.0	0.0016	110	37.00	8	14373.	0.0	0.0	0.0148

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	36.00	12	87688.	0.3	0.3	0.0903*
112	35.00	14	9011.	0.5	0.0	0.0093*

8V7AV.1 [TIC-98476544, 188X-33825824] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	1221.	0.1	0.0	0.0013	56	89.00	21	292976.	0.9	0.9	0.3238
2	248.00	10	24282.	0.1	0.1	0.0268	57	88.00	10	7386.	0.0	0.0	0.0032
3	247.00	21	381616.	1.2	0.1	0.0268*	58	87.00	12	22307.	0.1	0.1	0.0247*
4	246.00	35	3028224.	9.2	9.2	3.3470	59	86.00	10	18119.	0.1	0.1	0.0200*
5	231.00	12	62818.	0.2	0.2	0.0694	60	85.00	12	10583.	0.0	0.0	0.0117
6	229.00	6	1840.	0.0	0.0	0.0020	61	84.00	10	19018.	0.1	0.1	0.0210
7	203.00	17	117324.	0.4	0.4	0.1297	62	83.00	35	2172800.	6.6	6.6	2.4015
8	191.00	6	9468.	0.0	0.0	0.0105	63	81.00	6	1885.	0.0	0.0	0.0021
9	190.00	17	280896.	0.9	0.9	0.3105	64	80.00	21	170112.	0.5	0.5	0.1880*
10	189.00	29	3337088.	10.1	10.1	3.6883*	65	79.00	29	2611840.	7.9	7.9	2.8868
11	188.00	8	1461.	0.0	0.0	0.0016	66	78.00	35	2211200.	6.7	6.7	2.4439*
12	181.00	6	1156.	0.0	0.0	0.0013	67	77.00	21	4074944.	12.3	12.3	4.5039*
13	169.00	10	9091.	0.0	0.0	0.0100	68	76.00	21	316944.	1.0	1.0	0.3503
14	165.00	6	1730.	0.0	0.0	0.0019	69	75.00	21	240736.	0.7	0.7	0.2661*
15	149.00	8	3203.	0.0	0.0	0.0035	70	74.00	21	212796.	0.6	0.6	0.2352*
16	148.00	14	71124.	0.2	0.2	0.0786	71	73.00	29	212780.	0.6	0.6	0.0019
17	147.00	21	39657.	0.1	0.1	0.0438	72	72.00	6	1678.	0.0	0.0	0.0019
18	146.00	10	53024.	0.2	0.2	0.08465	73	69.00	29	480928.	1.5	1.5	0.5315
19	145.00	14	1170.	0.0	0.0	0.0586*	74	67.00	10	6753.	0.0	0.0	0.0075
20	144.00	6	23210.	0.0	0.0	0.0013	75	66.00	14	80880.	0.2	0.2	0.0894*
21	142.00	10	1963.	0.1	0.1	0.0257	76	65.00	25	773424.	2.3	2.3	0.8548
22	141.00	6	1991.	0.0	0.0	0.0022	77	64.00	25	238532.	0.7	0.7	0.2636
23	135.00	6	14743.	0.0	0.0	0.0022	78	63.00	25	758976.	2.3	2.3	0.8389
24	133.00	8	33656.	0.1	0.1	0.0163	79	62.00	21	161332.	0.5	0.5	0.1783*
25	132.00	10	38480.	1.2	0.1	0.0372*	80	61.00	17	99704.	0.3	0.3	0.1102*
26	129.00	8	5540.	0.0	1.2	0.4294	81	59.00	8	2708.	0.0	0.0	0.0030
27	128.00	8	4593.	0.0	0.0	0.0051	82	58.00	21	82360.	0.2	0.2	0.0910*
28	127.00	17	72488.	0.2	0.0	0.0051	83	58.00	35	260536.	0.8	0.8	0.2880*
29	123.00	10	22639.	0.1	0.1	0.0250*	84	57.00	43	301456.	0.9	0.9	0.3332*
30	122.00	10	41587.	0.1	0.1	0.0460*	85	56.00	12	21588.	0.1	0.1	0.0239*
31	121.00	21	351088.	1.1	1.1	0.3800	86	55.00	12	24917.	0.1	0.1	0.0275
32	120.00	14	64405.	0.2	0.2	0.0712*	87	53.00	21	267792.	0.8	0.8	0.2960
33	119.00	25	1095744.	3.3	3.3	1.2111*	88	52.00	25	561312.	1.7	1.7	0.6204
34	118.00	51	8188160.	24.8	24.8	9.0500*	89	51.00	35	2372352.	7.2	7.2	2.6221*
35	117.00	29	1333760.	4.0	4.0	1.4742*	90	50.00	25	711216.	2.2	2.2	0.7861*
36	116.00	35	251188.	0.8	0.8	0.2776*	91	49.00	10	8119.	0.0	0.0	0.0090
37	115.00	25	725776.	2.2	2.2	0.8022	92	47.00	8	11263.	0.0	0.0	0.0124
38	114.00	8	2173.	0.0	0.0	0.0024	93	45.00	14	46952.	0.1	0.1	0.0519
39	113.00	8	13657.	0.0	0.0	0.0015	94	44.00	17	92128.	0.3	0.3	0.1018*
40	110.00	6	1073.	0.0	0.0	0.0012	95	43.00	25	472656.	1.4	1.4	0.5224
41	109.00	21	186572.	0.6	0.6	0.2062	96	42.00	29	882496.	2.7	2.7	0.9754
42	107.00	21	145220.	0.4	0.4	0.1605*	97	41.00	35	1288576.	3.9	3.9	1.4242*
43	106.00	35	2691776.	8.2	8.2	2.9751*	98	40.00	29	160140.	0.5	0.5	0.1770*
44	105.00	71	33025024.	100.0	100.0	*36.50*	99	39.00	29	1633152.	4.9	4.9	1.8051
45	104.00	43	2465184.	7.5	7.5	2.7291*	100	38.00	21	155800.	0.5	0.5	0.1722*
46	102.00	35	2976256.	9.0	9.0	3.2895*	101	37.00	12	17744.	0.1	0.1	0.0196*
47	102.00	25	431552.	1.3	1.3	0.4770*	102	36.00	14	39699.	0.1	0.1	0.0439*
48	101.00	21	96868.	0.3	0.3	0.1071*							
49	98.00	8	2278.	0.0	0.0	0.0025							
50	97.00	6	1606.	0.0	0.0	0.0018							
51	93.00	8	7867.	0.0	0.0	0.0087							
52	92.00	21	210536.	0.6	0.6	0.0327*							
53	91.00	29	2725504.	8.3	8.3	3.0124							
54	91.00	12	63894.	0.2	0.2	0.0706*							
55	90.00												

8XAV8.1 [TIC-128884688, 188X-36115456] E1

4-phenylbutyric acid,
2,2,2-trifluoroethyl ester

A-137

808PA.1 [TIC-81846272, 188X-15967488] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	281.00	6	1178.	0.0	0.0	0.0014
2	248.00	14	80412.	0.5	0.5	0.0982*
3	247.00	21	923408.	5.8	5.8	1.1282*
4	246.00	43	7215616.	45.2	45.2	8.8161*
5	245.00	21	277440.	1.7	1.7	0.3390
6	232.00	10	11221.	0.1	0.1	0.0137
7	231.00	17	215264.	1.3	1.3	0.2630
8	228.00	10	42152.	0.3	0.3	0.0515
9	227.00	17	413808.	2.6	2.6	0.5056
10	219.00	8	4756.	0.0	0.0	0.0058
11	217.00	10	36976.	0.2	0.2	0.0452
12	183.00	6	8694.	0.1	0.1	0.0106
13	181.00	8	3897.	0.0	0.0	0.0048
14	175.00	8	15105.	0.1	0.1	0.0185
15	169.00	8	20232.	0.1	0.1	0.0247
16	165.00	8	10404.	0.1	0.1	0.0127
17	164.00	12	55060.	0.3	0.3	0.0673
18	163.00	21	609408.	3.8	3.8	0.7446
19	162.00	12	46820.	0.3	0.3	0.0572*
20	161.00	17	130756.	0.9	0.9	0.1695
21	159.00	6	968.	0.0	0.0	0.0012
22	155.00	6	1273.	0.0	0.0	0.0016
23	150.00	6	963.	0.0	0.0	0.0012
24	149.00	17	123520.	0.8	0.8	0.1509
25	148.00	35	1642048.	10.3	10.3	2.0063*
26	147.00	59	15967488.	100.0	100.0	*12.57*
27	146.00	51	10290176.	64.4	64.4	0.0933*
28	145.00	14	76372.	0.5	0.5	0.0027
29	142.00	8	2189.	0.0	0.0	0.0071*
30	137.00	10	33112.	0.2	0.2	0.0405
31	135.00	14	58222.	0.4	0.4	0.0711*
32	134.00	17	47888.	0.3	0.3	0.0585*
33	133.00	17	189780.	1.2	1.2	0.2319
34	132.00	14	69224.	0.4	0.4	0.0846*
35	131.00	12	66268.	0.0	0.0	0.0810*
36	123.00	6	1961.	0.0	0.0	0.0024
37	121.00	10	23196.	0.1	0.1	0.0283
38	120.00	25	652000.	4.1	4.1	0.7966
39	119.00	43	6953216.	43.5	43.5	8.4955*
40	118.00	29	2231552.	14.0	14.0	2.7265*
41	117.00	43	2436096.	15.3	15.3	2.9764*
42	116.00	29	402224.	2.5	2.5	0.4914*
43	115.00	35	1424704.	8.9	8.9	1.7407*
44	114.00	12	19654.	0.1	0.1	0.0240*
45	113.00	10	29709.	0.2	0.2	0.0363*
46	109.00	8	2189.	0.0	0.0	0.0027
47	107.00	21	198484.	1.2	1.2	0.2425
48	106.00	14	58803.	0.4	0.4	0.0719*
49	105.00	21	497648.	3.1	3.1	0.6080
50	104.00	21	978672.	6.1	6.1	1.1957
51	103.00	25	1677312.	10.5	10.5	2.0493
52	102.00	21	316096.	2.6	2.6	0.3862
53	101.00	10	41145.	0.3	0.3	0.0503
54	100.00	6	2014.	0.0	0.0	0.0025
55	99.00	6	1131.	0.0	0.0	0.0014

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
56	98.00	8	7112.	0.0	0.0	0.0087
57	97.00	12	30121.	0.2	0.2	0.0368*
58	96.00	21	63837.	0.4	0.4	0.0780*
59	95.00	10	23575.	0.1	0.1	0.0288*
60	94.00	8	935.	0.0	0.0	0.0011
61	93.00	21	296208.	1.9	1.9	0.3619
62	92.00	21	433808.	2.7	2.7	0.5300
63	91.00	29	4548352.	28.5	28.5	5.5572*
64	90.00	17	122264.	0.8	0.8	0.1494*
65	89.00	21	316432.	2.0	2.0	0.3866
66	88.00	10	21960.	0.1	0.1	0.0268
67	87.00	17	95984.	0.6	0.6	0.1173*
68	86.00	12	41991.	0.3	0.3	0.0513*
69	85.00	8	1558.	0.0	0.0	0.0019
70	83.00	21	519120.	3.3	3.3	0.6343
71	81.00	8	4634.	0.0	0.0	0.0057
72	80.00	14	68180.	0.4	0.4	0.0833*
73	79.00	25	916480.	5.7	5.7	1.1198
74	78.00	25	953568.	6.0	6.0	1.1651*
75	77.00	29	2454528.	15.4	15.4	2.9989*
76	76.00	21	175416.	1.1	1.1	0.2143*
77	75.00	21	237444.	1.5	1.5	0.2901*
78	74.00	25	250912.	1.6	1.6	0.3066*
79	73.00	43	939168.	5.9	5.9	1.1475*
80	72.00	12	47973.	0.3	0.3	0.0586*
81	70.00	6	6061.	0.0	0.0	0.0074
82	69.00	25	631568.	4.0	4.0	0.7717
83	67.00	21	155604.	1.0	1.0	0.1901*
84	66.00	25	444144.	2.8	2.8	0.5427*
85	65.00	35	1277312.	8.0	8.0	1.5606*
86	64.00	25	354064.	2.2	2.2	0.4326
87	63.00	25	836256.	5.2	5.2	1.0217
88	62.00	21	230288.	1.4	1.4	0.2814*
89	61.00	12	55038.	0.3	0.3	0.0672*
90	59.00	10	32559.	0.2	0.2	0.0398*
91	58.00	35	525152.	3.3	3.3	0.6416*
92	57.00	35	393632.	2.5	2.5	0.4809*
93	55.00	17	97164.	0.6	0.6	0.1187*
94	54.00	12	43130.	0.3	0.3	0.0527*
95	53.00	25	696240.	4.4	4.4	0.8507
96	52.00	25	547824.	3.4	3.4	0.6693
97	51.00	29	1648960.	10.3	10.3	2.0147*
98	50.00	25	457920.	2.9	2.9	0.5595
99	49.00	6	1791.	0.0	0.0	0.0022
100	45.00	10	41090.	0.3	0.3	0.0502
101	44.00	14	65952.	0.4	0.4	0.0806*
102	43.00	25	211528.	1.3	1.3	0.2584*
103	42.00	10	31470.	0.2	0.2	0.0385*
104	41.00	29	1573248.	9.9	9.9	1.9222
105	40.00	29	269344.	1.7	1.7	0.3291*
106	39.00	29	1759168.	11.0	11.0	2.1494
107	38.00	21	159032.	1.0	1.0	0.1943*
108	37.00	8	5901.	0.0	0.0	0.0072
109	36.00	14	75416.	0.5	0.5	0.0921*
110	35.00	10	2076.	0.0	0.0	0.0025

PAGE	3	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
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BH9AV.1 [TIC=106319872, 100X=33700064] EI

5-phenylpentanoic acid,

2,2,2-trifluoroethyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	262.00	10	10280.	0.0	0.0	0.0097	56	98.00	14	9893.	0.0	0.0	0.0093*
2	261.00	17	282640.	0.0	0.0	0.2658*	57	95.00	6	712.	0.0	0.0	0.0007
3	260.00	21	2224576.	6.6	6.6	2.0923	58	93.00	21	283376.	0.0	0.0	0.2665*
4	203.00	6	2166.	0.0	0.0	0.0020	59	92.00	35	5186304.	15.4	15.4	4.8780*
5	189.00	8	2201.	0.0	0.0	0.0021	60	91.00	59	33700864.	100.0	100.0	*31.69*
6	178.00	8	33837.	0.1	0.1	0.0318*	61	90.00	25	408336.	1.2	1.2	0.3841*
7	169.00	21	774560.	2.3	2.3	0.07285	62	89.00	25	686048.	2.0	2.0	0.6453
8	163.00	10	12538.	0.0	0.0	0.0118	63	87.00	10	30344.	0.1	0.1	0.0285*
9	162.00	17	248268.	0.7	0.7	0.2335*	64	86.00	8	12967.	0.0	0.0	0.0122
10	161.00	25	2381760.	7.1	7.1	2.2402*	65	85.00	6	1639.	0.0	0.0	0.0015
11	159.00	35	58823.	0.2	0.2	0.0553	66	84.00	10	26262.	0.1	0.1	0.0247*
12	156.00	8	20386.	0.1	0.1	0.0192	67	83.00	25	2809216.	8.3	8.3	2.6422
13	155.00	17	253436.	0.0	0.0	0.2384*	68	82.00	10	33532.	0.1	0.1	0.0315*
14	149.00	6	2517.	0.0	0.0	0.0024	69	81.00	21	225884.	0.7	0.7	0.2125*
15	145.00	12	67280.	0.2	0.2	0.0633*	70	80.00	25	235180.	0.7	0.7	0.2212*
16	144.00	8	3952.	0.0	0.0	0.0037	71	79.00	25	1158592.	3.4	3.4	1.0897
17	143.00	17	178480.	0.5	0.5	0.1679	72	78.00	29	2395008.	7.1	7.1	2.2526
18	142.00	25	1103168.	3.3	3.3	1.0376	73	77.00	25	2323776.	6.9	6.9	2.1856
19	141.00	8	19955.	0.1	0.1	0.0188*	74	76.00	17	189836.	0.6	0.6	0.1786*
20	140.00	8	780.	0.0	0.0	0.0007	75	75.00	17	172836.	0.5	0.5	0.1628*
21	139.00	12	45427.	0.1	0.1	0.0427	76	74.00	17	138160.	0.4	0.4	0.1299*
22	137.00	8	1223.	0.0	0.0	0.0012	77	73.00	10	8411.	0.1	0.1	0.0079
23	136.00	8	14636.	0.0	0.0	0.0138	78	70.00	12	39053.	0.1	0.1	0.0367
24	135.00	17	227976.	0.7	0.7	0.2144*	79	69.00	25	599824.	1.8	1.8	0.5642*
25	134.00	8	11144.	0.0	0.0	0.0105*	80	68.00	6	5965.	0.0	0.0	0.0056
26	133.00	21	404864.	1.2	1.2	0.3808	81	67.00	12	48123.	0.1	0.1	0.0453*
27	132.00	25	2238976.	6.6	6.6	2.1059	82	66.00	25	310816.	0.9	0.9	0.2923*
28	131.00	21	314816.	0.9	0.9	0.2961*	83	65.00	29	4294144.	12.7	12.7	4.0389*
29	129.00	21	530480.	1.6	1.6	0.4989	84	64.00	25	535728.	3.1	3.1	0.9783
30	128.00	17	31776.	0.9	0.9	0.2932*	85	63.00	25	1046160.	0.5	0.5	0.1559*
31	127.00	25	1378368.	4.1	4.1	1.2964	86	62.00	17	165804.	0.5	0.5	0.1580*
32	126.00	10	6025.	0.0	0.0	0.0057*	87	61.00	17	160296.	0.0	0.0	0.0027
33	123.00	6	1508.	0.0	0.0	0.0014	88	60.00	8	2848.	0.0	0.0	0.0149*
34	122.00	17	139264.	0.4	0.4	0.1310*	89	59.00	12	15866.	0.1	0.1	0.0295*
35	121.00	6	2123.	0.0	0.0	0.0020	90	58.00	12	31315.	0.1	0.1	0.0295*
36	120.00	8	8979.	0.0	0.0	0.0084	91	57.00	21	175056.	0.5	0.5	0.1647*
37	119.00	21	462976.	1.4	1.4	0.4355*	92	56.00	17	115560.	0.3	0.3	0.1087*
38	118.00	25	1865664.	5.5	5.5	1.7548	93	55.00	29	960784.	2.9	2.9	0.9037
39	117.00	35	4009024.	11.9	11.9	3.7707*	94	54.00	12	44390.	0.1	0.1	0.0416*
40	116.00	21	396352.	1.2	1.2	0.3728	95	53.00	21	373040.	1.1	1.1	0.3509*
41	115.00	21	869616.	2.6	2.6	0.8179	96	52.00	25	488912.	1.5	1.5	0.4599
42	114.00	6	1420.	0.0	0.0	0.0013	97	51.00	29	2025472.	6.0	6.0	1.9051
43	113.00	12	47726.	0.1	0.1	0.0449*	98	50.00	25	624976.	1.9	1.9	0.5878*
44	110.00	6	3001.	0.0	0.0	0.0028	99	49.00	10	6018.	0.0	0.0	0.0057
45	109.00	17	157996.	0.5	0.5	0.1486*	100	48.00	14	77312.	0.2	0.2	0.0727*
46	108.00	6	7979.	0.0	0.0	0.0075	101	46.00	12	5590.	0.0	0.0	0.0053*
47	107.00	17	215920.	0.6	0.6	0.2031	102	45.00	17	106872.	0.3	0.3	0.1005*
48	106.00	29	2708032.	8.0	8.0	2.5471*	103	44.00	25	2108956.	0.6	0.6	0.1934*
49	105.00	35	6593280.	19.6	19.6	6.2014*	104	43.00	25	1515632.	1.5	1.5	0.4850*
50	104.00	29	1218368.	3.6	3.6	1.1459*	105	42.00	35	1617792.	4.8	4.8	1.5216
51	103.00	17	262416.	0.8	0.8	0.2468	106	41.00	29	1499520.	4.4	4.4	1.4104
52	102.00	10	20728.	0.1	0.1	0.0195	107	40.00	25	262028.	0.8	0.8	0.2455*
53	101.00	17	8868.	0.0	0.0	0.0083*	108	39.00	25	252768.	7.6	7.6	2.4010
54	99.00	17					109	38.00	21	176328.	0.5	0.5	0.1658*
55		17					110	37.00	17	10927.	0.0	0.0	0.0103*

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	36.00	14	81956.	0.2	0.2	0.0771*
112	35.00	10	8808.	0.0	0.0	0.0083

8H12AV.1 [TIC-89321472, 100X=1251456X]. EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	381.00	6	826.	0.0	0.0	0.0009	56	159.00	17	232620.	1.9	1.9	0.2604*
2	305.00	6	1923.	0.0	0.0	0.0022	57	158.00	8	1547.	0.0	0.0	0.0017
3	304.00	8	34539.	0.3	0.3	0.0387	58	157.00	8	4506.	0.0	0.0	0.0050
4	303.00	17	494832.	4.0	4.0	0.5540*	59	155.00	8	789.	0.0	0.0	0.0009
5	302.00	25	3003904.	24.0	24.0	3.3630	60	154.00	10	10350.	0.1	0.1	0.0116
6	301.00	10	33364.	0.3	0.3	0.0374*	61	153.00	10	7339.	0.1	0.1	0.0092
7	287.00	6	1899.	0.0	0.0	0.0021	62	151.00	8	1859.	0.0	0.0	0.0021
8	284.00	14	72524.	0.6	0.6	0.0081	63	149.00	12	28495.	0.2	0.2	0.0319
9	283.00	17	517072.	4.1	4.1	0.5789	64	148.00	17	5444.	0.0	0.0	0.0061
10	274.00	8	3942.	0.0	0.0	0.0044	65	147.00	12	96900.	0.0	0.0	0.1085*
11	273.00	12	84848.	0.7	0.7	0.0950	66	146.00	10	31192.	0.2	0.2	0.0349
12	261.00	8	7205.	0.1	0.1	0.0081	67	145.00	17	301472.	2.4	2.4	0.3375*
13	250.00	17	165048.	1.3	1.3	0.1848	68	143.00	10	34947.	0.3	0.3	0.0391*
14	259.00	21	722912.	5.8	5.8	0.8093	69	142.00	8	2745.	0.0	0.0	0.0031
15	258.00	12	6699.	0.1	0.1	0.0075	70	141.00	10	10620.	0.1	0.1	0.0119
16	247.00	6	1722.	0.0	0.0	0.0019	71	137.00	8	4350.	0.0	0.0	0.0049
17	246.00	10	59524.	0.5	0.5	0.0666*	72	136.00	17	126876.	1.0	1.0	0.1420*
18	245.00	17	254228.	2.0	2.0	0.2846	73	135.00	25	1686556.	13.5	13.5	1.8883
19	244.00	8	10862.	0.1	0.1	0.0122	74	134.00	10	31621.	0.3	0.3	0.0354*
20	235.00	8	6264.	0.1	0.1	0.0070	75	133.00	17	191432.	1.5	1.5	0.2142*
21	232.00	12	72048.	0.6	0.6	0.0807*	76	132.00	25	236956.	1.9	1.9	0.2653*
22	231.00	17	321680.	2.6	2.6	0.3601	77	131.00	17	1798720.	14.4	14.4	2.0138
23	230.00	17	289216.	2.3	2.3	0.3238	78	130.00	10	22019.	0.2	0.2	0.0247*
24	221.00	10	2414.	0.0	0.0	0.0027	79	129.00	14	103756.	0.8	0.8	0.1162*
25	220.00	14	120564.	1.0	1.0	0.1350*	80	128.00	14	122976.	1.0	1.0	0.1377*
26	219.00	29	1370944.	11.0	11.0	1.5348*	81	127.00	17	109744.	0.9	0.9	0.1229*
27	218.00	43	12514560.	100.0	100.0	*14.01*	82	122.00	12	52467.	0.4	0.4	0.0587*
28	217.00	35	5309952.	42.4	42.4	5.9448*	83	121.00	8	7319.	0.1	0.1	0.0082
29	216.00	8	5151.	0.0	0.0	0.0058	84	120.00	17	115348.	0.9	0.9	0.1291*
30	211.00	12	43019.	0.3	0.3	0.0482	85	119.00	25	1329280.	10.6	10.6	1.4882
31	207.00	10	38525.	0.3	0.3	0.0431	86	118.00	25	1855680.	14.8	14.8	2.0775
32	206.00	8	8664.	0.1	0.1	0.0097	87	117.00	21	497920.	4.0	4.0	0.5574*
33	205.00	17	130876.	1.0	1.0	0.1465*	88	116.00	21	243248.	1.9	1.9	0.2723*
34	204.00	21	336896.	2.7	2.7	0.3772*	89	115.00	21	695616.	5.6	5.6	0.7788
35	203.00	25	2163776.	17.3	17.3	2.4225	90	114.00	6	1560.	0.0	0.0	0.0017
36	202.00	8	17962.	0.1	0.1	0.0201	91	110.00	8	16382.	0.1	0.1	0.0183*
37	201.00	8	16970.	0.1	0.1	0.0190	92	109.00	10	42818.	0.3	0.3	0.0479*
38	199.00	8	9406.	0.1	0.1	0.0105	93	108.00	10	21659.	0.2	0.2	0.0242*
39	198.00	14	132996.	1.1	1.1	0.1489*	94	107.00	21	527584.	4.2	4.2	0.5907*
40	193.00	8	2275.	0.0	0.0	0.0025	95	106.00	17	219236.	1.8	1.8	0.2454*
41	190.00	17	188244.	1.5	1.5	0.2187*	96	105.00	25	1003768.	8.6	8.6	1.2100
42	189.00	25	2163776.	17.3	17.3	2.4225	97	104.00	25	792912.	6.3	6.3	0.8877
43	187.00	6	1773.	0.0	0.0	0.0020	98	103.00	25	1007744.	8.1	8.1	1.1282*
44	185.00	8	10407.	0.1	0.1	0.0117	99	102.00	17	185756.	1.5	1.5	0.2090
45	177.00	8	2558.	0.0	0.0	0.0029	100	101.00	12	24354.	0.2	0.2	0.0273*
46	176.00	14	88152.	0.7	0.7	0.0987*	101	98.00	6	5725.	0.0	0.0	0.0064
47	175.00	21	554912.	4.4	4.4	0.6213	102	97.00	8	16576.	0.1	0.1	0.0186*
48	174.00	10	22545.	0.2	0.2	0.0252	103	96.00	12	41368.	0.3	0.3	0.0463
49	173.00	14	82036.	0.7	0.7	0.0918*	104	95.00	8	6905.	0.1	0.1	0.0077
50	169.00	6	4883.	0.0	0.0	0.0055	105	94.00	6	2825.	0.0	0.0	0.0032
51	166.00	6	4492.	0.0	0.0	0.0050	106	93.00	10	34723.	0.3	0.3	0.0389*
52	165.00	6	1482.	0.0	0.0	0.0017	107	92.00	25	781008.	6.2	6.2	0.8744
53	164.00	6	4458.	0.0	0.0	0.0050	108	91.00	35	10779648.	86.1	86.1	*12.06*
54	163.00	6	1222.	0.0	0.0	0.0014	109	90.00	29	2893632.	23.1	23.1	3.2396
55	160.00	10	19440.	0.2	0.2	0.0210	110	89.00	25	1367424.	10.9	10.9	1.5309

PEAK NO.	MEASURED MASS	N ^o . POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TO ION
111	88.00	14	23131.	0.2	0.2	0.0259*
112	87.00	10	9776.	0.1	0.1	0.0109
113	86.00	8	5986.	0.0	0.0	0.0067
114	85.00	21	370544.	3.0	3.0	0.4148*
115	84.00	14	64900.	0.5	0.5	0.0727*
116	83.00	29	1334336.	10.7	10.7	1.4939
117	82.00	10	50593.	0.4	0.4	0.0566*
118	81.00	12	29347.	0.2	0.2	0.0329
119	80.00	10	20262.	0.2	0.2	0.0227
120	79.00	21	233612.	1.9	1.9	0.2615*
121	78.00	25	701024.	5.6	5.6	0.7848
122	77.00	25	1046192.	8.4	8.4	1.1713
123	76.00	17	205208.	1.6	1.6	0.2297*
124	75.00	14	111948.	0.9	0.9	0.1253*
125	74.00	10	28260.	0.2	0.2	0.0316*
126	73.00	6	2242.	0.0	0.0	0.0025
127	72.00	6	4942.	0.0	0.0	0.0055
128	71.00	12	43385.	3.3	0.3	0.0486*
129	70.00	14	93944.	0.8	0.8	0.1052*
130	69.00	29	417632.	3.3	3.3	0.4676*
131	68.00	8	17481.	0.1	0.1	0.0196
132	67.00	14	109560.	0.9	0.9	0.1227*
133	66.00	8	24405.	0.2	0.2	0.0273
134	65.00	25	578192.	4.6	4.6	0.6473*
135	64.00	25	336144.	2.7	2.7	0.3763*
136	63.00	25	446048.	3.6	3.6	0.4994*
137	62.00	12	45300.	0.4	0.4	0.0507*
138	61.00	12	37436.	0.3	0.3	0.0419
139	58.00	10	45719.	0.4	0.4	0.0512*
140	57.00	25	1150336.	9.2	9.2	1.2879
141	56.00	25	434224.	3.5	3.5	0.4861*
142	55.00	25	1266368.	10.1	10.1	1.4178
143	54.00	17	95896.	0.8	0.8	0.1074*
144	53.00	21	268992.	2.1	2.1	0.3012*
145	52.00	17	130940.	1.0	1.0	0.1466*
146	51.00	25	525312.	4.2	4.2	0.5881*
147	50.00	21	242944.	1.9	1.9	0.2720*
148	49.00	8	3314.	0.0	0.0	0.0037
149	45.00	8	16325.	0.1	0.1	0.0183
150	44.00	29	369728.	3.1	3.1	0.4363*
151	43.00	35	10490112.	83.8	83.8	*11.74*
152	42.00	25	530480.	4.2	4.2	0.5939*
153	41.00	35	4330496.	34.5	34.6	4.8412
154	40.00	21	209780.	1.7	1.7	0.2349*
155	39.00	29	1318592.	10.5	10.5	1.4762
156	38.00	17	62532.	0.5	0.5	0.0700*
157	37.00	6	1966.	0.0	0.0	0.0022
158	36.00	3	22134.	0.2	0.2	0.0248

ED11PA.1 [TIC-156246144, 100X-25294040] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	381.00	14	95972.	0.4	0.4	0.0003	56	121.00	8	4644.	0.0	0.0	0.0044
2	380.00	17	535600.	2.1	2.1	0.5041	57	120.00	8	29240.	0.1	0.1	0.0275
3	281.00	14	4243.	0.0	0.0	0.0040	58	119.00	21	727648.	0.0	0.0	0.0049
4	280.00	8	6654.	0.0	0.0	0.0081	59	118.00	35	6807808.	23.8	23.8	5.6546*
5	254.00	6	1323.	0.0	0.0	0.0012	60	117.00	25	832848.	3.3	3.3	0.7839*
6	235.00	6	1796.	0.0	0.0	0.0007	61	116.00	21	530368.	2.1	2.1	0.4992
7	230.00	10	1399.	0.0	0.0	0.0013	62	115.00	25	1706176.	6.7	6.7	1.0059
8	222.00	6	500.	0.0	0.0	0.0005	63	114.00	12	20153.	0.1	0.1	0.0190
9	221.00	8	6044.	0.0	0.0	0.0057	64	113.00	10	25358.	0.1	0.1	0.0239
10	220.00	17	235216.	0.9	0.9	0.2214*	65	112.00	8	10625.	0.0	0.0	0.0100
11	219.00	35	2759936.	10.9	10.9	2.5977*	66	109.00	21	243216.	1.0	1.0	0.0228
12	218.00	59	25294848.	100.0	100.0	*23.80*	67	108.00	12	42589.	0.2	0.2	0.0401
13	217.00	21	154884.	0.6	0.6	0.0026	68	107.00	25	709328.	2.8	2.8	0.0676
14	215.00	10	2726.	0.0	0.0	0.0087	69	106.00	17	100084.	0.4	0.4	0.0942*
15	207.00	10	9275.	0.0	0.0	0.00319	70	105.00	25	680112.	2.7	2.7	0.16401
16	200.00	10	33935.	0.1	0.1	0.03168	71	104.00	21	281216.	1.1	1.1	0.02647
17	199.00	17	336576.	1.3	1.3	0.01847	72	103.00	21	404864.	1.6	1.6	0.03811
18	198.00	17	196232.	0.8	0.8	0.0025	73	102.00	17	223360.	0.9	0.9	0.2102*
19	191.00	6	2628.	0.0	0.0	0.00370*	74	101.00	10	30510.	0.1	0.1	0.0287
20	190.00	10	39354.	0.2	0.2	0.0479*	75	100.00	8	1546.	0.0	0.0	0.0015
21	189.00	17	525856.	2.1	2.1	0.0479*	76	95.00	21	216772.	0.9	0.9	0.2040
22	181.00	12	50873.	0.0	0.0	0.0007	77	94.00	6	2380.	0.0	0.0	0.0022
23	180.00	6	700.	0.0	0.0	0.0007	78	93.00	17	89320.	0.4	0.4	0.0841*
24	174.00	17	144444.	0.6	0.6	0.1360	79	92.00	25	676224.	2.7	2.7	0.6365
25	173.00	21	1016032.	4.0	4.0	0.9563	80	91.00	35	8193792.	32.4	32.4	7.7121*
26	172.00	12	44562.	0.2	0.2	0.0419*	81	90.00	25	1273856.	5.0	5.0	1.1990
27	171.00	17	130580.	0.5	0.5	0.1228	82	89.00	25	697024.	2.8	2.8	0.6560*
28	169.00	8	9680.	0.0	0.0	0.0091	83	88.00	8	20812.	0.1	0.1	0.0196
29	167.00	8	4034.	0.0	0.0	0.0038	84	88.00	10	16058.	0.0	0.0	0.0151
30	166.00	8	1757.	0.0	0.0	0.0017	85	86.00	8	7970.	0.0	0.0	0.0075
31	165.00	10	5110.	0.0	0.0	0.0048	86	85.00	17	5824.	0.0	0.0	0.0055*
32	159.00	10	15242.	0.1	0.1	0.0143	87	84.00	21	492096.	1.9	1.9	0.4632
33	157.00	10	13123.	0.1	0.1	0.0124*	88	83.00	35	9287168.	36.7	36.7	8.7412*
34	156.00	10	4131.	0.0	0.0	0.0039	89	82.00	21	479440.	1.9	1.9	0.4513
35	154.00	6	21347.	0.1	0.1	0.0201*	90	81.00	25	1055232.	4.2	4.2	0.9932
36	153.00	17	5989.	0.0	0.0	0.0056	91	80.00	21	151196.	0.6	0.6	0.1423*
37	152.00	8	76724.	0.3	0.3	0.0722	92	79.00	25	1395584.	5.5	5.5	1.3135
38	152.00	8	15137.	0.1	0.1	0.0142	93	78.00	21	528848.	2.1	2.1	0.4978
39	145.00	6	1155.	0.0	0.0	0.0011	94	77.00	25	1196992.	4.7	4.7	1.1266
40	144.00	10	3414.	0.0	0.0	0.0032	95	76.00	17	141424.	0.6	0.6	0.1331*
41	143.00	17	132776.	0.5	0.5	0.1250	96	75.00	17	89828.	0.4	0.4	0.0845*
42	142.00	12	41211.	0.2	0.2	0.0388	97	74.00	10	22497.	0.1	0.1	0.0212
43	141.00	17	145444.	0.6	0.6	0.1369	98	73.00	8	1610.	0.0	0.0	0.0015
44	139.00	8	22171.	0.1	0.1	0.0209	99	71.00	12	13781.	0.1	0.1	0.0130*
45	136.00	17	134036.	0.5	0.5	0.1262	100	70.00	10	1718.	0.0	0.0	0.0016
46	135.00	25	1772736.	7.0	7.0	1.6685	101	69.00	35	533360.	2.1	2.1	0.5028
47	134.00	10	40283.	0.2	0.2	0.0379*	102	68.00	14	86076.	5.2	5.2	1.2297
48	132.00	8	18307.	0.1	0.1	0.0172	103	67.00	25	1306560.	0.3	0.3	0.0810*
49	130.00	8	8636.	0.0	0.0	0.0081	104	66.00	17	155036.	0.6	0.6	0.1459*
50	131.00	21	218004.	0.9	0.9	0.2052	105	65.00	25	917648.	3.6	3.6	0.8637*
51	129.00	21	408768.	1.6	1.6	0.3847	106	64.00	35	333792.	1.3	1.3	0.3142*
52	129.00	25	877904.	3.5	3.5	0.8263*	107	63.00	25	478608.	1.9	1.9	0.4505*
53	128.00	25	744240.	2.9	2.9	0.7005*	108	62.00	12	60486.	0.2	0.2	0.0569*
54	127.00	21	256708.	1.0	1.0	0.2416	109	61.00	10	15282.	0.1	0.1	0.0144
55	126.00	10	9292.	0.0	0.0	0.0087	110	59.00	6	5120.	0.0	0.0	0.0048

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. MREF	% TOT. ION
111	57.00	12	33226.	6.1	0.1	0.0313*
112	56.00	25	609952.	2.4	2.4	0.5741*
113	55.00	43	1450188.	57.3	57.3	*13.64*
114	54.00	25	648032.	2.6	2.6	0.6099
115	53.00	25	780992.	3.1	3.1	0.7351
116	52.00	21	188800.	0.7	0.7	0.1777*
117	51.00	25	761360.	3.0	3.0	0.7166
118	50.00	21	183732.	0.7	0.7	0.1729
119	45.00	14	29342.	0.1	0.1	0.0276
120	44.00	12	50453.	0.2	0.2	0.0475*
121	43.00	25	497472.	2.0	2.0	0.4682*
122	42.00	25	306600.	1.2	1.2	0.2886*
123	41.00	35	6267904.	24.8	24.8	5.8994
124	40.00	29	230840.	0.9	0.9	0.2173*
125	39.00	29	1787320.	7.1	7.1	1.6823
126	38.00	17	61032.	0.2	0.2	0.0574*
127	37.00	10	16499.	0.1	0.1	0.0155*
128	36.00	21	87448.	0.3	0.3	0.0823*
129	35.00	6	3276.	0.0	0.0	0.0031

809PA.1 [TIC-6758288, 188X-15613952] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	282.00	6	1384.	0.0	0.0	0.0020	56	98.00	21	258636.	1.7	1.7	0.3832
2	281.00	6	4153.	0.0	0.0	0.0062	57	97.00	8	4098.	0.0	0.0	0.0061
3	256.00	14	113008.	0.7	0.7	0.1674*	58	96.00	8	3385.	0.0	0.0	0.0050
4	255.00	25	1474176.	9.4	9.4	2.1839*	59	95.00	17	29142.	0.2	0.2	0.0432*
5	254.00	43	10661120.	68.3	68.3	*15.79*	60	94.00	6	4661.	0.0	0.0	0.0069
6	253.00	17	86076.	0.6	0.6	0.1275*	61	89.00	17	82020.	0.5	0.5	0.1215
7	252.00	5	773.	0.0	0.0	0.0011	62	88.00	17	115092.	0.7	0.7	0.1705*
8	236.00	10	39641.	0.3	0.3	0.0587	63	87.00	21	354608.	2.3	2.3	0.5253*
9	235.00	17	279248.	1.8	1.8	0.4137	64	86.00	17	183652.	1.2	1.2	0.2721*
10	234.00	8	14372.	0.1	0.1	0.0213	65	85.00	10	9603.	0.1	0.1	0.0142
11	231.00	6	1293.	0.0	0.0	0.0019	66	83.00	21	301696.	1.9	1.9	0.4469
12	219.00	8	2140.	0.0	0.0	0.0032	67	80.00	6	891.	0.0	0.0	0.0013
13	209.00	8	14402.	0.1	0.1	0.0213	68	79.00	8	7647.	0.0	0.0	0.0113
14	208.00	6	1825.	0.0	0.0	0.0027	69	78.00	43	1297472.	8.3	8.3	1.9221*
15	207.00	10	6728.	0.0	0.0	0.0100	70	77.00	35	2108352.	13.5	13.5	3.1234*
16	186.00	18	3509.	0.0	0.0	0.0052	71	76.00	25	551600.	3.5	3.5	0.8172
17	185.00	10	22187.	0.1	0.1	0.0329	72	75.00	25	1228160.	7.9	7.9	1.8194
18	181.00	6	3465.	0.0	0.0	0.0051	73	74.00	25	866544.	5.5	5.5	1.2837
19	171.00	14	114696.	0.7	0.7	0.1699	74	73.00	12	58501.	0.4	0.4	0.0867*
20	170.00	17	169104.	1.1	1.1	0.2505	75	69.00	21	504992.	3.2	3.2	0.7481
21	169.00	12	54360.	0.3	0.3	0.0805*	76	65.00	10	22873.	0.1	0.1	0.0339
22	157.00	17	105036.	0.7	0.7	0.1556*	77	64.00	35	1663168.	10.7	10.7	2.4639*
23	156.00	35	1807808.	11.6	11.6	2.6782*	78	63.00	43	2522432.	16.2	16.2	3.7368*
24	155.00	51	15613952.	100.0	100.0	*23.13*	79	62.00	25	384160.	2.5	2.5	0.5691*
25	154.00	21	215132.	1.4	1.4	0.3187*	80	61.00	14	76172.	0.5	0.5	0.1128
26	153.00	10	22821.	0.1	0.1	0.0338*	81	53.00	8	16755.	0.1	0.1	0.0159
27	144.00	6	902.	0.0	0.0	0.0013	82	52.00	17	113140.	0.7	0.7	0.1676*
28	143.00	8	27400.	0.2	0.2	0.0406	83	51.00	29	1110976.	7.1	7.1	1.6458
29	142.00	10	25270.	0.2	0.2	0.0374	84	50.00	29	660448.	4.2	4.2	0.9784*
30	141.00	8	23432.	0.2	0.2	0.0347	85	49.00	12	13938.	0.1	0.1	0.0206*
31	133.00	8	6943.	0.0	0.0	0.0103	86	45.00	10	7348.	0.0	0.0	0.0109
32	131.00	10	21103.	0.1	0.1	0.0313	87	44.00	17	102208.	0.7	0.7	0.1514*
33	129.00	14	95376.	0.6	0.6	0.1413	88	41.00	8	2858.	0.0	0.0	0.0042
34	128.00	25	1685632.	10.8	10.8	2.4972*	89	40.00	10	27400.	0.2	0.2	0.0406*
35	127.00	51	14503168.	92.9	92.9	*21.48*	90	39.00	21	239600.	1.5	1.5	0.3541*
36	126.00	35	2496640.	16.0	16.0	3.6986*	91	38.00	14	87712.	0.6	0.6	0.1299*
37	125.00	21	263536.	1.7	1.7	0.3004*	92	37.00	10	8494.	0.1	0.1	0.0126*
38	124.00	6	1115.	0.0	0.0	0.0017	93	36.00	10	27072.	0.2	0.2	0.0401*
39	123.00	8	7081.	0.0	0.0	0.0105	94	35.00	8	2069.	0.0	0.0	0.0031
40	122.00	10	29353.	0.2	0.2	0.0435							
41	121.00	6	1715.	0.0	0.0	0.0025							
42	119.00	12	36594.	0.2	0.2	0.0542							
43	117.00	16	1672.	0.0	0.0	0.0025							
44	116.00	10	9317.	0.1	0.1	0.0138							
45	115.00	17	248004.	1.6	1.6	0.3686							
46	114.00	21	299488.	1.9	1.9	0.4437							
47	113.00	14	83064.	0.5	0.5	0.1231*							
48	111.00	10	3020.	0.0	0.0	0.0045							
49	105.00	8	1520.	0.0	0.0	0.0023							
50	104.00	17	31488.	0.2	0.2	0.0466*							
51	103.00	8	1619.	0.0	0.0	0.0024							
52	102.00	17	133768.	0.9	0.9	0.1982*							
53	101.00	25	1117056.	7.2	7.2	1.6548							
54	100.00	21	240152.	1.5	1.5	0.3558							
55	99.00	21	222836.	1.4	1.4	0.3301*							

8Y8AV.1 [TIC-62626064, 188X-13418496] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	257.00	10	2010.	0.0	0.0	0.0032	56	98.00	21	230496.	1.7	1.7	0.3680
2	256.00	17	133412.	1.0	1.0	0.2130	57	96.00	8	2073.	0.0	0.0	0.0033
3	255.00	35	1448960.	10.8	10.8	2.3136*	58	95.00	17	28659.	0.2	0.2	0.0458*
4	254.00	43	10620416.	79.1	79.1	*16.95*	59	94.00	12	10977.	0.1	0.1	0.0175*
5	253.00	21	142728.	1.1	1.1	0.2279*	60	93.00	8	2140.	0.0	0.0	0.0034
6	252.00	8	3077.	0.0	0.0	0.0049	61	92.00	14	124520.	0.9	0.9	0.1988
7	236.00	10	38424.	0.3	0.3	0.0614*	62	89.00	12	41251.	0.3	0.3	0.0659
8	235.00	17	293872.	2.2	2.2	0.4692	63	88.00	17	85832.	0.5	0.6	0.1370
9	210.00	6	1475.	0.0	0.0	0.0024	64	87.00	21	303008.	2.3	2.3	0.4838
10	209.00	10	27177.	0.2	0.2	0.0434*	65	86.00	21	164452.	1.2	1.2	0.2626*
11	207.00	8	1625.	0.0	0.0	0.0026	66	85.00	10	28549.	0.2	0.2	0.0456
12	190.00	10	3057.	0.0	0.0	0.0049	67	83.00	21	190640.	1.4	1.4	0.3044*
13	189.00	10	4155.	0.0	0.0	0.0066	68	78.00	25	410992.	3.1	3.1	0.6562*
14	186.00	10	9384.	0.1	0.1	0.0150*	69	77.00	59	4292608.	32.0	32.0	6.8540*
15	185.00	17	103980.	0.8	0.8	0.1660	70	76.00	21	535808.	4.0	4.0	0.8555
16	181.00	6	2564.	0.0	0.0	0.0041	71	75.00	25	1033968.	7.7	7.7	1.6509
17	171.00	10	5308.	0.7	0.7	0.0085	72	74.00	25	738160.	5.5	5.5	1.1786
18	170.00	17	94412.	0.7	0.7	0.1507	73	73.00	12	35431.	0.3	0.3	0.0566*
19	169.00	14	28561.	0.2	0.2	0.0456*	74	69.00	21	360096.	2.7	2.7	0.5750
20	159.00	17	6041.	0.0	0.0	0.0096	75	65.00	14	14397.	0.1	0.1	0.0230*
21	157.00	17	102856.	0.8	0.8	0.1642	76	64.00	25	440400.	3.3	3.3	0.7032
22	156.00	35	1549312.	11.5	11.5	2.4738*	77	63.00	71	4330752.	32.3	32.3	6.9149*
23	155.00	51	13418496.	100.0	100.0	*21.42*	78	62.00	35	383632.	2.9	2.9	0.6125*
24	154.00	21	113416.	0.8	0.8	0.1811*	79	61.00	17	73644.	0.5	0.5	0.1176*
25	153.00	6	2417.	0.0	0.0	0.0039	80	53.00	12	26069.	0.2	0.2	0.0416*
26	145.00	8	1730.	0.0	0.0	0.0028	81	52.00	17	97668.	0.7	0.7	0.1559*
27	143.00	8	3666.	0.0	0.0	0.0059	82	51.00	29	998768.	7.4	7.4	1.5947
28	142.00	14	52866.	0.4	0.4	0.0844*	83	50.00	29	733728.	5.5	5.5	1.1715*
29	141.00	17	47595.	0.4	0.4	0.0760	84	49.00	8	15770.	0.1	0.1	0.0252*
30	133.00	10	8354.	0.1	0.1	0.0133	85	47.00	8	1996.	0.0	0.0	0.0032
31	131.00	10	2689.	0.0	0.0	0.0043	86	45.00	10	7830.	0.1	0.1	0.0125
32	129.00	17	73868.	0.6	0.6	0.1179*	87	44.00	17	61611.	0.5	0.5	0.0984*
33	128.00	29	1466624.	10.9	10.9	2.3418*	88	40.00	12	29790.	0.2	0.2	0.0476*
34	127.00	51	12343040.	92.0	92.0	*19.70*	89	39.00	25	245924.	1.8	1.8	0.3943
35	126.00	35	2089024.	15.6	15.6	3.3356*	90	38.00	21	125328.	0.9	0.9	0.2001*
36	125.00	29	251776.	1.9	1.9	0.4020*	91	37.00	8	9869.	0.1	0.1	0.0158
37	124.00	6	2264.	0.0	0.0	0.0036	92	36.00	8	16913.	0.1	0.1	0.0270*
38	123.00	8	3658.	0.0	0.0	0.0058							
39	122.00	10	16545.	0.1	0.1	0.0264							
40	121.00	8	3670.	0.0	0.0	0.0059							
41	117.00	8	6004.	0.0	0.0	0.0096							
42	116.00	6	1050.	0.0	0.0	0.0017							
43	115.00	17	111576.	0.8	0.8	0.1782*							
44	114.00	21	162676.	1.2	1.2	0.2597							
45	113.00	14	50496.	0.4	0.4	0.0806*							
46	112.00	8	1896.	0.0	0.0	0.0030							
47	111.00	10	6829.	0.1	0.1	0.0109							
48	107.00	8	9894.	0.1	0.1	0.0158							
49	105.00	12	9093.	0.1	0.1	0.0145*							
50	104.00	21	60179.	0.4	0.4	0.0961*							
51	103.00	6	1105.	0.0	0.0	0.0018							
52	102.00	17	119476.	0.9	0.9	0.1908							
53	101.00	25	90464.	7.0	7.0	1.4921							
54	100.00	21	10576.	1.5	1.5	0.3172*							
55	99.00	21	13344.	1.5	1.5	0.3135							

BH18AV.1 [TIC=77733888, 188X-29637632] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	271.00	6	2497.	0.0	0.0	0.0032	56	93.00	8	4193.	0.0	0.0	0.0054
2	270.00	14	126504.	0.4	0.4	0.1627*	57	92.00	8	1997.	0.0	0.0	0.0026
3	269.00	25	1244992.	4.2	4.2	1.6016*	58	91.00	21	319008.	1.1	1.1	0.4104*
4	268.00	35	8942080.	30.2	30.2	*11.50*	59	90.00	10	55075.	0.2	0.2	0.0789*
5	267.00	12	37980.	0.1	0.1	0.0489*	60	89.00	25	888672.	3.0	3.0	1.1432
6	250.00	8	1985.	0.0	0.0	0.0026	61	88.00	17	267792.	0.9	0.9	0.3445*
7	249.00	14	128540.	0.4	0.4	0.1654	62	87.00	21	490192.	1.7	1.7	0.6306*
8	240.00	6	805.	0.0	0.0	0.0010	63	86.00	21	282704.	1.0	1.0	0.3637*
9	239.00	8	11237.	0.0	0.0	0.0145	64	85.00	12	65525.	0.2	0.2	0.0843*
10	226.00	10	40835.	0.1	0.1	0.0525	65	84.00	12	59776.	0.2	0.2	0.0769*
11	207.00	8	3618.	0.0	0.0	0.0047	66	83.00	25	1714496.	5.8	5.8	2.2056
12	185.00	12	82800.	0.3	0.3	0.1065*	67	81.00	6	10383.	0.0	0.0	0.0134
13	184.00	10	21475.	0.1	0.1	0.0276	68	80.00	8	1727.	0.0	0.0	0.0022
14	170.00	8	6026.	0.0	0.0	0.0078	69	78.00	12	32937.	0.1	0.1	0.0437*
15	169.00	17	154424.	0.5	0.5	0.1987*	70	77.00	21	195316.	0.7	0.7	0.2513*
16	168.00	17	421152.	1.4	1.4	0.5418*	71	76.00	21	254444.	0.9	0.9	0.3273*
17	159.00	6	4622.	0.0	0.0	0.0059	72	75.00	25	443184.	1.5	1.5	0.5701*
18	157.00	14	72104.	0.2	0.2	0.0928*	73	74.00	29	485168.	1.6	1.6	0.6241*
19	156.00	17	162364.	0.5	0.5	0.2089*	74	73.00	8	8928.	0.0	0.0	0.0115
20	155.00	17	177612.	0.6	0.6	0.2285*	75	71.00	43	1770496.	6.0	6.0	2.2776*
21	153.00	8	4914.	0.0	0.0	0.0063	76	70.00	35	518896.	1.8	1.8	0.6675*
22	152.00	8	9285.	0.0	0.0	0.0119	77	69.00	29	849360.	2.9	2.9	1.0927*
23	150.00	8	1748.	0.0	0.0	0.0022	78	66.00	8	5435.	0.0	0.0	0.0070
24	143.00	17	211760.	0.7	0.7	0.2724*	79	65.00	21	405936.	1.4	1.4	0.5222*
25	142.00	35	3558208.	12.0	12.0	4.5774*	80	64.00	21	392192.	1.3	1.3	0.5045*
26	141.00	59	2963732.	100.0	100.0	*38.12*	81	63.00	25	1612480.	5.4	5.4	2.0744
27	140.00	35	1585728.	5.4	5.4	2.0399*	82	62.00	25	517280.	1.7	1.7	0.6654*
28	139.00	35	3780036.	12.8	12.8	4.8629*	83	61.00	17	171632.	0.6	0.6	0.2208
29	138.00	21	217536.	0.7	0.7	0.2798*	84	58.00	21	629936.	2.1	2.1	0.8104*
30	137.00	17	100940.	0.3	0.3	0.1299*	85	57.00	17	427536.	1.4	1.4	0.5500
31	134.00	6	2305.	0.0	0.0	0.0030	86	56.00	12	3401.	0.0	0.0	0.0044
32	131.00	10	7393.	0.0	0.0	0.0095*	87	53.00	8	4113.	0.0	0.0	0.0053
33	130.00	8	1599.	0.0	0.0	0.0021	88	52.00	17	156852.	0.5	0.5	0.2018*
34	129.00	14	114068.	0.4	0.4	0.1467*	89	51.00	25	795024.	2.7	2.7	1.0228*
35	128.00	21	500736.	1.7	1.7	0.6442*	90	50.00	25	526768.	1.8	1.8	0.6777*
36	127.00	21	347616.	1.2	1.2	0.4472	91	49.00	8	14665.	0.0	0.0	0.0189
37	126.00	17	163224.	0.6	0.6	0.2100*	92	47.00	6	3364.	0.0	0.0	0.0043
38	125.00	6	1521.	0.0	0.0	0.0020	93	45.00	10	23727.	0.1	0.1	0.0305*
39	117.00	8	12576.	0.0	0.0	0.0162	94	44.00	21	235308.	0.8	0.8	0.3027*
40	116.00	21	719120.	2.4	2.4	0.9251*	95	43.00	6	2932.	0.0	0.0	0.0038
41	115.00	35	7843328.	26.5	26.5	*10.09*	96	42.00	10	25971.	0.1	0.1	0.0334*
42	114.00	17	352176.	1.2	1.2	0.4531	97	41.00	18	18702.	0.1	0.1	0.0241*
43	113.00	21	521360.	1.8	1.8	0.6767*	98	40.00	12	32694.	0.1	0.1	0.0421*
44	112.00	8	18174.	0.1	0.1	0.0234	99	39.00	25	816448.	2.8	2.8	1.0503
45	111.00	10	54006.	0.2	0.2	0.0695	100	38.00	21	150248.	0.5	0.5	0.1933*
46	110.00	12	26971.	0.1	0.1	0.0347*	101	37.00	8	7946.	0.0	0.0	0.0102
47	109.00	6	1799.	0.0	0.0	0.0023	102	36.00	10	40910.	0.1	0.1	0.0526
48	103.00	8	13938.	0.0	0.0	0.0179							
49	102.00	21	239540.	0.8	0.8	0.3082*							
50	101.00	10	59241.	0.2	0.2	0.0762*							
51	100.00	12	40678.	0.1	0.1	0.0523*							
52	99.00	14	65474.	0.2	0.2	0.0842							
53	98.00	12	92552.	0.3	0.3	0.1191*							
54	95.00	10	10918.	0.0	0.0	0.0140*							
55	94.00	17	31307.	0.1	0.1	0.0403*							

8018PA.1 [TIC=75538248, 188X-18555984] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	319.00	6	2508.	0.0	0.0	0.0033	56	118.00	8	6906.	0.0	0.0	0.0021
2	283.00	8	5442.	0.0	0.0	0.0085	57	117.00	17	24230.	0.1	0.1	0.0321*
3	282.00	17	147564.	0.0	0.0	0.1954*	58	116.00	10	19202.	0.1	0.1	0.0254
4	281.00	25	1427320.	7.7	7.7	1.8897*	59	115.00	21	334832.	1.8	1.8	0.4433
5	280.00	43	10093056.	54.4	54.4	*13.36*	60	114.00	14	67416.	0.4	0.4	0.0993
6	279.00	35	1061312.	5.7	5.7	1.4051*	61	113.00	17	150444.	0.8	0.8	0.1992
7	278.00	14	51099.	0.3	0.3	0.0677*	62	112.00	6	1997.	0.0	0.0	0.0026
8	263.00	10	23162.	0.1	0.1	0.0307	63	111.00	16	25455.	0.1	0.1	0.0337*
9	262.00	10	8088.	0.0	0.0	0.0107	64	110.00	8	16068.	0.1	0.1	0.0213
10	261.00	17	149776.	0.0	0.0	0.1983*	65	109.00	6	1253.	0.0	0.0	0.0017
11	254.00	10	23898.	0.1	0.1	0.0316	66	108.00	8	27834.	0.2	0.2	0.0369
12	235.00	8	2875.	0.0	0.0	0.0038	67	104.00	10	15121.	0.1	0.1	0.0200
13	221.00	8	2750.	0.0	0.0	0.0036	68	103.00	10	28979.	0.2	0.2	0.0384*
14	219.00	8	1683.	0.0	0.0	0.0022	69	102.00	17	236520.	1.3	1.3	0.3131
15	215.00	8	1706.	0.0	0.0	0.0023	70	101.00	21	273488.	1.5	1.5	0.3621*
16	211.00	6	727.	0.0	0.0	0.0010	71	100.00	17	122388.	0.7	0.7	0.1620
17	207.00	8	5465.	0.0	0.0	0.0072	72	99.00	17	165656.	0.9	0.9	0.2193*
18	199.00	10	5729.	0.0	0.0	0.0076	73	98.00	17	152136.	0.8	0.8	0.2014*
19	198.00	10	1817.	0.0	0.0	0.0024	74	97.00	6	1359.	0.0	0.0	0.0018
20	197.00	17	151012.	0.0	0.0	0.1999	75	91.00	43	1814848.	9.8	9.8	2.4028*
21	196.00	17	272224.	1.5	1.5	0.3604	76	90.00	10	15135.	0.1	0.1	0.0200*
22	195.00	8	9936.	0.1	0.1	0.0132	77	89.00	17	145292.	0.8	0.8	0.1924
23	193.00	6	1323.	0.0	0.0	0.0018	78	88.00	17	127692.	0.7	0.7	0.1691*
24	184.00	8	3244.	0.0	0.0	0.0043	79	87.00	21	272336.	1.5	1.5	0.3606
25	183.00	17	209292.	1.1	1.1	0.2771*	80	86.00	17	150016.	0.8	0.8	0.1986
26	182.00	35	2503424.	13.5	13.5	3.3145*	81	85.00	8	1749.	0.0	0.0	0.0099
27	181.00	51	18555904.	100.0	100.0	*24.56*	82	84.00	6	477552.	0.0	0.0	0.0023
28	180.00	25	282320.	1.5	1.5	0.3738	83	83.00	21	477552.	2.6	2.6	0.6323
29	179.00	12	21579.	0.1	0.1	0.0284*	84	79.00	8	3646.	0.0	0.0	0.0048
30	170.00	0	11074.	0.1	0.1	0.0147	85	78.00	17	79512.	0.4	0.4	0.1053*
31	169.00	14	77856.	0.4	0.4	0.1031	86	77.00	51	2123840.	11.4	11.4	2.8119*
32	168.00	17	231668.	1.2	1.2	0.3067	87	76.00	51	4427776.	23.9	23.9	5.8623*
33	165.00	10	28285.	0.2	0.2	0.0374*	88	75.00	29	828912.	4.5	4.5	1.0975*
34	155.00	14	103992.	0.6	0.6	0.1377	89	74.00	25	549680.	3.0	3.0	0.7278*
35	154.00	25	841984.	4.5	4.5	1.1148*	90	73.00	10	6363.	0.0	0.0	0.0084*
36	153.00	51	6654720.	35.9	35.9	8.0107*	91	71.00	6	2439.	0.0	0.0	0.0032
37	152.00	59	8933632.	48.1	48.1	*11.82*	92	70.00	10	7446.	0.0	0.0	0.0099
38	151.00	59	2635200.	14.2	14.2	3.4889*	93	69.00	25	362688.	2.0	2.0	0.4802
39	150.00	35	741408.	4.0	4.0	0.9816*	94	66.00	6	2100.	0.0	0.0	0.0028
40	149.00	21	90300.	0.5	0.5	0.1196*	95	65.00	17	103524.	0.6	0.6	0.1371*
41	141.00	17	159948.	0.9	0.9	0.2118*	96	64.00	25	226176.	1.2	1.2	0.2995*
42	140.00	17	167716.	0.9	0.9	0.2221	97	63.00	35	1153472.	6.2	6.2	1.5272*
43	139.00	21	373088.	2.0	2.0	0.4940	98	62.00	25	287984.	1.6	1.6	0.3813*
44	137.00	8	3159.	0.0	0.0	0.0042	99	61.00	10	32790.	0.2	0.2	0.0434
45	131.00	10	23606.	0.1	0.1	0.0313	100	57.00	8	2527.	0.0	0.0	0.0033
46	130.00	21	59077.	0.3	0.3	0.0782*	101	53.00	10	40810.	0.2	0.2	0.0540*
47	129.00	17	48091.	0.3	0.3	0.0637*	102	52.00	21	155640.	0.8	0.8	0.2061*
48	128.00	14	95036.	0.5	0.5	0.1258*	103	51.00	25	980224.	5.3	5.3	1.2978
49	127.00	21	809952.	4.4	4.4	1.0724*	104	50.00	25	563648.	3.0	3.0	0.7463
50	126.00	21	832912.	4.5	4.5	1.1028	105	49.00	6	1540.	0.0	0.0	0.0020
51	125.00	17	138016.	0.7	0.7	0.1827	106	45.00	8	9099.	0.0	0.0	0.0120
52	124.00	6	2708.	0.0	0.0	0.0036	107	44.00	12	48059.	0.3	0.3	0.0636*
53	123.00	8	1863.	0.0	0.0	0.0025	108	41.00	6	4137.	0.0	0.0	0.0055
54	122.00	10	11178.	0.1	0.1	0.0148	109	40.00	12	44300.	0.2	0.2	0.0587*
55	119.00	14	69296.	0.4	0.4	0.0917*	110	39.00	25	501728.	2.7	2.7	0.6643*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	38.00	17	88100.	0.5	0.5	0.1166*
112	37.00	12	11694.	0.1	0.1	0.0155
113	36.00	8	24768.	0.1	0.1	0.0328*

8Y9AV.1 [TIC-58628896, 188X-12914176] EI

8H11AV.1 [TIC=92397568, 188X=38488576] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	310.00	8	2694.	0.0	0.0	0.0029	56	127.00	17	196540.	0.6	0.6	0.2127
2	309.00	14	130364.	0.4	0.4	0.1411*	57	126.00	17	175120.	0.6	0.6	0.1895*
3	308.00	17	652528.	2.1	2.1	0.7062	58	125.00	8	5959.	0.0	0.0	0.0064
4	293.00	10	5622.	0.0	0.0	0.0072	59	123.00	6	1657.	0.0	0.0	0.0018
5	266.00	8	5213.	0.0	0.0	0.0056	60	119.00	8	13138.	0.0	0.0	0.0142
6	265.00	14	82592.	0.3	0.3	0.0894*	61	118.00	8	1873.	0.0	0.0	0.0020
7	231.00	6	2625.	0.0	0.0	0.0028	62	116.00	12	57825.	0.2	0.2	0.0026*
8	211.00	8	10877.	0.0	0.0	0.0118	63	115.00	21	689200.	2.3	2.3	0.7459
9	209.00	8	7274.	0.0	0.0	0.0079	64	114.00	10	44101.	0.1	0.1	0.0477
10	208.00	8	7495.	0.0	0.0	0.0081	65	113.00	14	109784.	0.4	0.4	0.1188
11	207.00	12	56310.	0.2	0.2	0.0609*	66	112.00	6	1994.	0.0	0.0	0.0022
12	203.00	8	31645.	0.1	0.1	0.0342	67	111.00	8	8168.	0.0	0.0	0.0088
13	195.00	6	1968.	0.0	0.0	0.0021	68	110.00	8	3841.	0.0	0.0	0.0042
14	194.00	8	11284.	0.0	0.0	0.0122	69	109.00	8	15437.	0.1	0.1	0.0167
15	193.00	8	9636.	0.0	0.0	0.0104	70	107.00	6	1269.	0.0	0.0	0.0014
16	189.00	12	45519.	0.1	0.1	0.0493	71	106.00	10	28056.	0.1	0.1	0.0304*
17	184.00	6	1458.	0.0	0.0	0.0016	72	105.00	21	561184.	1.8	1.8	0.6074*
18	183.00	21	295616.	1.0	1.0	0.3199*	73	104.00	25	872144.	2.9	2.9	0.9439
19	182.00	35	448464.	14.7	14.7	4.8539*	74	103.00	43	9127168.	23.9	23.9	9.8781*
20	181.00	71	30488576.	100.0	100.0	*32.99*	75	102.00	25	663056.	2.2	2.2	0.7176*
21	180.00	35	912400.	3.0	3.0	0.9875*	76	101.00	17	146644.	0.5	0.5	0.1587*
22	179.00	35	1962752.	6.4	6.4	2.1242*	77	100.00	10	16007.	0.1	0.1	0.0173*
23	178.00	35	1743040.	5.7	5.7	1.8865*	78	99.00	10	27367.	0.1	0.1	0.0296*
24	177.00	35	428768.	1.4	1.4	0.4640*	79	98.00	10	26606.	0.1	0.1	0.0288
25	176.00	21	351520.	1.2	1.2	0.3804*	80	92.00	6	4136.	0.0	0.0	0.0045
26	175.00	17	25155.	0.1	0.1	0.0272	81	91.00	29	362912.	1.2	1.2	0.3328*
27	174.00	10	3755.	0.0	0.0	0.0041	82	90.00	35	562768.	1.8	1.8	0.6091*
28	169.00	8	3462.	0.0	0.0	0.0037	83	89.00	35	1221888.	4.0	4.0	1.3224*
29	168.00	10	36821.	0.1	0.1	0.0399	84	88.00	17	217588.	0.7	0.7	0.2355*
30	167.00	25	662944.	2.2	2.2	0.7175*	85	87.00	14	153676.	0.5	0.5	0.1653*
31	166.00	35	4721152.	15.5	15.5	5.1096*	86	86.00	10	47218.	0.2	0.2	0.0511*
32	165.00	51	6485504.	21.3	21.3	7.0191*	87	85.00	16	1247.	0.3	0.3	0.1144*
33	164.00	35	577184.	1.9	1.9	0.6247*	88	84.00	17	105672.	0.3	0.3	0.0013
34	163.00	21	315120.	1.0	1.0	0.3410*	89	83.00	51	3950912.	13.0	13.0	4.2760*
35	162.00	12	25689.	0.1	0.1	0.0278	90	82.00	29	614944.	2.0	2.0	0.6655*
36	155.00	10	27856.	0.1	0.1	0.0301	91	81.00	17	65484.	0.2	0.2	0.0709*
37	154.00	17	136332.	0.4	0.4	0.1475*	92	79.00	17	132736.	0.4	0.4	0.1437*
38	153.00	35	781392.	2.6	2.6	0.8457*	93	78.00	25	860768.	2.8	2.8	0.9316
39	152.00	43	1031312.	3.4	3.4	1.1162*	94	77.00	35	5110272.	16.8	16.8	5.5307*
40	151.00	21	318018.	1.0	1.0	0.3442*	95	76.00	25	836480.	2.7	2.7	0.9053*
41	150.00	14	99992.	0.3	0.3	0.1082*	96	75.00	21	394480.	1.3	1.3	0.4269*
42	147.00	6	2058.	0.0	0.0	0.0022	97	74.00	21	239848.	0.8	0.8	0.2596*
43	144.00	6	1126.	0.0	0.0	0.0012	98	73.00	12	4598.	0.0	0.0	0.0050
44	142.00	10	25285.	0.1	0.1	0.0274	99	70.00	12	37873.	0.1	0.1	0.0410*
45	141.00	21	268992.	0.9	0.9	0.2911	100	69.00	21	283548.	0.9	0.9	0.3070*
46	140.00	8	42494.	0.1	0.1	0.0460	101	65.00	21	318784.	1.0	1.0	0.3450*
47	139.00	21	417520.	1.4	1.4	0.4519	102	64.00	21	311616.	1.0	1.0	0.3373
48	138.00	10	17911.	0.1	0.1	0.0320	103	63.00	25	806608.	2.6	2.6	0.8730
49	137.00	12	29552.	0.1	0.1	0.0194	104	62.00	14	136904.	0.4	0.4	0.1482*
50	133.00	8	2555.	0.0	0.0	0.0028	105	61.00	10	34684.	0.1	0.1	0.0375*
51	132.00	10	29797.	0.1	0.1	0.0322	106	59.00	8	4064.	0.0	0.0	0.0044
52	131.00	10	13240.	0.0	0.0	0.0143	107	58.00	10	7869.	0.0	0.0	0.0085*
53	130.00	6	1138.	0.0	0.0	0.0012	108	55.00	6	4150.	0.0	0.0	0.0045
54	129.00	10	54208.	0.2	0.2	0.0587	109	53.00	17	217948.	0.7	0.7	0.2359*
55	128.00	17	259464.	0.9	0.9	0.2809*	110	52.00	21	396352.	1.3	1.3	0.4290*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	51.00	29	2185152.	7.2	7.2	2.3649
112	50.00	25	604016.	2.0	2.0	0.6537
113	45.00	10	28934.	0.1	0.1	0.0313*
114	44.00	17	127148.	0.4	0.4	0.1376*
115	43.00	17	129008.	0.4	0.4	0.1396
116	41.00	10	33350.	0.1	0.1	0.0361*
117	40.00	10	28675.	0.1	0.1	0.0310*
118	39.00	25	795152.	2.6	2.6	0.8606
119	38.00	12	44759.	0.1	0.1	0.0484*
120	37.00	6	1744.	0.0	0.0	0.0019
121	36.00	10	27360.	0.1	0.1	0.0296

BL73PK.1 [TIC-66926592, 100X-21053440] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	430.00	6	1053.	0.0	0.0	0.0016
2	429.00	6	885.	0.0	0.0	0.0013
3	357.00	6	1318.	0.0	0.0	0.0020
4	355.00	8	740.	0.0	0.0	0.0022
5	343.00	8	1457.	0.0	0.0	0.0052
6	341.00	8	3509.	0.0	0.0	0.0016
7	327.00	6	1096.	0.0	0.0	0.0143*
8	325.00	12	9579.	0.0	0.0	0.1375*
9	324.00	21	92024.	0.4	0.4	0.1375*
10	323.00	25	814480.	3.9	3.9	6.5241*
11	322.00	43	4366336.	20.7	20.7	0.0292*
12	321.00	14	19553.	0.1	0.1	0.0211*
13	320.00	17	14098.	0.0	0.0	0.0026
14	319.00	8	1735.	0.0	0.0	0.0070
15	318.00	8	4695.	0.0	0.0	0.0033
16	303.00	8	544.	0.0	0.0	0.0015
17	294.00	14	2211.	0.0	0.0	0.0089
18	292.00	8	987.	0.0	0.0	0.0165
19	283.00	8	5969.	0.1	0.1	0.0778
20	281.00	10	11018.	0.1	0.1	0.0122
21	281.00	17	52101.	0.2	0.2	0.0121
22	279.00	10	8177.	0.0	0.0	0.0027
23	269.00	8	1018.	0.0	0.0	0.0023
24	267.00	10	8123.	0.0	0.0	0.0154
25	266.00	6	1513.	0.0	0.0	0.0056
26	261.00	12	10294.	0.0	0.0	0.0014
27	261.00	10	3770.	0.0	0.0	0.0026
28	250.00	6	965.	0.0	0.0	0.0012
29	249.00	10	1716.	0.0	0.0	0.0046
30	241.00	10	3076.	0.0	0.0	0.0416*
31	240.00	12	27811.	0.1	0.1	0.0021
32	239.00	8	1413.	0.0	0.0	0.0359*
33	231.00	12	24021.	0.1	0.1	0.0048
34	224.00	12	124528.	0.6	0.6	0.0362
35	223.00	17	32479.	0.2	0.2	0.0485
36	222.00	14	24196.	0.1	0.1	0.0362
37	221.00	14	2702.	0.0	0.0	0.0044
38	219.00	8	945.	0.0	0.0	0.0041
39	217.00	6	2732.	0.0	0.0	0.0046
40	211.00	8	3074.	0.0	0.0	0.0055
41	210.00	8	33775.	0.0	0.0	0.0051
42	209.00	17	43589.	0.2	0.2	0.02625
43	208.00	14	175704.	0.8	0.8	0.0126
44	207.00	21	8410.	0.1	0.1	0.0316*
45	206.00	12	21121.	0.0	0.0	0.0019
46	205.00	10	1243.	0.0	0.0	0.0205
47	204.00	8	13722.	0.1	0.1	0.0506*
48	203.00	10	33835.	0.2	0.2	0.0131
49	202.00	17	8740.	0.0	0.0	0.0209*
50	201.00	8	13962.	0.1	0.1	0.0390
51	200.00	12	26131.	0.1	0.1	0.0062
52	199.00	12	4131.	0.0	0.0	0.0163
53	198.00	8	10882.	0.1	0.1	
54	197.00	10				
55						
56	196.00	14	27569.	0.1	0.1	0.0412
57	195.00	17	76340.	0.4	0.4	0.1141
58	194.00	21	129792.	0.6	0.6	0.1939*
59	193.00	25	204184.	1.0	1.0	0.3051*
60	192.00	21	66344.	0.3	0.3	0.0991
61	191.00	25	165872.	0.8	0.8	0.2478*
62	190.00	21	99132.	0.5	0.5	0.1481*
63	189.00	25	187572.	0.9	0.9	0.2803*
64	188.00	14	27179.	0.1	0.1	0.0406*
65	187.00	17	42426.	0.2	0.2	0.0534*
66	186.00	21	4082.	0.0	0.0	0.0061*
67	184.00	10	15555.	0.1	0.1	0.0232
68	183.00	25	229260.	1.1	1.1	0.3426*
69	182.00	43	3202368.	15.2	15.2	4.7849*
70	181.00	59	21053440.	100.0	100.0	*31.45*
71	180.00	51	2717696.	12.9	12.9	4.0507*
72	179.00	51	2342144.	11.1	11.1	3.4936*
73	178.00	51	2206272.	19.5	19.5	3.2366*
74	177.00	51	427456.	2.0	2.0	0.6387*
75	176.00	51	396448.	1.9	1.9	0.5924*
76	175.00	29	79248.	0.4	0.4	0.1184*
77	174.00	17	34957.	0.2	0.2	0.0522*
78	173.00	14	7174.	0.0	0.0	0.0107*
79	172.00	10	3814.	0.0	0.0	0.0057
80	171.00	12	5323.	0.0	0.0	0.0080*
81	170.00	8	7403.	0.0	0.0	0.0111
82	169.00	12	10830.	0.1	0.1	0.0162
83	168.00	21	95208.	0.5	0.5	0.1423*
84	167.00	43	805568.	3.8	3.8	1.2037*
85	166.00	51	4385792.	20.8	20.8	6.5531*
86	165.00	59	5035520.	23.9	23.9	7.5239*
87	164.00	51	505616.	2.4	2.4	0.7555*
88	163.00	51	286656.	1.4	1.4	0.4283*
89	162.00	29	61647.	0.3	0.3	0.0921*
90	161.00	21	75916.	0.4	0.4	0.1134*
91	160.00	12	14346.	0.1	0.1	0.0214*
92	158.00	8	4773.	0.0	0.0	0.0071
93	157.00	12	3191.	0.0	0.0	0.0048*
94	156.00	12	15295.	0.1	0.1	0.0229*
95	155.00	21	127476.	0.6	0.6	0.1905*
96	154.00	35	738816.	3.5	3.5	1.1039*
97	153.00	59	1089280.	5.2	5.2	1.6276*
98	152.00	71	1401664.	6.7	6.7	2.0943*
99	151.00	51	562704.	2.7	2.7	0.8408*
100	150.00	35	190092.	0.9	0.9	0.2840*
101	149.00	21	32224.	0.2	0.2	0.0481*
102	148.00	8	4313.	0.0	0.0	0.0064
103	147.00	10	6260.	0.0	0.0	0.0094*
104	146.00	6	1084.	0.0	0.0	0.0016
105	143.00	12	9976.	0.0	0.0	0.0149
106	142.00	25	157916.	0.8	0.8	0.2360*
107	141.00	29	697808.	3.3	3.3	1.0426*
108	140.00	25	108464.	0.5	0.5	0.1621*
109	139.00	25	369312.	1.8	1.8	0.5518*
110	138.00	17	35191.	0.2	0.2	0.0526*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	137.00	12	22789.	0.1	0.1	0.0341	166	80.00	17	51153.	0.2	0.2	0.0764
112	135.00	10	4256.	0.0	0.0	0.0064	167	79.00	12	15249.	0.1	0.1	0.0228*
113	134.00	8	1490.	0.0	0.0	0.0022	168	78.00	21	52334.	0.2	0.2	0.0782*
114	133.00	12	17627.	0.1	0.1	0.0263*	169	77.00	21	204664.	1.0	1.0	0.3058*
115	132.00	8	1586.	0.0	0.0	0.0024	170	76.00	43	527120.	2.5	2.5	0.7876*
116	131.00	25	1978.	0.0	0.0	0.0019*	171	75.00	29	191700.	0.9	0.9	0.2864*
117	130.00	14	25700.	0.1	0.1	0.0384*	172	74.00	21	79428.	0.4	0.4	0.1187
118	129.00	35	102132.	0.5	0.5	0.1526*	173	73.00	14	35596.	0.2	0.2	0.0532*
119	128.00	25	275280.	1.3	1.3	0.4113	174	71.00	8	2683.	0.0	0.0	0.0040
120	127.00	25	165704.	0.8	0.8	0.2476*	175	70.00	17	42929.	0.2	0.2	0.0641*
121	126.00	21	140116.	0.7	0.7	0.2094*	176	69.00	43	223956.	1.1	1.1	0.3346*
122	125.00	14	27574.	0.1	0.1	0.0412*	177	68.00	12	8877.	0.0	0.0	0.0133*
123	124.00	6	1459.	0.0	0.0	0.0022	178	67.00	14	18928.	0.1	0.1	0.0283*
124	123.00	8	8846.	0.0	0.0	0.0132	179	66.00	10	9533.	0.0	0.0	0.0142
125	122.00	12	37829.	0.2	0.2	0.0565	180	65.00	21	103344.	0.5	0.5	0.1544*
126	121.00	8	2108.	0.0	0.0	0.0031	181	64.00	25	110128.	0.5	0.5	0.1646*
127	120.00	17	3881.	0.0	0.0	0.0058*	182	63.00	25	302240.	1.4	1.4	0.4516
128	119.00	12	9868.	0.0	0.0	0.0147	183	62.00	17	60139.	0.3	0.3	0.0899
129	118.00	8	1949.	0.0	0.0	0.0029	184	61.00	17	63760.	0.3	0.3	0.0953*
130	117.00	10	8466.	0.0	0.0	0.0126*	185	60.00	10	11873.	0.1	0.1	0.0177
131	116.00	17	59614.	0.3	0.3	0.0891	186	59.00	10	3024.	0.0	0.0	0.0045
132	115.00	25	547184.	2.6	2.6	0.8176*	187	57.00	12	24663.	0.1	0.1	0.0369*
133	114.00	14	37587.	0.2	0.2	0.0562*	188	56.00	10	3284.	0.0	0.0	0.0049*
134	113.00	21	63467.	0.3	0.3	0.0948*	189	55.00	17	33928.	0.2	0.2	0.0507*
135	112.00	14	23459.	0.1	0.1	0.0351	190	54.00	10	11322.	0.1	0.1	0.0169
136	111.00	29	144842.	0.7	0.7	0.2164*	191	53.00	21	138708.	0.7	0.7	0.2073*
137	110.00	17	20921.	0.1	0.1	0.0313*	192	52.00	21	42384.	0.2	0.2	0.0633*
138	109.00	8	4139.	0.0	0.0	0.0062*	193	51.00	29	216512.	1.0	1.0	0.3235
139	108.00	6	1059.	0.0	0.0	0.0016	194	50.00	21	99632.	0.5	0.5	0.1489
140	106.00	6	649.	0.0	0.0	0.0010	195	49.00	8	5414.	0.0	0.0	0.0081
141	105.00	8	1595.	0.0	0.0	0.0024	196	47.00	8	3990.	0.0	0.0	0.0060
142	104.00	8	4051.	0.0	0.0	0.0061	197	46.00	10	2421.	0.0	0.0	0.0036
143	103.00	43	89668.	0.4	0.4	0.1340*	198	45.00	21	64812.	0.3	0.3	0.0968*
144	102.00	51	151744.	0.7	0.7	0.2267*	199	44.00	29	174084.	0.8	0.8	0.2601*
145	101.00	35	100372.	0.5	0.5	0.1500*	200	43.00	29	381472.	1.8	1.8	0.5700
146	100.00	12	26248.	0.1	0.1	0.0392	201	42.00	29	505488.	2.4	2.4	0.7553
147	99.00	14	31568.	0.1	0.1	0.0472	202	41.00	25	122294.	0.6	0.6	0.1826*
148	98.00	17	42541.	0.2	0.2	0.0636*	203	40.00	14	25433.	0.1	0.1	0.0380
149	97.00	29	210644.	1.0	1.0	0.3147*	204	39.00	25	213540.	1.0	1.0	0.3191
150	96.00	43	230636.	1.1	1.1	0.3446*	205	38.00	17	34026.	0.2	0.2	0.0508*
151	95.00	35	132684.	0.6	0.6	0.1983*	206	37.00	8	6682.	0.0	0.0	0.0100*
152	94.00	29	143416.	0.7	0.7	0.2143*	207	36.00	17	40846.	0.2	0.2	0.0610*
153	93.00	14	32621.	0.2	0.2	0.0487*	208	35.00	8	2965.	0.0	0.0	0.0044
154	92.00	17	3772.	0.0	0.0	0.0056*							
155	91.00	14	66600.	0.3	0.3	0.0995							
156	90.00	29	143336.	0.7	0.7	0.2142*							
157	89.00	51	873760.	4.2	4.2	1.3055*							
158	88.00	35	281264.	1.3	1.3	0.4203*							
159	87.00	25	113480.	0.5	0.5	0.1696*							
160	86.00	17	34492.	0.2	0.2	0.0515							
161	85.00	12	11673.	0.1	0.1	0.0174*							
162	84.00	12	17063.	0.1	0.1	0.0255*							
163	83.00	43	739344.	3.5	3.5	1.1047*							
164	82.00	51	571312.	2.7	2.7	0.8536*							
165	81.00	43	153076.	0.7	0.7	0.2287*							

FV5AV.1 [TIC-49985536, 188X-18626816] EI

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	82.00	71	2873024.	27.0	27.0	5.7477*
112	81.00	59	1143296.	10.8	10.8	2.2873*
113	80.00	10	11642.	0.1	0.1	0.0233*
114	79.00	8	4161.	0.0	0.0	0.0083
115	78.00	8	5091.	0.0	0.0	0.0102
116	77.00	17	70428.	0.7	0.7	0.1409*
117	76.00	21	147500.	1.4	1.4	0.2951*
118	75.00	25	232428.	2.2	2.2	0.4650*
119	74.00	25	254784.	2.4	2.4	0.5097
120	73.00	10	22665.	0.2	0.2	0.0453*
121	71.00	6	1322.	0.0	0.0	0.0026
122	70.00	21	87028.	0.8	0.8	0.1741*
123	69.00	59	1024240.	9.6	9.6	2.0491*
124	68.00	17	55846.	0.5	0.5	0.1117*
125	66.00	8	866.	0.0	0.0	0.0017
126	65.00	17	90476.	0.9	0.9	0.1810*
127	64.00	21	147724.	1.4	1.4	0.2955*
128	63.00	29	613600.	5.8	5.8	1.2276*
129	62.00	25	244348.	2.3	2.3	0.4888
130	61.00	14	59005.	0.6	0.6	0.1180*
131	56.00	12	28688.	0.3	0.3	0.0574*
132	55.00	10	17970.	0.2	0.2	0.0360*
133	53.00	12	6011.	0.1	0.1	0.0120
134	52.00	10	25409.	0.2	0.2	0.0508*
135	51.00	29	269360.	2.5	2.5	0.5389*
136	50.00	25	239076.	2.2	2.2	0.4783*
137	49.00	12	6357.	0.1	0.1	0.0127*
138	48.00	8	3257.	0.0	0.0	0.0065
139	47.00	10	7319.	0.1	0.1	0.0146*
140	45.00	10	30216.	0.3	0.3	0.0604*
141	44.00	21	113820.	1.1	1.1	0.2277*
142	43.00	8	4154.	0.0	0.0	0.0083
143	41.00	6	4845.	0.0	0.0	0.0097
144	40.00	8	8281.	0.1	0.1	0.0166
145	39.00	29	292096.	2.7	2.7	0.5844*
146	38.00	17	69580.	0.7	0.7	0.1392*
147	37.00	8	5020.	0.0	0.0	0.0100
148	36.00	17	112332.	1.1	1.1	0.2247*
149	35.00	14	20379.	0.2	0.2	0.0400*

8012PA.1 [TIC=42631168, 189X=7565824] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	5	1025.	0.0	0.0	0.0024
2	365.00	17	139589.	1.8	17.5	3.0924
3	305.00	21	1321536.	17.5	17.5	3.0999*
4	304.00	43	7325440.	95.8	96.8	*17.18*
5	303.00	17	42119.	0.6	0.6	0.0988*
6	296.00	10	22159.	0.3	0.3	0.0520
7	285.00	17	125600.	1.7	1.7	0.2946
8	284.00	8	2371.	0.0	0.0	0.0056
9	283.00	8	6170.	0.1	0.1	0.0145
10	282.00	6	4759.	0.1	0.1	0.0112
11	281.00	14	58775.	0.8	0.8	0.1379
12	267.00	8	4934.	0.1	0.1	0.0116
13	235.00	6	1057.	0.0	0.0	0.0025
14	222.00	10	7531.	0.1	0.1	0.0177
15	221.00	14	8394.	1.1	1.1	0.1969
16	220.00	17	105148.	1.4	1.4	0.2466
17	219.00	6	5318.	0.1	0.1	0.0125
18	209.00	10	36432.	0.5	0.5	0.0855
19	208.00	14	62544.	0.8	0.8	0.1467
20	207.00	21	378272.	5.0	5.0	0.8873*
21	205.00	25	1230272.	16.3	16.3	2.8859*
22	205.00	43	7565824.	100.0	100.0	*17.74*
23	204.00	12	44057.	0.6	0.6	0.1033
24	203.00	8	4010.	0.1	0.1	0.0094
25	194.00	8	24014.	0.3	0.3	0.0563*
26	193.00	17	165900.	2.2	2.2	0.3893
27	192.00	10	19377.	0.3	0.3	0.0455
28	191.00	10	20405.	0.3	0.3	0.0479
29	179.00	17	102368.	1.4	1.4	0.2401
30	178.00	25	1034896.	13.7	13.7	2.4276
31	177.00	43	5678000.	75.0	75.0	*13.31*
32	176.00	51	3291072.	43.5	43.5	7.7199*
33	175.00	43	582064.	7.7	7.7	1.3653*
34	174.00	21	296144.	3.9	3.9	0.5947
35	173.00	10	11903.	0.2	0.2	0.0279*
36	169.00	6	2423.	0.0	0.0	0.0057
37	165.00	10	10582.	0.1	0.1	0.0246
38	165.00	17	177908.	2.4	2.4	0.4175
39	164.00	21	207752.	2.7	2.7	0.4873
40	163.00	21	220348.	2.9	2.9	0.5169
41	162.00	8	19392.	0.3	0.3	0.0455
42	159.00	8	2984.	0.0	0.0	0.0049
43	154.00	12	2945.	0.0	0.0	0.0069
44	153.00	29	102332.	1.4	1.4	0.2414*
45	152.00	25	406400.	5.4	5.4	0.9533
46	151.00	21	1064128.	14.1	14.1	2.4961
47	150.00	21	683104.	9.0	9.0	1.6024*
48	149.00	17	133276.	1.8	1.8	0.3126
49	147.00	14	4886.	0.1	0.1	0.0115
50	140.00	12	3873.	0.1	0.1	0.0091*
51	139.00	21	55281.	0.7	0.7	0.1297*
52	138.00	14	31749.	0.4	0.4	0.0745*
53	137.00	14	27017.	0.4	0.4	0.0634*
54	135.00	6	1499.	0.0	0.0	0.0035
55	134.00	8	2733.	0.0	0.0	0.0064

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. REF	% TOT. ION
111	41.98	6	1813.	0.0	0.0	0.0043
112	48.00	14	3574.	0.0	0.0	0.0084*
113	39.00	17	9898.	1.3	1.3	0.2322*
114	38.00	12	12950.	0.2	0.2	0.0304*
115	36.00	8	10490.	0.1	0.1	0.0246

8L74PK.1 [TIC=28363776, 188X=4514816] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	415.00	6	1201.	0.0	0.0	0.0042
2	355.00	6	3642.	0.1	0.1	0.0128
3	341.00	12	7425.	0.2	0.2	0.0262*
4	327.00	8	873.	0.0	0.0	0.0031
5	322.00	6	1066.	0.0	0.0	0.0038
6	309.00	6	1408.	0.0	0.0	0.0050
7	307.00	10	5988.	0.1	0.1	0.0211
8	306.00	17	8048.	1.8	1.8	0.0836*
9	305.00	29	805104.	17.8	17.8	2.8385*
10	304.00	43	4514815.	100.0	100.0	15.91*
11	303.00	17	36315.	0.8	0.8	0.0382*
12	302.00	12	10834.	0.0	0.0	0.0012
13	301.00	8	339.	0.0	0.0	0.00119
14	287.00	19	3377.	0.1	0.1	0.0514
15	286.00	16	14590.	0.3	0.3	0.03940
16	285.00	17	111748.	2.5	2.5	0.08131
17	284.00	10	3723.	0.1	0.1	0.0336*
18	283.00	10	9526.	0.2	0.2	0.0566
19	282.00	10	16067.	0.4	0.4	0.01894
20	281.00	17	53732.	1.2	1.2	0.0041
21	269.00	8	1160.	0.3	0.3	0.0047
22	267.00	12	12047.	0.1	0.1	0.0085
23	265.00	8	2416.	0.0	0.0	0.0425
24	260.00	8	1346.	0.0	0.0	0.0047
25	259.00	12	7281.	0.2	0.2	0.0043
26	258.00	6	1217.	0.0	0.0	0.0032
27	257.00	6	900.	0.0	0.0	0.0043
28	253.00	8	1206.	0.0	0.0	0.0064
29	251.00	10	1828.	0.0	0.0	0.0045
30	240.00	8	1283.	0.0	0.0	0.0045
31	239.00	8	8858.	0.2	0.2	0.0312
32	238.00	14	1520.	0.1	0.1	0.0054
33	235.00	6	5114.	0.0	0.0	0.0054
34	233.00	6	1273.	0.0	0.0	0.0045
35	223.00	6	1383.	0.0	0.0	0.0049
36	222.00	10	8250.	0.2	0.2	0.0291
37	221.00	17	47820.	1.1	1.1	0.1686
38	220.00	14	55036.	1.2	1.2	0.0044
39	219.00	8	1261.	0.0	0.0	0.0052
40	216.00	10	1461.	0.0	0.0	0.0054
41	211.00	6	1532.	0.0	0.0	0.0052
42	210.00	8	5123.	0.1	0.1	0.0181
43	209.00	17	45868.	1.0	1.0	0.1617*
44	208.00	21	67188.	1.5	1.5	0.2369*
45	206.00	25	341872.	7.6	7.6	1.2053*
46	205.00	29	565104.	14.7	14.7	2.3449*
47	204.00	43	4113216.	91.1	91.1	14.50*
48	203.00	21	52258.	1.2	1.2	0.1842*
49	200.00	17	33210.	0.7	0.7	0.1171-
50	196.00	6	1825.	0.0	0.0	0.0064
51	195.00	6	1063.	0.0	0.0	0.0037
52	194.00	8	1578.	0.0	0.0	0.0037
53	193.00	6	1064.	0.0	0.0	0.0038
54	193.00	10	19933.	0.4	0.4	0.0083
55	192.00	12	26251.	0.6	0.6	0.0926*
56	191.00	17	48757.	1.1	1.1	0.1719*
57	189.00	10	6857.	0.2	0.2	0.0242
58	189.00	10	7253.	0.2	0.2	0.0256
59	188.00	6	471.	0.0	0.0	0.0017
60	187.00	8	4867.	0.1	0.1	0.0172
61	183.00	12	2991.	0.1	0.1	0.0105
62	181.00	10	2523.	0.1	0.1	0.0089
63	179.00	17	74104.	1.6	1.6	0.2613*
64	178.00	35	689712.	15.3	15.3	2.4317*
65	177.00	51	3972288.	88.0	88.0	14.00*
66	176.00	43	2000256.	44.3	44.3	7.0521*
67	175.00	51	438352.	9.7	9.7	1.5455*
68	174.00	35	217796.	4.8	4.8	0.7679*
69	173.00	21	18750.	0.4	0.4	0.0661*
70	172.00	8	1539.	0.0	0.0	0.0054
71	169.00	12	10495.	0.2	0.2	0.0370*
72	168.00	6	432.	0.0	0.0	0.0015
73	167.00	6	857.	0.0	0.0	0.0030
74	166.00	12	10893.	0.2	0.2	0.0384
75	165.00	21	92392.	2.0	2.0	0.3257*
76	164.00	25	101176.	2.2	2.2	0.3567*
77	163.00	21	2080.	2.7	2.7	0.4304*
78	162.00	17	28704.	0.6	0.6	0.1012*
79	161.00	12	14748.	0.3	0.3	0.0520
80	159.00	6	1326.	0.0	0.0	0.004-
81	157.00	8	2151.	0.0	0.0	0.0076
82	156.00	10	3100.	0.1	0.1	0.0109*
83	155.00	8	2726.	0.1	0.1	0.0096
84	154.00	21	13083.	0.3	0.3	0.0461*
85	153.00	35	71464.	1.6	1.6	0.2520*
86	152.00	29	223580.	5.0	5.0	0.7883*
87	151.00	29	645120.	14.3	14.3	2.2745
88	150.00	29	412240.	9.1	9.1	1.4534*
89	149.00	25	89864.	2.0	2.0	0.3168*
90	148.00	6	1584.	0.0	0.0	0.0056
91	147.00	12	10468.	0.2	0.2	0.0370*
92	146.00	10	4215.	0.1	0.1	0.0149
93	143.00	8	697.	0.0	0.0	0.0025
94	141.00	6	958.	0.0	0.0	0.0034
95	140.00	21	14363.	0.3	0.3	0.0506*
96	139.00	35	64928.	1.4	1.4	0.2289*
97	138.00	35	50003.	1.1	1.1	0.1763*
98	137.00	17	31697.	0.7	0.7	0.1118*
99	136.00	8	3511.	0.1	0.1	0.0124
100	135.00	12	11282.	0.2	0.2	0.0398
101	134.00	10	8740.	0.2	0.2	0.0308
102	133.00	14	33088.	0.7	0.7	0.1167
103	132.00	6	985.	0.0	0.0	0.0035
104	131.00	8	2838.	0.1	0.1	0.0100
105	130.00	12	1297.	0.0	0.0	0.0046
106	129.00	6	7777.	0.2	0.2	0.0274*
107	128.00	8	3338.	0.1	0.1	0.0118
108	127.00	17	48427.	1.1	1.1	0.1707
109	126.00	21	93952.	2.1	2.1	0.3312*
110	125.00	17	38112.	0.8	0.8	0.1344

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	124.00	17	22633.	0.5	0.5	0.0798
112	123.00	12	35538.	0.8	0.8	0.1253
113	122.00	12	27965.	0.3	0.6	0.0984
114	119.00	12	15727.	0.3	0.3	0.0554
115	118.00	10	3766.	0.1	0.1	0.0133
116	117.00	6	2675.	0.1	0.1	0.0094
117	116.00	8	940.	0.0	0.0	0.0033
118	115.00	12	15366.	0.3	0.3	0.0542*
119	114.00	10	6949.	0.2	0.2	0.0245
120	113.00	12	25947.	0.6	0.6	0.0915
121	112.00	12	12361.	0.3	0.3	0.0436*
122	111.00	17	47122.	1.0	1.0	0.1661
123	110.00	14	39497.	0.9	0.9	0.1393*
124	109.00	8	6334.	0.1	0.1	0.0223*
125	108.00	6	1146.	0.0	0.0	0.0046
126	105.00	12	2806.	0.1	0.1	0.0099*
127	104.00	8	1145.	0.0	0.0	0.0040
128	103.00	25	138960.	3.1	3.1	0.4899*
129	102.00	43	703744.	15.6	15.6	2.4811*
130	101.00	21	41263.	0.9	0.9	0.1455*
131	100.00	17	47614.	1.1	1.1	0.1679
132	99.00	21	77820.	1.7	1.7	0.2744*
133	98.00	21	105116.	2.3	2.3	0.3706
134	97.00	14	19389.	0.4	0.4	0.0584*
135	96.00	29	79632.	1.8	1.8	0.2808*
136	95.00	6	2187.	0.0	0.0	0.0077
137	94.00	8	2121.	0.0	0.0	0.0075
138	91.00	8	1588.	0.5	0.0	0.0056
139	89.00	29	178592.	4.0	4.0	0.6296*
140	88.00	71	2809856.	62.2	62.2	9.9065*
141	87.00	59	446864.	9.9	9.9	1.5755*
142	86.00	21	95896.	2.1	2.1	0.3381*
143	85.00	10	18826.	0.4	0.4	0.0664*
144	84.00	6	2939.	0.1	0.1	0.0104
145	83.00	25	152004.	3.4	3.4	0.5359*
146	82.00	29	75868.	1.7	1.7	0.2675*
147	81.00	17	31491.	0.7	0.7	0.1110*
148	79.00	10	7037.	0.2	0.2	0.0248
149	78.00	14	8052.	0.2	0.2	0.0284
150	77.00	17	58733.	1.3	1.3	0.2071*
151	76.00	29	147660.	3.3	3.3	0.5206*
152	75.00	43	549152.	12.2	12.2	1.9361*
153	74.00	29	182904.	4.1	4.1	0.6449*
154	73.00	21	59244.	1.3	1.3	0.2089*
155	72.00	8	2676.	0.0	0.0	0.0073
156	71.00	8	1098.	0.0	0.0	0.0039
157	70.00	6	1356.	0.0	0.0	0.0048
158	69.00	29	114288.	2.5	2.5	0.4029*
159	68.00	8	1489.	0.0	0.0	0.0052
160	67.00	8	1188.	0.0	0.0	0.0042
161	66.00	8	1410.	0.0	0.0	0.0050
162	65.00	12	8744.	0.2	0.2	0.0308
163	64.00	21	63610.	1.4	1.4	0.2243*
164	63.00	25	172368.	3.8	3.8	0.6077*
165	62.00	25	106280.	2.4	2.4	0.3747*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
166	61.00	17	25171.	0.6	0.6	0.0887*
167	59.00	8	4571.	0.1	0.1	0.0161
168	58.00	8	2955.	0.1	0.1	0.0104
169	57.00	10	1927.	0.0	0.0	0.0068
170	55.00	12	7153.	0.2	0.2	0.0252*
171	53.00	8	2589.	0.1	0.1	0.0091
172	52.00	17	15459.	0.3	0.3	0.0545*
173	51.00	25	139276.	3.1	3.1	0.4910*
174	50.00	21	108104.	2.4	2.4	0.3811*
175	49.00	8	3920.	0.1	0.1	0.0138
176	47.00	6	2230.	0.0	0.0	0.0079
177	45.00	17	22010.	0.5	0.5	0.0776*
178	44.00	25	89692.	2.0	2.0	0.3162*
179	43.00	12	14932.	0.3	0.3	0.0526*
180	42.00	10	2192.	0.0	0.0	0.0077
181	41.00	8	2945.	0.1	0.1	0.0104
182	40.00	10	8797.	0.2	0.2	0.0310*
183	39.00	21	74636.	1.7	1.7	0.2631
184	38.00	21	26172.	0.6	0.6	0.0923*
185	37.00	10	1819.	0.0	0.0	0.0064
186	36.00	17	29338.	0.6	0.6	0.1034
187	35.00	10	5054.	0.1	0.1	0.0178

8CA7PK.1 [TIC-39227392, 188X-5114624] EI

2-hydroxybenzoic acid,
2,2,2-trifluoroethyl, trifluoroacetate diester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	459.00	8	1026.	0.0	0.0	0.0026	56	188.00	17	34534.	0.7	0.7	0.0883*
2	415.00	6	1166.	0.0	0.0	0.0030	57	185.00	8	2585.	0.1	0.1	0.0066
3	401.00	6	1173.	0.0	0.0	0.0030	58	184.00	10	1014.	0.0	0.0	0.0026
4	381.00	8	1525.	0.0	0.0	0.0039	59	183.00	12	39345.	0.8	0.8	0.1003
5	319.00	6	2834.	0.1	0.1	0.0072	60	182.00	8	1799.	0.0	0.0	0.0046
6	318.00	12	57582.	1.1	1.1	0.1468*	61	181.00	10	5187.	0.1	0.1	0.0132
7	317.00	21	345408.	6.8	6.8	0.8805*	62	179.00	8	672.	0.0	0.0	0.0017
8	316.00	35	3232000.	63.2	63.2	8.2391*	63	177.00	10	18149.	0.4	0.4	0.0463
9	315.00	17	50097.	1.0	1.0	0.1277*	64	176.00	8	354.	0.0	0.0	0.0009
10	314.00	8	1611.	0.0	0.0	0.0041	65	175.00	10	15269.	0.3	0.3	0.0389
11	299.00	10	1402.	0.0	0.0	0.0036	66	174.00	12	31409.	0.6	0.6	0.0801*
12	298.00	10	45532.	0.9	0.9	0.1161	67	173.00	10	3761.	0.1	0.1	0.0096
13	297.00	17	319408.	6.2	6.2	0.8142*	68	172.00	8	1633.	0.0	0.0	0.0042
14	296.00	8	2465.	0.0	0.0	0.0063	69	171.00	10	19853.	0.4	0.4	0.0506
15	288.00	8	1148.	0.0	0.0	0.0029	70	170.00	14	1976.	0.0	0.0	0.0050*
16	287.00	8	5932.	0.1	0.1	0.0151	71	169.00	12	45755.	0.9	0.9	0.1165*
17	281.00	10	7516.	0.1	0.1	0.0192	72	168.00	6	1550.	0.0	0.0	0.0040
18	280.00	6	315.	0.0	0.0	0.0028	73	167.00	10	10799.	0.2	0.2	0.0275*
19	271.00	8	4895.	0.1	0.1	0.0125	74	166.00	8	3567.	0.1	0.1	0.0091
20	270.00	6	1096.	0.0	0.0	0.0028	75	165.00	12	9482.	0.2	0.2	0.0242*
21	269.00	12	42653.	0.8	0.8	0.1087	76	164.00	10	19823.	0.4	0.4	0.0505
22	267.00	10	14368.	0.3	0.3	0.0366	77	163.00	21	234936.	4.6	4.6	0.5989*
23	265.00	8	2866.	0.1	0.1	0.0073	78	162.00	10	14006.	0.3	0.3	0.0357*
24	253.00	14	47230.	0.9	0.9	0.1204	79	161.00	8	16664.	0.3	0.3	0.0425
25	249.00	8	7904.	0.2	0.2	0.0201	80	159.00	8	1676.	0.0	0.0	0.0043
26	248.00	10	30385.	0.6	0.6	0.0775	81	158.00	8	1985.	0.0	0.0	0.0051
27	247.00	17	225756.	4.4	4.4	0.5755	82	157.00	8	3315.	0.1	0.1	0.0085
28	243.00	8	721.	0.0	0.0	0.0018	83	155.00	10	24768.	0.5	0.5	0.0631
29	239.00	6	877.	0.0	0.0	0.0022	84	154.00	8	3446.	0.1	0.1	0.0088
30	238.00	6	929.	0.0	0.0	0.0024	85	153.00	6	4096.	0.1	0.1	0.0104
31	235.00	8	623.	0.0	0.0	0.0016	86	152.00	6	625.	0.0	0.0	0.0016
32	233.00	6	877.	0.0	0.0	0.0022	87	151.00	8	5485.	0.1	0.1	0.0140
33	225.00	6	1904.	0.0	0.0	0.0049	88	150.00	8	7509.	0.1	0.1	0.0191
34	221.00	10	5991.	0.1	0.1	0.0153	89	149.00	17	115600.	2.3	2.3	0.2947*
35	220.00	10	12230.	0.2	0.2	0.0312	90	147.00	10	8219.	0.2	0.2	0.0210
36	219.00	17	106668.	2.1	2.1	0.2720*	91	146.00	12	26190.	0.5	0.5	0.0668*
37	218.00	25	474912.	9.3	9.3	1.2107*	92	145.00	10	21311.	0.4	0.4	0.0543*
38	217.00	51	5114624.	100.0	100.0	*13.03*	93	144.00	6	1916.	0.0	0.0	0.0049
39	216.00	21	44291.	0.9	0.9	0.1129*	94	143.00	10	10045.	0.2	0.2	0.0256
40	215.00	12	9292.	0.2	0.2	0.0237*	95	142.00	8	2664.	0.1	0.1	0.0068
41	214.00	10	4126.	0.1	0.1	0.0105*	96	141.00	10	17316.	0.3	0.3	0.0441
42	207.00	6	7108.	0.1	0.1	0.0181	97	140.00	10	5029.	0.1	0.1	0.0128*
43	206.00	8	1561.	0.0	0.0	0.0040	98	139.00	17	122156.	2.4	2.4	0.3114
44	205.00	10	15105.	0.3	0.3	0.0385	99	138.00	8	6490.	0.1	0.1	0.0165
45	204.00	12	36594.	0.7	0.7	0.0933	100	137.00	10	6347.	0.1	0.1	0.0162*
46	203.00	17	254336.	5.0	5.0	0.6484	101	136.00	8	2667.	0.1	0.1	0.0068
47	202.00	17	70368.	1.4	1.4	0.1794*	102	135.00	8	5525.	0.1	0.1	0.0141
48	201.00	8	5565.	0.1	0.1	0.0142	103	134.00	8	4014.	0.1	0.1	0.0102
49	200.00	8	1650.	0.0	0.0	0.0042	104	133.00	14	80744.	1.6	1.6	0.2058
50	199.00	6	1280.	0.0	0.0	0.0033	105	132.00	10	6114.	0.1	0.1	0.0156
51	192.00	6	1327.	0.0	0.0	0.0034	106	131.00	10	17103.	0.3	0.3	0.0436*
52	193.00	8	8338.	0.2	0.2	0.0213	107	128.00	8	804.	0.0	0.0	0.0020
53	191.00	17	84880.	1.7	1.7	0.2164*	108	127.00	17	113532.	2.2	2.2	0.2894
54	190.00	21	250444.	4.9	4.9	0.6384*	109	126.00	8	9791.	0.2	0.2	0.0250
55	189.00	35	2986624.	58.4	58.4	7.6136*	110	125.00	10	15461.	0.3	0.3	0.0394

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	124.00	17	168592.	3.3	3.3	0.4298*	166	63.00	29	1303552.	25.5	25.5	3.3231
112	123.00	35	2323584.	45.4	45.4	5.3234*	167	62.00	25	250400.	4.9	4.9	0.6383*
113	122.00	14	47352.	0.9	0.9	0.1207*	168	61.00	17	84812.	1.7	1.7	0.2162*
114	121.00	25	523232.	10.2	10.2	1.3338*	169	60.00	8	4493.	0.1	0.1	0.0115
115	120.00	35	2785920.	54.5	54.5	7.1020*	170	59.00	10	7189.	0.1	0.1	0.0183*
116	119.00	21	140340.	2.7	2.7	0.3578*	171	57.00	12	27874.	0.5	0.5	0.0711*
117	117.00	8	2386.	0.0	0.0	0.0061	172	56.00	8	1719.	0.0	0.0	0.0044
118	115.00	10	28936.	0.6	0.6	0.0738	173	55.00	10	19268.	0.4	0.4	0.0491
119	114.00	12	14606.	0.3	0.3	0.0372*	174	54.00	12	28862.	0.6	0.6	0.0736
120	113.00	12	43514.	0.9	0.9	0.1109	175	53.00	25	239676.	4.7	4.7	0.6110*
121	112.00	8	8312.	0.2	0.2	0.0212	176	52.00	21	213000.	4.2	4.2	0.5430*
122	111.00	17	99832.	2.0	2.0	0.2545*	177	51.00	21	202104.	4.0	4.0	0.5152
123	110.00	8	831.	0.0	0.0	0.0021	178	50.00	29	513296.	10.0	10.0	1.3085
124	109.00	10	26091.	0.5	0.5	0.0665*	179	49.00	12	37513.	0.7	0.7	0.0956*
125	108.00	12	26872.	0.5	0.5	0.0685	180	48.00	5	1135.	0.0	0.0	0.0029
126	107.00	12	42256.	0.8	0.8	0.1077*	181	47.00	10	15320.	0.3	0.3	0.0391*
127	106.00	10	9552.	0.2	0.2	0.0244	182	46.00	6	9654.	0.2	0.2	0.0246
128	105.00	17	111420.	2.2	2.2	0.2840	183	45.00	17	41786.	0.8	0.8	0.1065*
129	104.00	17	106952.	2.1	2.1	0.2726	184	44.00	17	99056.	1.9	1.9	0.2525*
130	103.00	12	2137.	0.0	0.0	0.0054	185	43.00	8	2275.	0.0	0.0	0.0058
131	101.00	8	9124.	0.2	0.2	0.0233	186	42.00	8	4868.	0.1	0.1	0.0124
132	100.00	10	2628.	0.1	0.1	0.0067	187	41.00	8	7311.	0.1	0.1	0.0186
133	99.00	10	18831.	0.4	0.4	0.0480	188	40.00	10	14315.	0.3	0.3	0.0365
134	98.00	8	6600.	0.1	0.1	0.0168	189	39.00	21	294672.	5.8	5.8	0.7512*
135	97.00	21	209112.	4.1	4.1	0.5331*	190	38.00	25	461712.	9.0	9.0	1.1770
136	96.00	17	146844.	2.9	2.9	0.3743	191	37.00	25	123640.	2.4	2.4	0.3152*
137	95.00	29	2486464.	48.6	48.6	6.3386*	192	36.00	17	96404.	1.9	1.9	0.2458*
138	94.00	17	100992.	2.0	2.0	0.2575*	193	35.00	8	6860.	0.1	0.1	0.0175
139	93.00	21	291472.	5.7	5.7	0.7430*							
140	92.00	35	2058816.	40.3	40.3	5.2484*							
141	91.00	17	122232.	2.4	2.4	0.3116							
142	90.00	8	4315.	0.1	0.1	0.0110							
143	89.00	8	6564.	0.1	0.1	0.0167							
144	88.00	8	1137.	0.0	0.0	0.0029							
145	85.00	10	21613.	0.4	0.4	0.0551*							
146	84.00	12	36942.	0.7	0.7	0.0942*							
147	83.00	29	953024.	18.6	18.6	2.4295*							
148	82.00	10	16111.	0.3	0.3	0.0411*							
149	81.00	21	226532.	4.4	4.4	0.5775*							
150	80.00	25	162148.	3.2	3.2	0.4134*							
151	79.00	12	27415.	0.5	0.5	0.0699*							
152	78.00	14	60848.	1.2	1.2	0.1551*							
153	77.00	21	171956.	3.4	3.4	0.4384*							
154	76.00	21	252604.	4.9	4.9	0.6439							
155	75.00	21	340192.	6.7	6.7	0.8672*							
156	74.00	21	150624.	2.9	2.9	0.3840*							
157	73.00	29	64635.	1.3	1.3	0.1648*							
158	71.00	12	19866.	0.4	0.4	0.0506*							
159	70.00	17	50620.	1.0	1.0	0.1290*							
160	69.00	35	3765528.	73.6	73.6	9.6018*							
161	68.00	10	14641.	0.3	0.3	0.0373*							
162	67.00	8	845.	0.0	0.0	0.0022							
163	66.00	17	69916.	1.4	1.4	0.1782*							
164	65.00	25	291632.	5.7	5.7	0.7434*							
165	64.00	29	1293376.	25.3	25.3	3.2971*							

8L71PK.1 [TIC-50165760, 100X-12428280] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	385.00	8	3150	0.0	0.0	0.0063
2	331.00	6	1280	0.0	0.0	0.0026
3	319.00	10	4284	0.0	0.0	0.0084*
4	318.00	21	64797	0.5	0.5	0.1292*
5	317.00	29	479888	3.9	3.9	0.9566*
6	316.00	35	4150016	33.4	33.4	0.2726*
7	315.00	29	132348	1.1	1.1	0.2638*
8	314.00	14	11088	0.1	0.1	0.0221*
9	313.00	12	1179	0.0	0.0	0.0024
10	299.00	8	1542	0.0	0.0	0.0031
11	298.00	17	50493	0.4	0.4	0.1007
12	297.00	25	3473808	2.8	2.8	0.6853*
13	295.00	8	1691	0.0	0.0	0.0034
14	295.00	6	1123	0.0	0.0	0.0022
15	288.00	6	1565	0.0	0.0	0.0031
16	287.00	10	8209	0.1	0.1	0.0164
17	277.00	8	3025	0.0	0.0	0.0060
18	276.00	6	683	0.0	0.0	0.0014
19	272.00	10	1561	0.0	0.0	0.0031
20	271.00	8	4161	0.0	0.0	0.0083
21	270.00	8	3957	0.0	0.0	0.0079
22	269.00	17	85452	0.7	0.7	0.1703
23	267.00	8	4562	0.0	0.0	0.0091
24	265.00	12	16540	0.1	0.1	0.0330
25	254.00	12	4872	0.0	0.0	0.0097
26	253.00	14	62651	0.5	0.5	0.1253
27	252.00	12	7917	0.1	0.1	0.0158
28	249.00	10	17172	0.1	0.1	0.0342
29	248.00	12	28414	0.2	0.2	0.0566
30	247.00	12	27121	0.2	0.2	0.0541
31	245.00	10	1607	0.0	0.0	0.0032
32	241.00	8	2061	0.0	0.0	0.0041
33	239.00	8	2837	0.0	0.0	0.0057
34	231.00	6	1588	0.0	0.0	0.0032
35	225.00	12	3062	0.0	0.0	0.0061
36	221.00	14	5787	0.0	0.0	0.0115*
37	220.00	17	33604	0.3	0.3	0.0670*
38	219.00	25	180588	1.5	1.5	0.3600*
39	218.00	43	1116800	10.0	10.0	2.2262*
40	217.00	71	12428288	100.0	100.0	24.77*
41	216.00	29	82792	0.7	0.7	0.1650*
42	215.00	14	7720	0.1	0.1	0.0154*
43	214.00	21	12709	0.1	0.1	0.0253*
44	212.00	8	622	0.0	0.0	0.0012
45	211.00	6	1596	0.0	0.0	0.0029
46	207.00	10	1475	0.0	0.0	0.0026
47	206.00	10	1282	0.0	0.0	0.0026
48	205.00	10	8587	0.1	0.1	0.0171
49	204.00	17	51438	0.4	0.4	0.1025
50	203.00	25	480896	3.9	3.9	0.9585
51	202.00	17	36985	0.3	0.3	0.0737*
52	195.00	6	1808	0.0	0.0	0.0036
53	193.00	8	7868	0.1	0.1	0.0157
54	192.00	17	27733	0.2	0.2	0.0553
55	191.00	25	232708	1.9	1.9	0.4639*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	123.00	17	45710.	0.4	0.4	0.0911	166	64.00	43	1770944.	14.2	14.2	3.5302*
112	122.00	10	10823.	0.1	0.1	0.0216	167	63.00	43	1776256.	14.3	14.3	3.5408*
113	121.00	17	93312.	0.8	0.8	0.1860	168	62.00	43	437168.	3.5	3.5	0.8714*
114	120.00	29	474704.	3.8	3.8	0.9463*	169	61.00	25	112748.	0.9	0.9	0.2248*
115	119.00	25	268480.	2.2	2.2	0.5352*	170	60.00	25	19026.	0.2	0.2	0.0379*
116	118.00	12	6700.	0.1	0.1	0.0134*	171	59.00	6	6272.	0.1	0.1	0.0125
117	117.00	8	1038.	0.0	0.0	0.0021	172	58.00	5	1576.	0.0	0.0	0.0031
118	115.00	14	18316.	0.1	0.1	0.0365*	173	57.00	21	39555.	0.3	0.3	0.0788*
119	114.00	10	17853.	0.1	0.1	0.0356	174	56.00	17	16784.	0.1	0.1	0.0335*
120	113.00	25	130512.	1.1	1.1	0.2602	175	55.00	14	26367.	0.2	0.2	0.0538*
121	112.00	6	2812.	0.0	0.0	0.0056	176	54.00	17	52817.	0.4	0.4	0.1053
122	111.00	21	94752.	0.8	0.8	0.1889	177	53.00	29	193772.	1.6	1.6	0.3863
123	110.00	8	865.	0.0	0.0	0.0017	178	52.00	35	402864.	3.2	3.2	0.8031*
124	109.00	17	43443.	0.3	0.3	0.0866	179	51.00	25	218120.	1.8	1.8	0.4348*
125	108.00	17	111492.	0.9	0.9	0.2222	180	50.00	29	727504.	5.9	5.9	1.4502
126	107.00	17	54407.	0.4	0.4	0.1085	181	49.00	17	32006.	0.3	0.3	0.0638*
127	105.00	14	22747.	0.2	0.2	0.0453*	182	48.00	14	2334.	0.0	0.0	0.0047*
128	104.00	21	106868.	0.9	0.9	0.2130	183	47.00	8	11615.	0.1	0.1	0.0232
129	103.00	25	144344.	1.2	1.2	0.2877*	184	46.00	14	12452.	0.1	0.1	0.0248
130	102.00	12	7370.	0.1	0.1	0.0147*	185	45.00	17	46219.	0.4	0.4	0.0921*
131	101.00	12	8211.	0.1	0.1	0.0164	186	44.00	29	142180.	1.1	1.1	0.2834*
132	100.00	8	2496.	0.0	0.0	0.0050	187	43.00	14	16984.	0.1	0.1	0.0339
133	99.00	14	32352.	0.3	0.3	0.0645	188	42.00	12	22633.	0.2	0.2	0.0451
134	98.00	10	4372.	0.0	0.0	0.0087	189	41.00	14	12146.	0.1	0.1	0.0242*
135	97.00	25	314768.	2.5	2.5	0.6275*	190	40.00	10	7697.	0.1	0.1	0.0153*
136	96.00	25	157708.	1.3	1.3	0.3144	191	39.00	25	197584.	1.6	1.6	0.3939*
137	95.00	43	2460608.	19.8	19.8	4.9050*	192	38.00	35	667776.	5.4	5.4	1.3311*
138	94.00	17	68292.	0.5	0.5	0.1361	193	37.00	29	146344.	1.2	1.2	0.2917*
139	93.00	25	162860.	1.3	1.3	0.3246*	194	36.00	17	53196.	0.4	0.4	0.1060*
140	92.00	35	1755008.	14.1	14.1	3.4984*	195	35.00	10	5145.	0.0	0.0	0.0103*
141	91.00	21	69960.	0.6	0.6	0.1395*							
142	90.00	12	9155.	0.1	0.1	0.0182							
143	89.00	14	14553.	0.1	0.1	0.0290							
144	88.00	6	674.	0.0	0.0	0.0013							
145	85.00	21	66600.	0.5	0.5	0.1328*							
146	84.00	17	32801.	0.3	0.3	0.0654							
147	83.00	35	993216.	8.0	8.0	1.9799*							
148	82.00	21	40784.	0.3	0.3	0.0813*							
149	81.00	25	260076.	2.1	2.1	0.5184*							
150	80.00	21	191476.	1.5	1.5	0.3817							
151	79.00	21	74492.	0.6	0.6	0.1485							
152	78.00	21	62917.	0.5	0.5	0.1254							
153	77.00	21	95220.	0.8	0.8	0.1898							
154	76.00	25	359456.	2.9	2.9	0.7165							
155	75.00	35	1136192.	9.1	9.1	2.2649*							
156	74.00	25	296736.	2.4	2.4	0.5915*							
157	73.00	25	61769.	0.5	0.5	0.1231*							
158	72.00	8	1218.	0.0	0.0	0.0024							
159	71.00	14	22169.	0.2	0.2	0.0442*							
160	70.00	21	56162.	0.5	0.5	0.1120*							
161	69.00	51	5321216.	42.8	42.8	*10.60*							
162	68.00	12	12895.	0.1	0.1	0.0257*							
163	67.00	14	38832.	0.3	0.3	0.0774*							
164	66.00	25	168604.	1.4	1.4	0.3361							
165	65.00	25	207416.	1.7	1.7	0.4135*							

8V18AV.1 [TIC=32942888, 188X-19825928] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	389.00	12	66368.	0.3	0.3	0.2015	56	90.00	25	729840.	3.8	3.8	2.2155*
2	388.00	17	382624.	2.0	2.0	1.1615	57	89.00	14	40367.	0.2	0.2	0.1225*
3	387.00	8	1765.	0.0	0.0	0.0054	58	88.00	12	43555.	0.2	0.2	0.1322*
4	282.00	6	1360.	0.0	0.0	0.0041	59	87.00	17	90924.	0.5	0.5	0.2760*
5	281.00	12	61136.	0.3	0.3	0.1856	60	86.00	14	40903.	0.2	0.2	0.1242*
6	280.00	17	207640.	1.1	1.1	0.6303	61	85.00	6	2164.	0.0	0.0	0.0066
7	279.00	6	1503.	0.0	0.0	0.0046	62	84.00	14	3238.	0.0	0.0	0.0098*
8	261.00	8	3782.	0.0	0.0	0.0115	63	83.00	21	482688.	2.5	2.5	1.4653
9	260.00	6	12383.	0.1	0.1	0.0376	64	78.00	12	16593.	0.1	0.1	0.0504*
10	287.00	10	51519.	0.3	0.3	0.1564	65	77.00	29	292400.	1.5	1.5	0.8876*
11	197.00	8	3801.	0.0	0.0	0.0115	66	76.00	35	842128.	4.4	4.4	2.5564*
12	196.00	17	88200.	0.5	0.5	0.2678	67	75.00	35	386256.	2.0	2.0	1.1725*
13	184.00	12	9149.	0.0	0.0	0.0278	68	74.00	21	179844.	0.9	0.9	0.5459
14	183.00	17	201720.	1.1	1.1	0.6123*	69	73.00	8	2028.	0.0	0.0	0.0062
15	182.00	35	2570112.	13.5	13.5	0.6123*	70	69.00	21	144916.	0.8	0.8	0.4399*
16	181.00	59	19025920.	100.0	100.0	*57.75*	71	65.00	8	5575.	0.0	0.0	0.0169
17	180.00	29	414480.	2.2	2.2	1.2582*	72	64.00	17	90312.	0.5	0.5	0.2742*
18	179.00	17	98092.	0.5	0.5	0.2978*	73	63.00	35	456000.	2.4	2.4	1.3842*
19	178.00	8	1401.	0.0	0.0	0.0043	74	62.00	17	76688.	0.4	0.4	0.2328*
20	177.00	8	2087.	0.0	0.0	0.0063	75	61.00	10	6344.	0.0	0.0	0.0193
21	169.00	8	6496.	0.0	0.0	0.0197	76	57.00	6	1948.	0.0	0.0	0.0059
22	168.00	14	52297.	0.3	0.3	0.1588*	77	53.00	12	15970.	0.1	0.1	0.0485*
23	165.00	8	5592.	0.0	0.0	0.0170	78	52.00	17	24038.	0.1	0.1	0.0730*
24	155.00	8	15662.	0.1	0.1	0.0475	79	51.00	25	300864.	1.6	1.6	0.9133
25	154.00	8	24800.	0.1	0.1	0.0753	80	50.00	25	195876.	1.0	1.0	0.5946*
26	153.00	21	373728.	2.0	2.0	1.1345	81	44.00	21	99428.	0.5	0.5	0.3018*
27	152.00	29	2198144.	11.6	11.6	6.6728	82	40.00	10	22246.	0.1	0.1	0.0675*
28	151.00	25	621888.	3.3	3.3	1.8878*	83	39.00	25	227672.	1.2	1.2	0.6911
29	150.00	25	261440.	1.4	1.4	0.7936*	84	38.00	12	15816.	0.1	0.1	0.0480*
30	149.00	8	10100.	0.1	0.1	0.0307*	85	37.00	6	1694.	0.0	0.0	0.0051
31	148.00	8	2215.	0.0	0.0	0.0067	86	36.00	6	2777.	0.0	0.0	0.0084
32	142.00	10	8387.	0.0	0.0	0.0255							
33	140.00	10	3486.	0.0	0.0	0.0106							
34	139.00	12	40067.	0.2	0.2	0.1216*							
35	131.00	12	7203.	0.0	0.0	0.0219							
36	128.00	14	48560.	0.3	0.3	0.1474*							
37	127.00	21	340672.	1.8	1.8	1.0342							
38	126.00	21	296112.	1.6	1.6	0.6989*							
39	125.00	14	51569.	0.3	0.3	0.1565							
40	123.00	6	2839.	0.0	0.0	0.0086							
41	122.00	8	3209.	0.0	0.0	0.0097							
42	119.00	8	1458.	0.0	0.0	0.0044							
43	115.00	12	20706.	0.1	0.1	0.0629							
44	114.00	14	38592.	0.2	0.2	0.1172*							
45	113.00	12	37657.	0.2	0.2	0.1143*							
46	111.00	10	6352.	0.0	0.0	0.0193*							
47	110.00	6	3261.	0.0	0.0	0.0099							
48	103.00	10	9299.	0.0	0.0	0.0282							
49	102.00	17	91760.	0.5	0.5	0.2785*							
50	101.00	17	100376.	0.5	0.5	0.3047							
51	100.00	14	38174.	0.2	0.2	0.1159*							
52	99.00	12	29535.	0.2	0.2	0.0897*							
53	98.00	10	32536.	0.2	0.2	0.0988							
54	97.00	6	1744.	0.0	0.0	0.0053							
55	91.00	17	109984.	0.6	0.6	0.3339*							

BCA2PK.1 [TIC-176177152, 155X-4945952] EI

Malonic acid,
2,2,2-trifluoroethyl diester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	431.00	6	766.	0.0	0.0	0.0064	56	159.00	6	1382.	0.0	0.0	0.0008
2	355.00	10	4300.	0.0	0.0	0.0024	57	154.00	6	838.	0.0	0.0	0.0005
3	352.00	6	1244.	0.0	0.0	0.0007	58	151.00	8	4743.	0.0	0.0	0.0027
4	351.00	12	35596.	0.1	0.1	0.0202	59	150.00	17	52769.	0.1	0.1	0.0300
5	341.00	8	2715.	0.0	0.0	0.0015	60	149.00	25	767040.	1.6	1.6	0.4354*
6	319.00	6	1151.	0.0	0.0	0.0007	61	148.00	8	1887.	0.0	0.0	0.0011
7	301.00	10	1263.	0.0	0.0	0.0007	62	147.00	6	1837.	0.0	0.0	0.0019
8	295.00	10	4564.	0.0	0.0	0.0026	63	143.00	8	1166.	0.0	0.0	0.0007
9	293.00	8	1708.	0.0	0.0	0.0010	64	142.00	17	97316.	0.2	0.2	0.0552
10	289.00	6	624.	0.0	0.0	0.0004	65	141.00	21	457760.	0.9	0.9	0.2598*
11	282.00	10	1176.	0.0	0.0	0.0007	66	140.00	14	5053.	0.0	0.0	0.0029*
12	281.00	8	8243.	0.0	0.0	0.0047	67	135.00	6	784.	0.0	0.0	0.0004
13	271.00	10	1653.	0.0	0.0	0.0009	68	133.00	8	2524.	0.0	0.0	0.0014
14	270.00	10	10555.	0.0	0.0	0.0060	69	131.00	17	35526.	0.1	0.1	0.0202*
15	269.00	17	145188.	0.3	0.3	0.0824	70	129.00	8	1836.	0.0	0.0	0.0010
16	268.00	25	968752.	2.0	2.0	0.15499*	71	128.00	17	85488.	0.2	0.2	0.0485
17	267.00	6	2335.	0.0	0.0	0.0013	72	127.00	25	508464.	1.0	1.0	0.2886*
18	251.00	8	2476.	0.0	0.0	0.0014	73	126.00	59	17752064.	35.9	35.9	*10.07*
19	250.00	12	30716.	0.1	0.1	0.0174*	74	125.00	35	104592.	0.2	0.2	0.0594*
20	249.00	21	397232.	0.8	0.8	0.0225*	75	125.00	21	96346.	0.2	0.2	0.0547*
21	248.00	6	1029.	0.0	0.0	0.0006	76	123.00	8	2434.	0.0	0.0	0.0014
22	247.00	6	1495.	0.0	0.0	0.0008	77	122.00	17	123388.	0.2	0.2	0.0700
23	233.00	6	725.	0.0	0.0	0.0004	78	120.00	6	2008.	0.0	0.0	0.0011
24	224.00	12	21922.	0.0	0.0	0.0124	79	119.00	14	23389.	0.0	0.0	0.0133*
25	219.00	12	2227.	0.0	0.0	0.0013	80	118.00	14	8317.	0.0	0.0	0.0047*
26	212.00	8	1073.	0.0	0.0	0.0006	81	117.00	8	3360.	0.0	0.0	0.0019
27	211.00	8	8811.	0.0	0.0	0.0050	82	115.00	8	1476.	0.0	0.0	0.0008
28	210.00	8	1670.	0.0	0.0	0.0009	83	114.00	6	2915.	0.0	0.0	0.0017
29	209.00	10	26967.	0.1	0.1	0.0153	84	113.00	21	180732.	0.4	0.4	0.1026*
30	208.00	21	203848.	0.4	0.4	0.1157*	85	111.00	8	2546.	0.0	0.0	0.0014
31	207.00	43	4231680.	8.6	8.6	2.4019*	86	109.00	10	11250.	0.0	0.0	0.0064
32	206.00	17	3227.	0.0	0.0	0.0127*	87	108.00	10	6124.	0.0	0.0	0.0035
33	205.00	14	7193.	0.0	0.0	0.0018*	88	107.00	25	320640.	0.6	0.6	0.1820*
34	200.00	12	159328.	0.3	0.3	0.0041	89	106.00	17	19066.	0.0	0.0	0.0108*
35	199.00	17	753.	0.0	0.0	0.0004	90	105.00	10	7800.	0.0	0.0	0.0044
36	195.00	10	1863.	0.0	0.0	0.0011	91	101.00	14	18977.	0.0	0.0	0.0108*
37	191.00	6	500.	0.0	0.0	0.0003	92	99.00	17	50409.	0.1	0.1	0.0286*
38	187.00	8	1907.	0.0	0.0	0.0011	93	97.00	12	54306.	0.1	0.1	0.0308
39	185.00	6	410.	0.0	0.0	0.0002	94	97.00	21	26382.	0.1	0.1	0.0150*
40	183.00	6	278.	0.0	0.0	0.0002	95	96.00	35	231276.	0.5	0.5	0.1313*
41	181.00	6	7052.	0.0	0.0	0.0002	96	95.00	35	60674.	0.1	0.1	0.0344*
42	179.00	12	2323.	0.0	0.0	0.0002	97	94.00	71	294288.	0.6	0.6	0.1670*
43	178.00	8	1042.	0.0	0.0	0.0013	98	93.00	8	5868.	0.0	0.0	0.0033*
44	176.00	6	731.	0.0	0.0	0.0006	99	93.00	12	18030.	0.0	0.0	0.0107*
45	174.00	8	2451.	0.0	0.0	0.0004	100	91.00	14	34433.	0.1	0.1	0.0195*
46	173.00	10	14181.	0.0	0.0	0.0014	101	90.00	8	1490.	0.0	0.0	0.0008
47	172.00	35	69128.	0.1	0.1	0.0080*	102	89.00	21	56749.	0.1	0.1	0.0322*
48	171.00	35	368256.	0.7	0.7	0.0392*	103	88.00	6	1531.	0.0	0.0	0.0009
49	170.00	35	2436864.	4.9	4.9	0.2090*	104	87.00	17	42739.	0.1	0.1	0.0243*
50	169.00	43	49405952.	100.0	100.0	*28.01*	105	86.00	12	9560.	0.0	0.0	0.0054
51	168.00	71	422448.	0.9	0.9	0.2398*	106	85.00	14	42319.	0.1	0.1	0.0240*
52	167.00	51	47238.	0.1	0.1	0.0268*	107	84.00	35	797664.	1.6	1.6	0.4528*
53	166.00	12	5623.	0.0	0.0	0.0032*	108	83.00	87	4605248.	93.1	93.1	*26.11*
54	163.00	10	7833.	0.0	0.0	0.0044	109	82.00	59	355792.	0.7	0.7	0.2020*
55							110	81.00	21	115888.	0.2	0.2	0.0658*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	85.00	25	454576.	0.9	0.9	0.2580*
112	79.00	21	145476.	0.3	0.3	0.0826*
113	78.00	21	84300.	0.2	0.2	0.0478
114	77.00	25	647456.	1.3	1.3	0.3675*
115	76.00	8	2028.	0.0	0.0	0.0012
116	75.00	21	1011428.	0.2	0.2	0.0576*
117	74.00	12	46106.	0.1	0.1	0.0262
118	73.00	18	16602.	0.0	0.0	0.0094*
119	72.00	21	117916.	0.2	0.2	0.0669
120	71.00	17	53746.	0.1	0.1	0.0305
121	70.00	25	292512.	0.6	0.6	0.1660*
122	69.00	59	1234560.	25.0	25.0	7.0075*
123	68.00	43	197252.	0.4	0.4	0.1120*
124	67.00	6	3475.	0.0	0.0	0.0020
125	65.00	21	123380.	0.2	0.2	0.0700*
126	64.00	35	2298040.	4.7	4.7	1.3044*
127	63.00	35	1600960.	3.4	3.4	0.9541*
128	62.00	21	84132.	0.2	0.2	0.0478*
129	61.00	35	2704440.	5.6	5.6	1.5805*
130	60.00	21	84200.	0.2	0.2	0.0478*
131	59.00	8	10270.	0.0	0.0	0.0058
132	58.00	17	33596.	0.1	0.1	0.0191*
133	57.00	8	2909.	0.0	0.0	0.0017
134	56.00	12	21603.	0.0	0.0	0.0123*
135	55.00	21	63566.	0.1	0.1	0.0361*
136	54.00	71	110616.	0.2	0.2	0.0673*
137	53.00	17	44392.	0.1	0.1	0.0252*
138	52.00	14	36728.	0.1	0.1	0.0200*
139	51.00	29	1334336.	2.7	2.7	0.7574*
140	50.00	25	466560.	0.9	0.9	0.2648*
141	49.00	21	129860.	0.3	0.3	0.0737*
142	48.00	10	136400.	0.0	0.0	0.0077
143	47.00	29	167904.	0.3	0.3	0.0953*
144	46.00	12	25795.	0.1	0.1	0.0146*
145	45.00	29	550200.	1.1	1.1	0.3123*
146	44.00	35	814000.	1.6	1.6	0.4621*
147	43.00	43	2911600.	5.9	5.9	1.6527*
148	42.00	71	17633200.	35.7	35.7	10.00*
149	41.00	43	1731968.	3.5	3.5	0.9831*
150	40.00	43	177652.	0.4	0.4	0.1000*
151	39.00	6	2604.	0.0	0.0	0.0015
152	38.00	21	59156.	0.1	0.1	0.0336*
153	37.00	10	10423.	0.0	0.0	0.0059*
154	36.00	25	171336.	0.3	0.3	0.0973*
155	35.00	17	48602.	0.1	0.1	0.0276*

BCA3PK.1 [TIC-20041720, 100X-3957560] EI

Dimethylmalonic acid,
2,2,2-trifluoroethyl diester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	481.00	8	1487.	0.0	0.0	0.0074	150.00	12	35821.	0.9	0.9	0.1787
2	355.00	10	3359.	0.1	0.1	0.0168	149.00	21	385936.	9.8	9.8	1.9257*
3	325.00	6	870.	0.0	0.0	0.0043	148.00	6	6374.	0.2	0.2	0.0318
4	298.00	8	2990.	0.1	0.1	0.0149	145.00	21	8019.	0.2	0.2	0.0400*
5	297.00	10	37487.	0.9	0.9	0.1870	143.00	8	6594.	0.2	0.2	0.0329
6	296.00	17	317616.	8.0	8.0	1.5848	142.00	17	113372.	2.9	2.9	0.5657
7	295.00	10	1463.	0.0	0.0	0.0073	141.00	35	1921408.	48.6	48.6	9.5870*
8	293.00	8	1664.	0.0	0.0	0.0083	140.00	10	9828.	0.2	0.2	0.0490*
9	289.00	6	1042.	0.0	0.0	0.0052	139.00	8	4831.	0.1	0.1	0.0241
10	282.00	8	1137.	0.0	0.0	0.0057	135.00	12	60731.	1.5	1.5	0.3030
11	281.00	10	5354.	0.1	0.1	0.0267	132.00	6	1227.	0.0	0.0	0.0061
12	278.00	10	7031.	0.2	0.2	0.0351	131.00	17	44196.	1.1	1.1	0.2205*
13	277.00	17	127076.	3.2	3.2	0.6341	129.00	8	1592.	0.0	0.0	0.0079
14	269.00	8	5124.	0.1	0.1	0.0256	128.00	14	57456.	1.5	1.5	0.2867*
15	267.00	12	2803.	0.1	0.1	0.0140	126.00	29	1312832.	33.2	33.2	6.5505*
16	253.00	12	43054.	1.1	1.1	0.2148	125.00	8	4463.	0.1	0.1	0.0223
17	252.00	21	416482.	10.5	10.5	2.0781	123.00	10	4640.	0.1	0.1	0.0232
18	251.00	8	9398.	0.2	0.2	0.0469	122.00	8	5318.	0.1	0.1	0.0265
19	249.00	10	6409.	0.2	0.2	0.0320	121.00	6	666.	0.0	0.0	0.0033
20	238.00	10	24805.	0.6	0.6	0.1238	120.00	10	17839.	0.5	0.5	0.0890*
21	237.00	21	386416.	9.8	9.8	1.9281	119.00	6	625.	0.0	0.0	0.0031
22	236.00	6	1402.	0.0	0.0	0.0070	118.00	12	42722.	1.1	1.1	0.2132
23	231.00	8	5684.	0.1	0.1	0.0284	117.00	14	67316.	1.7	1.7	0.3359
24	225.00	8	2056.	0.1	0.1	0.0183	113.00	6	784.	0.0	0.0	0.0039
25	224.00	10	13760.	0.7	0.7	0.1293	109.00	17	82628.	2.1	2.1	0.4123
26	223.00	14	2106.	0.3	0.3	0.1293	108.00	6	1205.	0.0	0.0	0.0060
27	222.00	6	2863.	0.1	0.1	0.0185	107.00	8	4061.	0.1	0.1	0.0203
28	219.00	8	386.	0.1	0.1	0.0143	105.00	6	605.	0.0	0.0	0.0030
29	214.00	8	2491.	0.1	0.1	0.0124	104.00	8	1160.	0.0	0.0	0.0078
30	213.00	6	1102.	0.0	0.0	0.0019	103.00	8	2860.	0.1	0.1	0.0143
31	212.00	6	1142.	0.0	0.0	0.0057	101.00	8	36464.	0.9	0.9	0.1819
32	211.00	8	3486.	0.6	0.6	0.0055	100.00	12	19028.	0.5	0.5	0.0949
33	208.00	17	93068.	2.4	2.4	0.4644	99.00	10	887.	0.0	0.0	0.0044
34	207.00	8	8040.	0.2	0.2	0.0401	97.00	6	890.	0.0	0.0	0.0044
35	199.00	8	63393.	1.6	1.6	0.0401	95.00	6	2911.	0.1	0.1	0.0145
36	198.00	12	766368.	19.4	19.4	3.8239*	93.00	8	8821.	0.2	0.2	0.0440
37	197.00	21	154268.	3.9	3.9	0.7697*	90.00	6	1648.	0.0	0.0	0.0082
38	196.00	17	4511.	0.1	0.1	0.0225	89.00	6	1674.	0.0	0.0	0.0084
39	195.00	8	3844.	0.1	0.1	0.0192	87.00	8	5595.	0.1	0.1	0.0279
40	193.00	8	6623.	0.2	0.2	0.0330	86.00	8	8752.	0.2	0.2	0.0437
41	191.00	6	982.	0.0	0.0	0.0034	85.00	2	10416.	0.1	0.1	0.0520
42	183.00	6	690.	0.0	0.0	0.0049	84.00	20	100496.	2.5	2.5	0.5014*
43	182.00	8	2432.	0.1	0.1	0.0121	83.00	35	3957568.	100.0	100.0	*19.74*
44	181.00	10	50406.	1.3	1.3	0.02515*	82.00	10	8386.	0.2	0.2	0.0418*
45	177.00	10	9476.	0.2	0.2	0.0473	81.00	8	10190.	0.3	0.3	0.0508
46	172.00	10	765.	0.0	0.0	0.0038	80.00	8	10190.	0.1	0.1	0.0177
47	171.00	12	26417.	0.7	0.7	0.01318	79.00	8	1792.	0.0	0.0	0.0089
48	170.00	12	123428.	3.1	3.1	0.6159	77.00	8	8005.	0.2	0.2	0.0399
49	169.00	25	1493120.	37.7	37.7	7.4501*	74.00	10	939.	0.0	0.0	0.0047
50	168.00	17	161960.	4.1	4.1	0.8081*	73.00	6	14436.	0.4	0.4	0.0720*
51	167.00	21	62886.	1.6	1.6	0.3138*	72.00	10	16850.	0.4	0.4	0.0841
52	166.00	14	24028.	0.6	0.6	0.1199	71.00	12	36775.	0.9	0.9	0.1835*
53	155.00	12	29336.	0.7	0.7	0.1464	70.00	14	497680.	12.6	12.6	2.4832
54	153.00	12	4969.	0.1	0.1	0.0248	69.00	25	1783232.	45.1	45.1	8.8976*
55	151.00	8						35				

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	68.00	14	30787.	0.8	0.8	0.1536*
112	67.00	8	4413.	0.1	0.1	0.0220
113	65.00	10	18673.	0.5	0.5	0.0932
114	64.00	21	188136.	4.8	4.8	0.9387
115	63.00	17	108584.	2.7	2.7	0.5418
116	61.00	25	265120.	6.7	6.7	1.3228*
117	60.00	10	7970.	0.2	0.2	0.0398*
118	59.00	21	206124.	5.2	5.2	1.0285
119	58.00	6	1902.	0.0	0.0	0.0095
120	57.00	12	8585.	0.2	0.2	0.0428
121	56.00	10	30949.	0.8	0.8	0.1544*
122	55.00	25	169836.	4.3	4.3	0.8474*
123	54.00	12	23490.	0.6	0.6	0.1172*
124	53.00	17	51642.	1.3	1.3	0.2577*
125	52.00	6	1306.	0.0	0.0	0.0065
126	51.00	17	69808.	1.8	1.8	0.3483*
127	50.00	14	30107.	0.8	0.8	0.1502*
128	49.00	12	26462.	0.7	0.7	0.1320*
129	48.00	8	1431.	0.0	0.0	0.0071
130	47.00	17	64230.	1.6	1.6	0.3205*
131	46.00	8	2040.	0.1	0.1	0.0102
132	45.00	21	116108.	2.9	2.9	0.5793*
133	44.00	17	75560.	1.9	1.9	0.3770*
134	43.00	29	197048.	5.0	5.0	0.9832*
135	42.00	35	604368.	15.3	15.3	3.0155*
136	41.00	29	1419456.	35.9	35.9	7.0825*
137	40.00	29	202360.	5.1	5.1	1.0097*
138	39.00	25	574480.	14.5	14.5	2.8664
139	38.00	17	81684.	2.1	2.1	0.4076*
140	37.00	10	22565.	0.6	0.6	0.1126*
141	36.00	17	101520.	2.6	2.6	0.5065*
142	35.00	12	21403.	0.5	0.5	0.1068*

BCA4PK.1 [TIC=31681536, 188X=7299328] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	481.00	6	885.	0.0	0.0	0.0028	56	110.00	12	14251.	0.2	0.2	0.0450
2	415.00	8	802.	0.0	0.0	0.0025	57	108.00	10	2598.	0.7	0.7	0.0082
3	400.00	8	1835.	0.0	0.0	0.0058	58	107.00	14	48790.	0.7	0.7	0.1540*
4	355.00	8	5771.	0.1	0.1	0.0182	59	105.00	10	5035.	0.1	0.1	0.0159
5	341.00	10	4434.	0.1	0.1	0.0140	60	104.00	8	3804.	0.1	0.1	0.0120
6	331.00	6	1390.	0.0	0.0	0.0044	61	103.00	8	5380.	0.1	0.1	0.0170
7	282.00	10	9853.	0.1	0.1	0.0311	62	101.00	6	949.	0.0	0.0	0.0030
8	281.00	6	4728.	0.1	0.1	0.0149	63	100.00	10	14297.	0.2	0.2	0.0451
9	279.00	6	805.	0.0	0.0	0.0025	64	99.00	21	23980.	3.3	3.3	0.7575
10	270.00	6	1253.	0.0	0.0	0.0040	65	98.00	6	1667.	0.0	0.0	0.0053
11	269.00	8	893.	0.0	0.0	0.0028	66	93.00	12	12300.	0.2	0.2	0.0388
12	264.00	8	6298.	0.1	0.1	0.0199	67	91.00	12	31930.	0.4	0.4	0.1008*
13	263.00	14	104932.	1.4	1.4	0.3312*	68	90.00	10	23024.	0.3	0.3	0.0727
14	238.00	8	3792.	0.1	0.1	0.0120	69	89.00	6	813.	0.0	0.0	0.0026
15	237.00	12	23340.	0.3	0.3	0.0737	70	87.00	6	854.	0.0	0.0	0.0027
16	219.00	8	6165.	0.1	0.1	0.0195	71	86.00	10	4410.	0.1	0.1	0.0139
17	211.00	8	7577.	0.1	0.1	0.0239	72	85.00	12	21192.	0.3	0.3	0.0669*
18	207.00	8	2183.	0.0	0.0	0.0069	73	84.00	21	183912.	2.5	2.5	0.5805
19	191.00	6	2969.	0.0	0.0	0.0094	74	83.00	43	6432256.	88.1	88.1	*20.30*
20	186.00	8	737.	0.0	0.0	0.0023	75	81.00	25	92220.	1.3	1.3	0.2911*
21	185.00	6	1129.	0.0	0.0	0.0036	76	81.00	12	39981.	0.5	0.5	0.1262
22	184.00	12	59048.	0.8	0.8	0.1864	77	80.00	12	28139.	0.4	0.4	0.0888*
23	183.00	25	391296.	5.4	5.4	1.2351*	78	79.00	8	10812.	0.1	0.1	0.0341
24	182.00	43	6233088.	85.4	85.4	*19.67*	79	78.00	8	1951.	0.062	0.062	0.0082
25	181.00	17	2376256.	32.6	32.6	7.5004*	80	77.00	10	12922.	0.2	0.2	0.0408
26	179.00	8	53370.	0.7	0.7	0.1685*	81	75.00	8	5037.	0.1	0.1	0.0159
27	169.00	14	1667.	0.0	0.0	0.0053	82	73.00	12	22484.	0.3	0.3	0.0710
28	164.00	10	40348.	0.6	0.6	0.1274	83	72.00	10	14687.	0.2	0.2	0.0464
29	163.00	17	14512.	0.2	0.2	0.0458	84	71.00	10	10375.	0.1	0.1	0.0327
30	162.00	8	201800.	2.8	2.8	0.6372*	85	70.00	25	2796.	0.088	0.088	0.0088
31	157.00	6	1652.	0.0	0.0	0.0064	86	69.00	8	694592.	9.5	9.5	2.1924*
32	156.00	21	30255.	0.4	0.4	0.0052	87	68.00	6	1096.	0.0	0.0	0.0035
33	155.00	10	408080.	5.6	5.6	0.0955	88	67.00	12	1126.	0.036	0.036	0.0036
34	154.00	12	27322.	0.4	0.4	1.2881	89	65.00	12	23538.	0.3	0.3	0.0743
35	153.00	10	17810.	0.2	0.2	0.0862*	90	64.00	21	349664.	4.8	4.8	1.0337
36	143.00	6	854.	0.0	0.0	0.0562	91	63.00	21	217328.	3.0	3.0	0.6860
37	139.00	8	3046.	0.0	0.0	0.0027	92	61.00	21	119196.	1.6	1.6	0.3762*
38	137.00	8	5237.	0.1	0.1	0.0096	93	60.00	8	5552.	0.1	0.1	0.0175
39	136.00	14	66612.	0.9	0.9	0.0165	94	59.00	10	5245.	0.1	0.1	0.0166
40	135.00	25	957456.	13.1	13.1	0.2103*	95	58.00	12	8429.	0.1	0.1	0.0266*
41	134.00	8	2874.	0.0	0.0	0.0091	96	57.00	21	214148.	2.9	2.9	0.6759
42	132.00	8	630.	0.0	0.0	0.0020	97	56.00	29	755600.	10.4	10.4	2.3850*
43	131.00	12	31648.	0.4	0.4	0.0099*	98	55.00	51	7299328.	100.0	100.0	*23.03*
44	129.00	6	2534.	0.0	0.0	0.0080	99	54.00	21	68980.	0.9	0.9	0.2177*
45	128.00	12	35962.	0.5	0.5	0.1135	100	53.00	17	80706.	1.2	1.2	0.2740*
46	127.00	29	1285760.	17.6	17.6	4.0584*	101	51.00	21	151796.	2.1	2.1	0.4791*
47	126.00	6	946.	0.0	0.0	0.0030	102	50.00	14	50142.	0.7	0.7	0.1583*
48	122.00	12	5114.	0.1	0.1	0.0161	103	49.00	14	35084.	0.5	0.5	0.1107*
49	121.00	8	3441.	0.0	0.0	0.0109	104	47.00	21	180176.	2.5	2.5	0.5687*
50	120.00	6	1618.	0.0	0.0	0.0032	105	46.00	8	4831.	0.1	0.1	0.0152
51	119.00	12	24108.	0.3	0.3	0.0761	106	45.00	29	189296.	2.6	2.6	0.5975*
52	117.00	8	1380.	0.0	0.0	0.0044	107	44.00	17	121060.	1.7	1.7	0.3821
53	114.00	8	22315.	0.3	0.3	0.0704	108	43.00	17	91936.	1.3	1.3	0.2902*
54	113.00	21	537488.	7.4	7.4	1.6965	109	42.00	25	476864.	6.5	6.5	1.5052*
55							110	41.00	12	26819.	0.4	0.4	0.0847*

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	40.00	8	2367.	0.0	0.0	0.0075
112	39.00	12	12945.	0.2	0.2	0.0409*
113	38.00	14	42810.	0.6	0.6	0.1351*
114	37.00	10	16303.	0.2	0.2	0.0515*
115	36.00	17	8808.	1.2	1.2	0.2778
116	35.00	12	12366.	0.2	0.2	0.0390

APPENDIX B

MASS SPECTRA OF 2,2,3,3,4,4,4-HEPTAFLUORO-1-BUTYL ESTERS

TABLE B1. - Directory for spectra of 2,2,3,3,4,4,4-heptafluoro-1-butyl esters

Parent Acid				Heptafluorobutyl Ester			Page No.
Z-Series	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	
0(O ₂)	88	Butyric Acid	C ₄ H ₈ O ₂	270	83.37±0.04	0.77±0.05	B-4
0(O ₂)	102	Trimethylacetic Acid	C ₅ H ₁₀ O ₂	284	81.95±0.18	0.56±0.12	B-7
0(O ₂)	102	2-Methylbutyric Acid	C ₅ H ₁₀ O ₂	284	91.71±0.02	0.96±0.05	B-9
0(O ₂)	102	Pentanoic Acid	C ₅ H ₁₀ O ₂	284	103.49±0.07	0.84±0.04	B-12
0(O ₂)	116	2,2-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	298	99.48±0.02	0.92±0.02	B-15
0(O ₂)	116	3,3-Dimethylbutyric Acid	C ₆ H ₁₂ O ₂	298	100.24±0.10	0.85±0.08	B-18
0(O ₂)	116	2-Ethylbutyric acid	C ₆ H ₁₂ O ₂	298	107.11±0.47	0.83±0.02	B-21
0(O ₂)	116	2-Methylisopentanoic Acid	C ₆ H ₁₂ O ₂	298	104.76±0.03	0.55±0.04	B-24
0(O ₂)	116	2-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	298	107.82±0.03	0.98±0.05	B-27
0(O ₂)	116	3-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	298	111.70±0.03	0.77±0.12	B-30
0(O ₂)	116	4-Methylpentanoic Acid	C ₆ H ₁₂ O ₂	298	112.62±0.04	0.94±0.14	B-32
0(O ₂)	116	Hexanoic Acid	C ₆ H ₁₂ O ₂	298	122.17±0.04	0.90±0.05	B-35
0(O ₂)	130	2-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	312	127.25±0.02	0.97±0.04	B-38
0(O ₂)	130	5-Methylhexanoic Acid	C ₇ H ₁₄ O ₂	312	133.21±0.04	0.72±0.05	B-41
0(O ₂)	130	Heptanoic Acid	C ₇ H ₁₄ O ₂	312	142.22±0.05	0.95±0.03	B-44
0(O ₂)	144	Octanoic Acid	C ₈ H ₁₆ O ₂	326	162.36±0.04	1.000	B-47
0(O ₂)	158	Nonanoic Acid	C ₉ H ₁₈ O ₂	340	181.87±0.03	1.02±0.04	B-50
0(O ₂)	172	Decanoic Acid	C ₁₀ H ₂₀ O ₂	354	200.50±0.05	1.06±0.09	B-53
0(O ₂)	186	Undecanoic Acid	C ₁₁ H ₂₂ O ₂	368	219.14±0.04	1.01±0.08	B-56
0(O ₂)	200	Dodecanoic Acid	C ₁₂ H ₂₄ O ₂	382	237.03±0.04	1.14±0.09	B-59
0(O ₂)	214	Tridecanoic Acid	C ₁₃ H ₂₆ O ₂	396	253.94±0.04	1.13±0.10	B-62
0(O ₂)	228	2,6,10-Trimethylundecanoic Acid ³	C ₁₄ H ₂₈ O ₂	410	241.87	-	B-65
0(O ₂)	228	Tetradecanoic Acid	C ₁₄ H ₂₈ O ₂	410	270.12±0.06	1.21±0.11	B-67
0(O ₂)	242	3,7,11-Trimethyltridecanoic Acid ³	C ₁₅ H ₃₀ O ₂	424	259.91	-	B-70
0(O ₂)	242	Pentadecanoic Acid ³	C ₁₅ H ₃₀ O ₂	424	285.56	-	B-72
0(O ₂)	256	4,8,12-Trimethyltridecanoic Acid ³	C ₁₆ H ₃₂ O ₂	438	276.85	-	B-75
0(O ₂)	256	Hexadecanoic Acid	C ₁₆ H ₃₂ O ₂	438	300.29±0.07	1.19±0.09	B-77
0(O ₂)	270	5,9,13-Trimethyltetradecanoic Acid ³	C ₁₇ H ₃₄ O ₂	452	291.72	-	B-80
0(O ₂)	270	Heptadecanoic Acid	C ₁₇ H ₃₄ O ₂	452	314.42±0.07	1.24±0.13	B-82
0(O ₂)	284	Octadecanoic Acid	C ₁₈ H ₃₆ O ₂	466	328.06±0.08	1.32±0.15	B-85
0(O ₂)	298	2,6,10,14-Tetramethylpentadecanoic Acid ³	C ₁₉ H ₃₈ O ₂	480	308.37	-	B-89
0(O ₂)	298	Nonadecanoic Acid	C ₁₉ H ₃₈ O ₂	480	341.06±0.07	1.31±0.19	B-91
0(O ₂)	312	3,7,11,15-Tetramethylhexadecanoic Acid ³	C ₂₀ H ₄₀ O ₂	494	323.32	-	B-95
0(O ₂)	312	Eicosanoic Acid	C ₂₀ H ₄₀ O ₂	494	353.63±0.12	1.35±0.21	B-98
0(O ₂)	326	Henelicosanoic Acid ³	C ₂₁ H ₄₂ O ₂	508	365.73	-	-
-2(O ₂)	114	Cyclopentanecarboxylic Acid	C ₆ H ₁₀ O ₂	296	128.39±0.10	0.83±0.03	B-102
-2(O ₂)	128	Cyclohexanecarboxylic Acid	C ₇ H ₁₂ O ₂	310	149.59±0.02	0.95±0.05	B-105
-2(O ₂)	142	1-Methyl-1-cyclohexanecarboxylic Acid	C ₈ H ₁₄ O ₂	324	151.90±0.06	0.95±0.02	B-108
-2(O ₂)	156	3-Cyclohexylpropionic Acid	C ₉ H ₁₆ O ₂	338	191.49±0.04	1.05±0.04	B-111
-2(O ₂)	282	9-Octadecenoic Acid	C ₁₈ H ₃₄ O ₂	464	324.53±0.01	0.75±0.06	B-114

TABLE B1. - Directory for spectra of 2,2,3,3,4,4,4-heptafluoro-1-butyl esters (contd)

Parent Acid				Heptafluorobutyl Ester			Page No.
Z-Series	MW	Name	Empirical Formula	MW	GC Retention Index ¹	Relative TIC Response ²	
-8(O ₂)	122	Benzoic Acid	C ₇ H ₆ O ₂	304	154.76±0.11	0.52±0.04	B-118
-8(O ₂)	136	2-Methylbenzoic Acid	C ₈ H ₈ O ₂	318	173.31±0.02	0.86±0.08	B-120
-8(O ₂)	136	3-Methylbenzoic Acid	C ₈ H ₈ O ₂	318	175.81±0.08	0.75±0.03	B-122
-8(O ₂)	136	4-Methylbenzoic Acid	C ₈ H ₈ O ₂	318	179.62±0.02	0.85±0.04	B-125
-8(O ₂)	136	Phenylacetic Acid	C ₈ H ₈ O ₂	318	169.40±0.03	0.97±0.05	B-128
-8(O ₂)	150	2,3-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	332	198.72±0.05	0.78±0.01	B-130
-8(O ₂)	150	2,6-Dimethylbenzoic Acid	C ₉ H ₁₀ O ₂	332	183.23±0.01	0.86±0.12	B-133
-8(O ₂)	150	2-Ethylbenzoic Acid	C ₉ H ₁₀ O ₂	332	185.83±0.04	0.77±0.03	B-135
-8(O ₂)	150	4-Methylphenylacetic Acid	C ₉ H ₁₀ O ₂	332	188.76±0.03	0.83±0.06	B-138
-8(O ₂)	164	2-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	346	188.76±0.03	0.92±0.05	B-141
-8(O ₂)	164	3-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	346	197.82±0.06	0.91±0.02	B-144
-8(O ₂)	164	4-Phenylbutyric Acid	C ₁₀ H ₁₂ O ₂	346	212.38±0.09	1.02±0.02	B-147
-8(O ₂)	164	2,4,6-Trimethylbenzoic Acid	C ₁₀ H ₁₂ O ₂	346	204.28±0.05	0.89±0.19	B-150
-8(O ₂)	178	5-Phenylpentanoic Acid	C ₁₁ H ₁₄ O ₂	360	232.12±0.04	0.86±0.10	B-153
-8(O ₂)	220	4-Heptylbenzoic Acid	C ₁₄ H ₂₀ O ₂	402	285.01±0.05	0.75±0.15	B-156
-10(O ₂)	218	Cyclohexylphenylacetic Acid	C ₁₄ H ₁₈ O ₂	400	262.18±0.07	1.04±0.29	B-159
-14(O ₂)	172	1-Naphthoic Acid	C ₁₁ H ₈ O ₂	354	253.57±0.04	0.87±0.25	B-162
-14(O ₂)	172	2-Naphthoic Acid	C ₁₁ H ₈ O ₂	354	256.58±0.19	0.69±0.16	B-165
-14(O ₂)	186	1-Naphthylacetic Acid	C ₁₂ H ₁₀ O ₂	368	260.74±0.05	0.73±0.12	B-168
-16(O ₂)	198	Biphenyl-2-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	380	255.75±0.04	0.90±0.23	B-171
-16(O ₂)	198	Biphenyl-4-Carboxylic Acid	C ₁₃ H ₁₀ O ₂	380	289.68±0.17	0.66±0.14	B-174
-16(O ₂)	226	2,2-Diphenylpropionic Acid	C ₁₅ H ₁₄ O ₂	408	271.80±0.06	0.49±0.05	B-177
-16(O ₂)	240	1,2,5,4-Tetrahydro-4-phenanthreneacetic Acid	C ₁₆ H ₁₆ O ₂	422	332.73±0.04	0.54	B-180
-18(O ₂)	210	1-Fluorene-carboxylic Acid	C ₁₄ H ₁₀ O ₂	392	314.09±0.03	0.59±0.08	B-184
-20(O ₂)	222	Anthracene-9-Carboxylic Acid	C ₁₅ H ₁₀ O ₂	404	329.19±0.04	0.51±0.08	B-187
-20(O ₂)	222	9-Phenanthroic Acid	C ₁₅ H ₁₀ O ₂	404	339.05±0.00	0.40	B-190
-8(O ₃)	138	2-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	416	181.19±0.33	0.56±0.03	B-194
-8(O ₃)	138	4-Hydroxybenzoic Acid	C ₇ H ₆ O ₃	416	185.23±0.23	0.80±0.06	B-196
-18(O ₃)	226	9-Xanthanecarboxylic Acid	C ₁₄ H ₁₀ O ₃	408	286.12±0.09	0.26±0.13	B-200

¹ Based on assigned indices of 100, 200 and 300 for trifluoroacetyl esters of 4-fluorophenol, 1-naphthol, and 9-phenanthrol, respectively. Uncertainties shown are standard deviations.

² Response of octanoic acid esters was assumed = 1.00. TIC = total ion current. Uncertainties shown are standard deviations.

³ From analysis of petroleum fractions. Other data from pure compounds.

Dash - Not available.

ALIPA.1 [TIC=135778304, 100X=39384064] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	381.00	6	3558.	0.0	0.0	0.0026
2	331.00	6	2263.	0.0	0.0	0.0017
3	281.00	10	3992.	0.0	0.0	0.0029
4	272.00	12	5606.	0.0	0.0	0.0041
5	271.00	14	162804.	0.4	0.4	0.1199
6	270.00	17	187196.	0.5	0.5	0.1379
7	269.00	12	61268.	0.2	0.2	0.0451
8	268.00	6	728.	0.0	0.0	0.0005
9	257.00	8	8953.	0.0	0.0	0.0066
10	256.00	17	222792.	0.6	0.6	0.1641
11	255.00	35	3593344.	9.1	9.1	2.6465*
12	254.00	12	9060.	0.0	0.0	0.0067*
13	253.00	8	1237.	0.0	0.0	0.0009
14	252.00	8	16738.	0.0	0.0	0.0123
15	251.00	17	362928.	0.9	0.9	0.2673
16	244.00	14	65478.	0.2	0.2	0.0482*
17	243.00	25	723152.	1.8	1.8	0.5326*
18	242.00	51	11071232.	28.1	28.1	8.1539
19	241.00	21	56756.	0.1	0.1	0.0418*
20	240.00	8	6307.	0.0	0.0	0.0046
21	235.00	12	77956.	0.2	0.2	0.0574
22	231.00	8	10533.	0.0	0.0	0.0078
23	229.00	6	1945.	0.0	0.0	0.0014
24	228.00	10	38861.	0.1	0.1	0.0286
25	227.00	17	674864.	1.7	1.7	0.4970
26	226.00	12	7371.	0.0	0.0	0.0054
27	223.00	6	2075.	0.0	0.0	0.0015
28	219.00	8	11646.	0.0	0.0	0.0086
29	218.00	8	1723.	0.0	0.0	0.0013
30	217.00	8	4699.	0.0	0.0	0.0035
31	213.00	14	74216.	0.2	0.2	0.0547
32	209.00	12	55451.	0.1	0.1	0.0408
33	183.00	14	114464.	0.3	0.3	0.0843
34	181.00	12	33162.	0.1	0.1	0.0244
35	180.00	10	2226.	0.0	0.0	0.0016
36	179.00	8	1550.	0.0	0.0	0.0011
37	169.00	17	220644.	0.6	0.6	0.1625
38	163.00	12	23707.	0.1	0.1	0.0175
39	161.00	12	52076.	0.1	0.1	0.0384
40	158.00	8	9128.	0.0	0.0	0.0067
41	152.00	8	5771.	0.0	0.0	0.0043
42	145616.	17	145616.	0.4	0.4	0.1072
43	150.00	14	58121.	0.1	0.1	0.0428
44	133.00	17	231400.	0.6	0.6	0.1704
45	132.00	6	5799.	0.0	0.0	0.0043
46	131.00	17	249396.	0.6	0.6	0.1837
47	123.00	17	136288.	0.3	0.3	0.1004
48	120.00	10	21136.	0.1	0.1	0.0156
49	119.00	25	191412.	4.9	4.9	1.4097
50	114.00	14	66040.	0.2	0.2	0.0486*
51	113.00	25	2099264.	5.3	5.3	1.5461*
52	112.00	8	4372.	0.0	0.0	0.0032
53	111.00	17	84340.	0.2	0.2	0.0621
54	109.00	14	63960.	0.2	0.2	0.0471
55	108.00	10	20999.	0.1	0.1	0.0155

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	40.00	29	761968.	1.9	1.9	0.5612*
112	39.00	71	4746752.	12.1	12.1	3.4960*
113	38.00	29	476080.	1.2	1.2	0.3506
114	37.00	21	151288.	0.4	0.4	0.1114*
115	36.00	21	147336.	0.4	0.4	0.1085*
116	35.00	10	19287.	0.0	0.0	0.0142*

ACIPK.1 [TIC-89727072, 1.00X-2711.0400] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	331.00	6	2368.	0.0	0.0	0.0040	56	60.00	10	4501.	0.0	0.0	0.0075*
2	285.00	10	2966.	0.0	0.0	0.0050	57	59.00	25	531744.	2.0	2.0	0.8903
3	281.00	10	7831.	0.0	0.0	0.0131	58	58.00	25	1115456.	4.1	4.1	1.8676
4	270.00	10	48436.	0.2	0.2	0.0811	59	57.00	71	27110400.	100.0	100.0	*45.38*
5	269.00	21	674336.	2.5	2.5	1.1290	60	56.00	25	908736.	3.1	3.1	1.4194*
6	268.00	12	37585.	0.1	0.1	0.0629	61	55.00	29	847792.	3.4	3.4	1.5215
7	267.00	6	7589.	0.0	0.0	0.0127	62	54.00	14	48077.	0.2	0.2	0.0805*
8	265.00	6	1713.	0.0	0.0	0.0029	63	53.00	21	208640.	0.8	0.8	0.3493
9	249.00	6	1445.	0.0	0.0	0.0024	64	52.00	8	9320.	0.0	0.0	0.0156
10	242.00	14	88464.	0.3	0.3	0.1481	65	51.00	29	1347392.	5.0	5.0	2.2559
11	241.00	21	1233408.	4.5	4.5	2.0650	66	50.00	17	77996.	0.3	0.3	0.1306*
12	231.00	10	9153.	0.0	0.0	0.0153	67	49.00	17	121136.	0.4	0.4	0.2028*
13	228.00	10	29188.	0.1	0.1	0.0489	68	47.00	17	83092.	0.3	0.3	0.1391*
14	227.00	21	580368.	2.1	2.1	0.9717	69	45.00	25	323136.	1.2	1.2	0.5418*
15	223.00	6	728.	0.0	0.0	0.0012	70	44.00	17	111456.	0.4	0.4	0.1866*
16	219.00	10	18030.	0.1	0.1	0.0302	71	43.00	25	390144.	1.4	1.4	0.6532*
17	213.00	6	2198.	0.0	0.0	0.0037	72	42.00	29	993488.	3.7	3.7	1.6634
18	209.00	14	77848.	0.3	0.3	0.1303	73	41.00	43	10623744.	39.2	39.2	*17.78*
19	183.00	8	5835.	0.0	0.0	0.0098	74	40.00	29	462224.	1.7	1.7	0.7739*
20	181.00	8	31162.	0.1	0.1	0.0522	75	39.00	29	2513592.	9.3	9.3	4.2168
21	169.00	14	116004.	0.4	0.4	0.1942	76	38.00	21	148340.	0.5	0.5	0.2484*
22	165.00	8	5936.	0.0	0.0	0.0099	77	37.00	12	40444.	0.1	0.1	0.0677*
23	163.00	6	2883.	0.0	0.0	0.0048	78	36.00	10	39535.	0.1	0.1	0.0662*
24	161.00	17	119408.	0.4	0.4	0.0604	79	35.00	6	1659.	0.0	0.0	0.0028
25	150.00	8	11461.	0.0	0.0	0.0199							
26	133.00	14	78436.	0.3	0.3	0.1313*							
27	131.00	17	128432.	0.5	0.5	0.2150							
28	119.00	21	726800.	2.7	2.7	1.2170							
29	114.00	6	1731.	0.0	0.0	0.0029							
30	113.00	21	514496.	1.9	1.9	0.0829							
31	109.00	10	28471.	0.1	0.1	0.0614							
32	107.00	8	9977.	0.0	0.0	0.0477							
33	105.00	6	1544.	0.0	0.0	0.0167							
34	101.00	8	7906.	0.0	0.0	0.0026							
35	100.00	21	297648.	1.1	1.1	0.0132							
36	95.00	21	427344.	1.6	1.6	0.4983							
37	87.00	21	248056.	0.9	0.9	0.7155							
38	86.00	21	175608.	0.6	0.6	0.4153*							
39	85.00	25	1323776.	4.9	4.9	0.2940*							
40	84.00	12	41503.	0.2	0.2	2.2163*							
41	83.00	21	154040.	0.6	0.6	0.0695*							
42	82.00	10	26123.	0.1	0.1	0.2579*							
43	81.00	8	15277.	0.1	0.1	0.0437							
44	75.00	8	22325.	0.1	0.1	0.0256							
45	73.00	6	5622.	0.0	0.0	0.0374							
46	72.00	6	5102.	0.0	0.0	0.0111							
47	71.00	12	51081.	0.2	0.2	0.0085							
48	70.00	21	171008.	0.6	0.6	0.0855*							
49	69.00	35	3549952.	13.1	13.1	0.2863*							
50	67.00	8	6093.	0.0	0.0	5.9435*							
51	65.00	8	10817.	0.0	0.0	0.0102							
52	64.00	21	471648.	1.7	1.7	0.0181							
53	63.00	10	11763.	0.0	0.0	0.7897							
54	62.00	6	1216.	0.0	0.0	0.0197							
55	61.00	10	29910.	0.1	0.1	0.0020							
						0.0501*							

AG2AV.1 [TIC-149888832. 180X-41861128] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	8	3590.	0.0	0.0	0.0024	56	133.00	17	255556.	0.6	0.6	0.1705
2	285.00	14	118488.	0.3	0.3	0.0791	57	132.00	6	1772.	0.0	0.0	0.0012
3	284.00	14	182436.	0.4	0.4	0.1217	58	131.00	17	26112.	0.6	0.6	0.1742
4	283.00	10	42409.	0.1	0.1	0.0283	59	127.00	6	1387.	0.0	0.0	0.0009
5	282.00	10	27830.	0.1	0.1	0.0186	60	123.00	10	16400.	0.0	0.0	0.0109
6	281.00	12	102792.	0.2	0.2	0.0686	61	120.00	10	16156.	0.0	0.0	0.0108*
7	271.00	10	7163.	0.0	0.0	0.0048	62	119.00	25	2012032.	4.8	4.8	1.3424
8	270.00	17	300816.	0.7	0.7	0.0048	63	114.00	10	54504.	0.0	0.0	0.0364*
9	269.00	29	3761408.	9.0	9.0	2.5096*	64	113.00	25	1712896.	4.1	4.1	1.1428
10	268.00	8	14944.	0.0	0.0	0.0100	65	112.00	10	4846.	0.0	0.0	0.0032
11	267.00	10	41155.	0.1	0.1	0.0275	66	111.00	8	20167.	0.0	0.0	0.0135
12	265.00	12	116324.	0.3	0.3	0.0776	67	109.00	17	290864.	0.7	0.7	0.1941
13	258.00	14	103984.	0.2	0.2	0.0694	68	103.00	8	20668.	0.0	0.0	0.0138
14	257.00	25	1310348.	3.1	3.1	0.8746*	69	101.00	12	30227.	0.1	0.1	0.0202
15	256.00	43	17443840.	41.7	41.7	*11.63*	70	100.00	21	903072.	2.2	2.2	0.6025
16	255.00	35	1130432.	2.7	2.7	0.7542*	71	99.00	8	4302.	0.0	0.0	0.0029
17	254.00	12	24470.	0.1	0.1	0.0163*	72	96.00	10	39007.	0.1	0.1	0.0266*
18	253.00	10	7216.	0.0	0.0	0.0048	73	95.00	21	1477632.	3.5	3.5	0.9859
19	249.00	10	29710.	0.1	0.1	0.0198	74	94.00	8	17463.	0.0	0.0	0.0117
20	243.00	6	1591.	0.0	0.0	0.0011	75	93.00	10	50126.	0.1	0.1	0.0334*
21	242.00	14	109136.	0.3	0.3	0.0728	76	91.00	12	50996.	0.1	0.1	0.0340*
22	241.00	17	449040.	1.1	1.1	0.2996	77	87.00	12	91204.	0.2	0.2	0.0609
23	236.00	8	2008.	0.0	0.0	0.0013	78	86.00	21	434224.	1.0	1.0	0.2897
24	235.00	12	54705.	0.2	0.2	0.0432	79	85.00	35	815488.	20.1	20.1	5.6148*
25	231.00	10	2985.	0.0	0.0	0.0020	80	84.00	17	87684.	0.2	0.2	0.0585*
26	229.00	10	4112.	0.0	0.0	0.0027	81	83.00	21	522784.	1.2	1.2	0.3488
27	228.00	10	69300.	0.2	0.2	0.0462	82	82.00	14	86684.	0.2	0.2	0.0578*
28	227.00	21	1435968.	3.4	3.4	0.9581	83	81.00	12	72568.	0.2	0.2	0.0484
29	224.00	14	1455.	0.0	0.0	0.0010	84	80.00	12	11514.	0.0	0.0	0.0077
30	223.00	10	100900.	0.2	0.2	0.0673	85	77.00	8	19151.	0.0	0.0	0.0128
31	219.00	10	19550.	0.0	0.0	0.0130	86	76.00	10	3851.	0.0	0.0	0.0026
32	217.00	8	3745.	0.0	0.0	0.0025	87	75.00	17	164728.	0.4	0.4	0.1099*
33	214.00	8	2039.	0.0	0.0	0.0014	88	74.00	10	53669.	0.1	0.1	0.0358*
34	213.00	10	45074.	0.1	0.1	0.0301	89	73.00	21	287776.	0.7	0.7	0.1920*
35	210.00	10	31335.	0.1	0.1	0.0209*	90	72.00	6	3891.	0.0	0.0	0.0026
36	209.00	17	771008.	1.8	1.8	0.5144	91	71.00	12	115744.	0.3	0.3	0.0072
37	207.00	8	21533.	0.1	0.1	0.0144	92	70.00	17	153524.	0.4	0.4	0.1024*
38	205.00	8	7404.	0.0	0.0	0.0049	93	69.00	43	9389312.	22.4	22.4	6.2645*
39	193.00	6	4577.	0.0	0.0	0.0031	94	68.00	12	49480.	0.1	0.1	0.0330*
40	191.00	10	40487.	0.1	0.1	0.0270	95	67.00	17	137496.	0.3	0.3	0.0917*
41	183.00	10	45926.	0.1	0.1	0.0306	96	65.00	12	54000.	0.1	0.1	0.0361*
42	181.00	12	88756.	0.2	0.2	0.0592*	97	64.00	25	1240576.	3.0	3.0	0.8277
43	179.00	6	2319.	0.0	0.0	0.0015	98	63.00	12	42384.	0.1	0.1	0.0203*
44	169.00	17	205996.	0.5	0.5	0.1374	99	62.00	18	16892.	0.0	0.0	0.0113
45	165.00	12	91432.	0.2	0.2	0.0610	100	61.00	17	91208.	0.2	0.2	0.0609*
46	164.00	8	4270.	0.0	0.0	0.0028	101	60.00	8	3484.	0.0	0.0	0.0023
47	163.00	10	19118.	0.0	0.0	0.0128	102	59.00	21	238272.	0.6	0.6	0.1590*
48	162.00	6	3392.	0.0	0.0	0.0023	103	58.00	29	1820352.	4.3	4.3	1.2145
49	161.00	14	108704.	0.3	0.3	0.0725	104	57.00	71	41861120.	100.0	100.0	*27.92*
50	160.00	8	2581.	0.0	0.0	0.0017	105	56.00	35	6006016.	14.3	14.3	4.0072
51	151.00	0	2807.	0.0	0.0	0.0019	106	55.00	35	5564416.	13.3	13.3	3.7126*
52	150.00	12	47344.	0.1	0.1	0.0316*	107	54.00	21	311696.	0.7	0.7	0.2000*
53	145.00	12	18132.	0.0	0.0	0.0121*	108	53.00	29	873808.	2.1	2.1	0.5830
54	137.00	14	76712.	0.2	0.2	0.0512*	109	52.00	17	122956.	0.3	0.3	0.0820*
55	135.00	10	22200.	0.1	0.1	0.0148	110	51.00	35	3922432.	9.4	9.4	2.6170*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	50.00	21	308704.	0.7	0.7	0.2060
112	49.00	17	112340.	0.3	0.3	0.9750
113	47.00	21	266832.	0.6	0.6	0.1780*
114	46.00	10	12863.	0.0	0.0	0.0086
115	45.00	35	1437248.	3.4	3.4	0.9589*
116	44.00	21	268448.	0.6	0.6	0.1791*
117	43.00	35	1135616.	2.7	2.7	0.7577
118	42.00	35	1425088.	3.4	3.4	0.9508*
119	41.00	43	20167680.	48.2	48.2	*13.45*
120	40.00	29	689440.	1.6	1.6	0.4600*
121	39.00	35	5263616.	12.6	12.6	3.5119
122	38.00	25	329536.	0.8	0.8	0.2199*
123	37.00	17	89960.	0.2	0.2	0.0600*
124	36.00	17	132372.	0.3	0.3	0.0883*
125	35.00	10	23911.	0.1	0.1	0.0160*

AL3PA.1 [TIC-123185288, 188X-1982592] EI

Pentanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester
 $\text{CH}_3(\text{CH}_2)_3\text{COOCH}_2\text{C}_3\text{F}_7$

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	56.00	35	4318200.	21.8	21.8	3.5077*
112	55.00	43	7081984.	35.7	35.7	5.7528*
113	54.00	21	295328.	1.5	1.5	0.2399
114	53.00	25	537232.	2.7	2.7	0.4364
115	52.00	21	121656.	0.6	0.6	0.0988
116	51.00	35	3342272.	16.9	16.9	2.7150
117	50.00	21	246008.	1.2	1.2	0.1998
118	49.00	17	58632.	0.3	0.3	0.0476*
119	47.00	25	195004.	1.0	1.0	0.1584*
120	46.00	8	15186.	0.1	0.1	0.0123
121	45.00	35	926656.	4.7	4.7	0.7527
122	44.00	35	1874176.	9.5	9.5	1.5224*
123	43.00	59	19822592.	100.0	100.0	*16.10*
124	42.00	35	3718592.	18.8	18.8	3.0207*
125	41.00	43	10459648.	52.8	52.8	8.4965*
126	40.00	25	476912.	2.4	2.4	0.3874
127	39.00	35	3676288.	18.5	18.5	2.9863*
128	38.00	35	264032.	1.3	1.3	0.2145*
129	37.00	21	73056.	0.4	0.4	0.0593*
130	36.00	21	133428.	0.7	0.7	0.1084*
131	35.00	8	23637.	0.1	0.1	0.0192

EXA92.1 (TIC-197816328, 188X-57188488) EI

2,2-dimethylbutyric acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	300.00	8	5472.	0.0	0.0	0.0028	56	111.00	6	2744.	0.0	0.0	0.0014
2	299.00	14	101368.	0.2	0.2	0.0512	57	109.00	12	23070.	0.0	0.0	0.0117*
3	298.00	6	13426.	0.0	0.0	0.0068	58	105.00	8	1348.	0.0	0.0	0.0007
4	284.00	12	101556.	0.0	0.0	0.0513	59	101.00	17	82080.	0.1	0.1	0.0415*
5	283.00	21	1185920.	2.1	2.1	0.5995	60	100.00	35	935312.	1.6	1.6	0.4728
6	282.00	12	45022.	0.1	0.1	0.0228*	61	99.00	25	1840128.	3.2	3.2	0.9302
7	281.00	18	25984.	0.0	0.0	0.0131	62	97.00	10	30159.	0.1	0.1	0.0152*
8	279.00	8	2736.	0.0	0.0	0.0014	63	96.00	12	49799.	0.1	0.1	0.0252*
9	272.00	8	16973.	0.0	0.0	0.0086	64	95.00	25	1160640.	2.0	2.0	0.5867
10	271.00	17	296576.	0.5	0.5	0.1499	65	94.00	8	2204.	0.0	0.0	0.0011
11	270.00	35	3561664.	6.2	6.2	1.8005*	66	93.00	10	25760.	0.0	0.0	0.0130
12	269.00	25	638200.	1.1	1.1	0.0433	67	91.00	8	6060.	0.0	0.0	0.0031
13	268.00	12	85568.	0.1	0.1	0.0433	68	88.00	8	4193.	0.0	0.0	0.0021
14	267.00	12	58464.	0.1	0.1	0.0296*	69	87.00	21	354448.	0.6	0.6	0.1792
15	257.00	8	3498.	0.0	0.0	0.0018	70	86.00	8	2617.	0.0	0.0	0.0013
16	256.00	17	142252.	0.2	0.2	0.0719	71	85.00	17	102952.	0.2	0.2	0.0520*
17	255.00	21	1092224.	1.9	1.9	0.5521	72	84.00	10	49359.	0.1	0.1	0.0250*
18	253.00	8	9243.	0.0	0.0	0.0047	73	83.00	29	1125120.	2.0	2.0	0.5688
19	249.00	8	4787.	0.0	0.0	0.0061	74	82.00	17	136780.	0.2	0.2	0.0691*
20	243.00	14	12111.	0.0	0.0	0.0076	75	81.00	21	140344.	0.2	0.2	0.0709*
21	242.00	25	151432.	0.3	0.3	0.0370	76	80.00	10	3338.	0.0	0.0	0.0017
22	241.00	6	1655680.	2.9	2.9	0.8370	77	79.00	6	3759.	0.0	0.0	0.0019
23	240.00	8	9831.	0.0	0.0	0.0050	78	77.00	10	27844.	0.0	0.0	0.0141
24	239.00	8	1800.	0.0	0.0	0.0010	79	76.00	8	4514.	0.0	0.0	0.0023
25	235.00	10	63079.	0.1	0.1	0.0313	80	75.00	17	125856.	0.2	0.2	0.0636*
26	229.00	8	1890.	0.0	0.0	0.0010	81	73.00	21	217724.	0.4	0.4	0.1101*
27	228.00	17	194720.	0.3	0.3	0.0984*	82	72.00	29	2924416.	5.1	5.1	1.4783*
28	227.00	35	3465600.	6.1	6.1	1.7519*	83	71.00	71	57100400.	100.0	100.0	*28.86*
29	226.00	8	3051.	0.0	0.0	0.0015	84	70.00	43	3460160.	6.1	6.1	1.7492*
30	224.00	12	47300.	0.1	0.1	0.0240	85	69.00	51	9447168.	16.5	16.5	4.7757*
31	223.00	21	968304.	1.7	1.7	0.4895*	86	68.00	17	95800.	0.2	0.2	0.0484*
32	213.00	14	102516.	0.2	0.2	0.0518	87	67.00	21	223700.	0.4	0.4	0.1131*
33	209.00	10	43844.	0.1	0.1	0.0222	88	66.00	6	5229.	0.0	0.0	0.0026
34	207.00	6	3977.	0.0	0.0	0.0020	89	65.00	17	106492.	0.2	0.2	0.0530*
35	205.00	12	59055.	0.1	0.1	0.0299	90	64.00	25	1062144.	1.9	1.9	0.5369
36	183.00	8	18173.	0.0	0.0	0.0092	91	63.00	12	61559.	0.1	0.1	0.0311*
37	182.00	10	2789.	0.0	0.0	0.0014	92	62.00	10	11073.	0.0	0.0	0.0056
38	181.00	10	31231.	0.1	0.1	0.0158	93	61.00	17	124260.	0.2	0.2	0.0628
39	177.00	8	2367.	0.0	0.0	0.0012	94	60.00	12	39186.	0.1	0.1	0.0198*
40	163.00	14	132420.	0.2	0.2	0.0670	95	59.00	29	1671936.	2.9	2.9	0.8452
41	163.00	8	22394.	0.0	0.0	0.0113	96	58.00	12	48443.	0.1	0.1	0.0245*
42	161.00	12	86600.	0.2	0.2	0.0438	97	57.00	25	338752.	0.6	0.6	0.1712*
43	159.00	8	1557.	0.0	0.0	0.0008	98	56.00	25	853936.	1.5	1.5	0.4317
44	151.00	6	1974.	0.0	0.0	0.0010	99	55.00	43	9396224.	16.5	16.5	4.7506*
45	150.00	12	43549.	0.1	0.1	0.0220*	100	54.00	21	309984.	0.5	0.5	0.1567*
46	149.00	10	7726.	0.0	0.0	0.0039	101	53.00	29	1471232.	2.6	2.6	0.7437
47	135.00	17	101228.	0.2	0.2	0.0512*	102	52.00	21	165636.	0.3	0.3	0.0837*
48	133.00	17	230260.	0.4	0.4	0.1164	103	51.00	35	3849792.	6.7	6.7	1.9461*
49	131.00	17	196592.	0.3	0.3	0.0994	104	50.00	21	247648.	0.4	0.4	0.1252
50	124.00	6	1307.	0.0	0.0	0.0007	105	49.00	10	33764.	0.1	0.1	0.0171
51	123.00	17	325936.	0.6	0.6	0.1648	106	47.00	21	305632.	0.5	0.5	0.1545*
52	120.00	8	12097.	0.0	0.0	0.0061	107	46.00	8	5237.	0.0	0.0	0.0026
53	119.00	25	1702464.	3.1	3.1	0.9011	108	45.00	35	1332544.	2.3	2.3	0.6736
54	114.00	14	50709.	0.1	0.1	0.0256*	109	44.00	35	1739840.	3.0	3.0	0.8795*
55	113.00	25	1518656.	2.7	2.7	0.7677	110	43.00	71	50700160.	88.9	88.9	*25.67*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	42.00	43	3865344.	6.8	6.8	1.9540*
112	41.00	43	13535744.	23.7	23.7	6.8426*
113	40.00	29	1089344.	1.9	1.9	0.5567*
114	39.00	51	6174464.	10.8	10.8	3.1213*
115	38.00	29	330240.	0.6	0.6	0.1669*
116	37.00	17	74084.	0.1	0.1	0.0325*
117	36.00	25	267568.	0.5	0.5	0.1353
118	35.00	12	54182.	0.1	0.1	0.0274*

AY2AV.1 [TIC-26865416, 165X-55933952] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	381.14	6	2728.	0.1	0.1	0.0013	56	113.00	25	1769488.	3.2	3.2	0.8504
2	299.00	12	58883.	0.1	0.1	0.0203	57	111.00	12	789996.	0.1	0.1	0.0380*
3	298.00	6	1631.	0.0	0.0	0.0008	58	109.00	8	107382.	0.0	0.0	0.0050
4	284.00	12	74432.	0.1	0.1	0.0358	59	107.00	6	2291.	0.0	0.0	0.0011
5	283.00	21	905408.	1.6	1.6	0.4352*	60	103.00	17	2697.	0.0	0.0	0.0013
6	282.00	17	208804.	0.4	0.4	0.1004*	61	101.00	8	64056.	0.1	0.1	0.0308
7	281.00	8	13466.	0.0	0.0	0.0065	62	100.00	35	1220544.	2.2	2.2	0.5866*
8	269.00	10	3735.	0.0	0.0	0.0013	63	99.00	43	5499648.	17.0	17.0	4.5658*
9	268.00	6	1178.	0.0	0.0	0.0006	64	98.00	8	10585.	0.0	0.0	0.0051
10	267.00	8	15357.	0.0	0.0	0.0074	65	97.00	14	60725.	0.1	0.1	0.0292
11	256.00	6	5648.	0.0	0.0	0.0027	66	96.00	25	18162.	0.0	0.0	0.0087
12	255.00	14	107680.	0.2	0.2	0.0518	67	95.00	22	1208192.	2.2	2.2	0.5807
13	254.00	17	266144.	0.5	0.5	0.1279	68	94.00	8	5661.	0.0	0.0	0.0027
14	253.00	10	10979.	0.0	0.0	0.0053	69	93.00	10	33012.	0.1	0.1	0.0159
15	244.00	10	24771.	0.0	0.0	0.0019*	70	91.00	8	3515.	0.0	0.0	0.0017
16	243.00	25	374896.	0.7	0.7	0.1802*	71	85.00	14	109008.	0.2	0.2	0.0524*
17	242.00	35	4958464.	0.9	0.9	2.3832*	72	84.00	21	404128.	0.7	0.7	0.1942*
18	241.00	51	27382784.	49.0	49.0	*13.16*	73	83.00	35	8933888.	16.0	16.0	4.2939*
19	240.00	25	162772.	0.3	0.3	0.0782*	74	82.00	25	624288.	1.1	1.1	0.3001*
20	239.00	29	349808.	0.6	0.6	0.1681*	75	81.00	29	547984.	1.0	1.0	0.2634*
21	238.00	8	4254.	0.0	0.0	0.0020	76	80.00	14	75436.	0.1	0.1	0.0363
22	235.00	8	2315.	0.0	0.0	0.0011	77	79.00	10	10444.	0.0	0.0	0.0089
23	231.00	8	9554.	0.0	0.0	0.0046	78	78.00	12	2284.	0.0	0.0	0.0011
24	227.00	14	102408.	0.2	0.2	0.0492	79	77.00	14	34694.	0.1	0.1	0.0167*
25	223.00	12	77300.	0.1	0.1	0.0372	80	76.00	12	18451.	0.0	0.0	0.0089
26	222.00	8	8178.	0.0	0.0	0.0014	81	75.00	17	145684.	0.3	0.3	0.0700
27	219.00	8	2891.	0.0	0.0	0.0039	82	74.00	6	6970.	0.0	0.0	0.0033
28	213.00	12	83224.	0.1	0.1	0.0400*	83	73.00	14	73548.	0.1	0.1	0.0353*
29	205.00	8	5206.	0.0	0.0	0.0025*	84	72.00	29	131372.	0.2	0.2	0.0631*
30	199.00	6	3458.	0.0	0.0	0.0017	85	71.00	29	1747456.	3.1	3.1	0.8399
31	183.00	10	30703.	0.1	0.1	0.0148	86	70.00	25	283152.	0.5	0.5	0.1361*
32	181.00	10	27634.	0.0	0.0	0.0133*	87	69.00	43	7796736.	13.9	13.9	3.7473
33	179.00	6	1281.	0.0	0.0	0.0006	88	68.00	17	106328.	0.2	0.2	0.0511*
34	172.00	6	2706.	0.0	0.0	0.0013	89	67.00	21	201020.	0.4	0.4	0.0970*
35	170.00	6	1281.	0.0	0.0	0.0006	90	66.00	8	1523.	0.0	0.0	0.0007
36	169.00	17	200700.	0.4	0.4	0.0965	91	65.00	17	102264.	0.2	0.2	0.0492*
37	163.00	10	20341.	0.0	0.0	0.0098	92	64.00	25	979136.	1.8	1.8	0.4706
38	161.00	10	42792.	0.1	0.1	0.0206	93	63.00	17	77896.	0.1	0.1	0.0374*
39	158.00	8	1365.	0.0	0.0	0.0007	94	62.00	8	21179.	0.0	0.0	0.0102
40	157.00	10	4126.	0.0	0.0	0.0020	95	61.00	29	554976.	1.0	1.0	0.2667
41	150.00	12	52887.	0.1	0.1	0.0254	96	60.00	17	143680.	0.3	0.3	0.0691*
42	149.00	6	7018.	0.0	0.0	0.0034	97	59.00	29	2024896.	3.6	3.6	0.9732*
43	145.00	8	5442.	0.0	0.0	0.0026	98	58.00	29	2350720.	4.2	4.2	1.1298*
44	135.00	8	4429.	0.0	0.0	0.0021	99	57.00	71	55933952.	100.0	100.0	*26.88*
45	133.00	17	264000.	0.5	0.5	0.1269	100	56.00	35	4332800.	7.7	7.7	2.0825*
46	132.00	6	3278.	0.0	0.0	0.0016	101	55.00	51	16114944.	28.8	28.8	7.7453*
47	131.00	17	274176.	0.5	0.5	0.1318	102	54.00	25	555648.	1.0	1.0	0.2671*
48	129.00	8	2104.	0.0	0.0	0.0010	103	53.00	29	1533056.	2.7	2.7	0.7368
49	127.00	8	4448.	0.0	0.0	0.0021	104	52.00	21	209660.	0.4	0.4	0.1008*
50	123.00	14	136972.	0.2	0.2	0.0658	105	51.00	35	4579328.	8.2	8.2	2.2010*
51	121.00	8	8006.	0.0	0.0	0.0038	106	50.00	21	341440.	0.6	0.6	0.1641*
52	120.00	10	33355.	0.1	0.1	0.0160	107	49.00	21	127030.	0.2	0.2	0.0610*
53	119.00	25	2054784.	3.7	3.7	0.9876*	108	47.00	17	128928.	0.2	0.2	0.0620*
54	118.00	6	1437.	0.0	0.0	0.0007	109	46.00	6	1998.	0.0	0.0	0.0010
55	114.00	12	43112.	0.1	0.1	0.0207*	110	45.00	29	590000.	1.1	1.1	0.2836

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	44.00	35	835120.	1.5	1.5	0.4014*
112	43.00	43	10065920.	18.0	18.0	4.8380*
113	42.00	35	3696768.	6.6	6.6	1.7768*
114	41.00	51	20258816.	36.2	36.2	9.7370*
115	40.00	35	1064576.	1.9	1.9	0.5117*
116	39.00	43	7044352.	12.6	12.6	3.3857*
117	38.00	25	377472.	0.7	0.7	0.1814
118	37.00	25	122808.	0.2	0.2	0.0590*
119	36.00	17	165644.	0.3	0.3	0.0796*
120	35.00	12	15829.	0.0	0.0	0.0076*

HEP1PK.1 (TIC-62629888, 188X-12243288) EI

2-ethylbutyric acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	305.00	6	413.	0.0	0.0	0.0007	56	228.00	14	37501.	0.3	0.3	0.0599
2	308.00	12	3124.	0.0	0.0	0.0050	57	227.00	21	508448.	4.2	4.2	0.8118
3	299.00	14	49694.	0.4	0.4	0.0793	58	226.00	6	1909.	0.0	0.0	0.0030
4	298.00	10	15726.	0.1	0.1	0.0251	59	223.00	8	3222.	0.0	0.0	0.0051
5	297.00	10	4465.	0.0	0.0	0.0071	60	217.00	12	11861.	0.1	0.1	0.0189
6	285.00	8	925.	0.0	0.0	0.0015	61	216.00	14	11111.	0.1	0.1	0.0177
7	284.00	14	28922.	0.2	0.2	0.0462	62	213.00	12	4629.	0.0	0.0	0.0074
8	283.00	21	262528.	2.1	2.1	0.4192	63	213.00	14	42473.	0.3	0.3	0.0678
9	282.00	10	5585.	0.0	0.0	0.0089	64	210.00	10	10492.	0.1	0.1	0.0168
10	281.00	8	4511.	0.0	0.0	0.0072	65	209.00	21	194380.	1.6	1.6	0.3104
11	280.00	10	8011.	0.1	0.1	0.0128	66	208.00	6	617.	0.0	0.0	0.0010
12	279.00	17	66020.	0.5	0.5	0.1054	67	207.00	12	15070.	0.1	0.1	0.0241
13	274.00	8	1583.	0.0	0.0	0.0025	68	191.00	8	568.	0.0	0.0	0.0009
14	273.00	17	2346.	0.0	0.0	0.0037	69	183.00	10	16421.	0.1	0.1	0.0262
15	272.00	14	41530.	0.3	0.3	0.0663	70	181.00	10	16160.	0.1	0.1	0.0258
16	271.00	29	404192.	3.3	3.3	0.6454	71	179.00	14	44898.	0.4	0.4	0.0717
17	270.00	43	4734976.	38.7	38.7	7.5602	72	169.00	17	59752.	0.5	0.5	0.0954
18	269.00	43	1727744.	14.1	14.1	2.7587	73	164.00	10	3092.	0.0	0.0	0.0049
19	268.00	21	43556.	0.4	0.4	0.0695	74	163.00	10	10027.	0.1	0.1	0.0173
20	257.00	21	33407.	0.3	0.3	0.0533	75	161.00	17	35525.	0.3	0.3	0.0567
21	256.00	8	3379.	0.0	0.0	0.0054	76	157.00	6	1389.	0.0	0.0	0.0022
22	265.00	8	637.	0.0	0.0	0.0010	77	154.00	8	875.	0.0	0.0	0.0014
23	263.00	6	1658.	0.0	0.0	0.0026	78	151.00	8	1428.	0.0	0.0	0.0023
24	262.00	8	716.	0.0	0.0	0.0011	79	150.00	12	18743.	0.2	0.2	0.0299
25	261.00	12	1954.	0.0	0.0	0.0031	80	149.00	8	2540.	0.0	0.0	0.0041
26	260.00	17	3028.	0.0	0.0	0.0051	81	145.00	6	3215.	0.0	0.0	0.0051
27	259.00	12	2407.	0.0	0.0	0.0038	82	142.00	6	1207.	0.0	0.0	0.0019
28	258.00	6	2303.	0.0	0.0	0.0038	83	138.00	6	999.	0.0	0.0	0.0016
29	257.00	21	43859.	0.4	0.4	0.0700	84	137.00	12	14007.	0.1	0.1	0.0225
30	256.00	29	416432.	3.4	3.4	0.6649	85	135.00	17	53744.	0.4	0.4	0.0858
31	255.00	51	4758016.	38.9	38.9	7.5970	86	134.00	6	933.	0.0	0.0	0.01296
32	254.00	21	38523.	0.3	0.3	0.0615	87	133.00	21	81176.	0.7	0.7	0.0078
33	253.00	25	35599.	0.3	0.3	0.0568	88	132.00	10	4858.	0.0	0.0	0.01155
34	252.00	10	5105.	0.0	0.0	0.0082	89	131.00	21	72344.	0.6	0.6	0.0028
35	251.00	8	4534.	0.0	0.0	0.0072	90	126.00	12	1769.	0.0	0.0	0.0044
36	250.00	6	2014.	0.0	0.0	0.0045	91	123.00	8	2731.	0.0	0.0	0.0026
37	249.00	12	18533.	0.2	0.2	0.0296	92	122.00	10	1647.	0.0	0.0	0.0057
38	248.00	6	1201.	0.0	0.0	0.0020	93	121.00	10	3565.	0.0	0.0	0.0076
39	247.00	6	1009.	0.0	0.0	0.0016	94	120.00	12	4749.	0.0	0.0	0.0043
40	246.00	6	3065.	0.0	0.0	0.0049	95	119.00	25	647696.	5.3	5.3	0.0024
41	245.00	8	1731.	0.0	0.0	0.0028	96	118.00	8	2717.	0.0	0.0	0.0301
42	244.00	8	2609.	0.0	0.0	0.0042	97	115.00	12	1522.	0.0	0.0	0.0715
43	243.00	17	22357.	0.2	0.2	0.0357	98	114.00	12	18840.	0.2	0.2	0.0084
44	242.00	35	198016.	1.6	1.6	0.3162	99	113.00	25	545824.	4.5	4.5	0.0030
45	241.00	51	265152.	2.2	2.2	0.4234	100	111.00	14	5285.	0.0	0.0	0.0022
46	240.00	17	37066.	0.3	0.3	0.0605	101	110.00	8	1878.	0.0	0.0	0.0007
47	239.00	10	10507.	0.1	0.1	0.0169	102	109.00	21	89100.	0.7	0.7	0.0495
48	238.00	12	4330.	0.0	0.0	0.0069	103	103.00	6	1349.	0.0	0.0	0.0022
49	237.00	17	66152.	0.5	0.5	0.1056	104	103.00	6	468.	0.0	0.0	0.0007
50	236.00	12	7007.	0.1	0.1	0.0125	105	101.00	21	30999.	0.3	0.3	0.0495
51	235.00	17	62111.	0.5	0.5	0.0992	106	99.00	35	360400.	2.9	2.9	0.5756
52	234.00	8	1369.	0.0	0.0	0.0022	107	99.00	35	1883328.	15.4	15.4	3.0071
53	233.00	8	1001.	0.0	0.0	0.0016	108	98.00	10	20215.	0.2	0.2	0.0323
54	231.00	6	1200.	0.0	0.0	0.0019	109	97.00	14	29217.	0.2	0.2	0.0467
55	229.00	10	9436.	0.1	0.1	0.0151	110	96.00	17	20756.	0.2	0.2	0.0331

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	95.00	25	462640.	3.8	3.8	0.7387	166	37.00	35	73372.	0.6	0.6	0.1172*
112	94.00	12	11836.	0.1	0.1	0.0189*	167	36.00	25	99508.	0.8	0.8	0.1589*
113	93.00	10	14223.	0.1	0.1	0.0227*	168	35.00	17	27388.	0.2	0.2	0.0437*
114	91.00	8	8210.	0.1	0.1	0.0131*							
115	90.00	8	1725.	0.0	0.0	0.0028							
116	89.00	10	2452.	0.0	0.0	0.0039							
117	88.00	6	1417.	0.0	0.0	0.0023							
118	87.00	21	58633.	0.5	0.5	0.0936*							
119	86.00	8	10469.	0.1	0.1	0.0167							
120	85.00	17	36293.	0.3	0.3	0.0579							
121	84.00	12	16931.	0.1	0.1	0.0270							
122	83.00	29	349552.	2.9	2.9	0.5581							
123	82.00	17	40872.	0.3	0.3	0.0653*							
124	81.00	25	114968.	0.9	0.9	0.1836							
125	80.00	14	14220.	0.1	0.1	0.0227*							
126	79.00	12	13910.	0.1	0.1	0.0222*							
127	77.00	14	26923.	0.2	0.2	0.0430*							
128	76.00	12	10799.	0.1	0.1	0.0172*							
129	75.00	17	56474.	0.5	0.5	0.0902							
130	74.00	10	8973.	0.1	0.1	0.0143*							
131	73.00	21	100264.	0.8	0.8	0.1601							
132	72.00	29	315120.	2.6	2.6	0.5031							
133	71.00	71	648268.	52.9	52.9	*10.35*							
134	70.00	43	1039184.	8.5	8.5	1.6592*							
135	69.00	51	4185248.	34.2	34.2	6.6889*							
136	68.00	29	153700.	1.3	1.3	0.2454*							
137	67.00	25	107528.	0.9	0.9	0.1717*							
138	66.00	17	25956.	0.2	0.2	0.0414							
139	65.00	21	60182.	0.5	0.5	0.0961							
140	64.00	21	352992.	2.9	2.9	0.5636							
141	63.00	21	42330.	0.3	0.3	0.0676*							
142	62.00	10	13614.	0.1	0.1	0.0217							
143	61.00	21	49155.	0.4	0.4	0.0785*							
144	60.00	8	5996.	0.0	0.0	0.0096							
145	59.00	21	105024.	0.8	0.8	0.1661							
146	58.00	14	22561.	0.2	0.2	0.0360*							
147	57.00	29	301232.	2.5	2.5	0.4810*							
148	56.00	29	324512.	2.7	2.7	0.5181*							
149	55.00	59	5304576.	43.3	43.3	8.4697*							
150	54.00	29	145654.	1.2	1.2	0.2326*							
151	53.00	35	438032.	3.6	3.6	0.6994							
152	52.00	25	66008.	0.5	0.5	0.1054*							
153	51.00	51	1394368.	11.4	11.4	2.2264*							
154	50.00	25	101928.	0.8	0.8	0.1627*							
155	49.00	21	34866.	0.3	0.3	0.0557*							
156	47.00	25	110960.	1.0	1.0	0.1899							
157	46.00	14	11060.	0.1	0.1	0.0177							
158	45.00	35	515952.	4.2	4.2	0.8238							
159	44.00	43	427488.	3.5	3.5	0.6826*							
160	43.00	87	12243200.	100.0	100.0	*19.54*							
161	42.00	51	1123264.	9.2	9.2	1.7935*							
162	41.00	59	4312832.	35.2	35.2	6.8862*							
163	40.00	43	377904.	3.1	3.1	0.6034*							
164	39.00	71	2242024.	18.3	18.3	3.5008*							
165	38.00	35	181040.	1.5	1.5	0.2891*							

EWIPK.1 [TIC-71442432, 100X-13621504] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	308.00	8	1371.	0.0	0.0	0.0019
2	298.00	14	48245.	0.4	0.4	0.0075
3	298.00	12	20261.	0.1	0.1	0.0284
4	289.00	6	774.	0.0	0.0	0.0011
5	285.00	8	4858.	0.0	0.0	0.0068
6	284.00	14	59776.	0.4	0.4	0.0037
7	283.00	25	717184.	5.3	5.3	1.0039*
8	282.00	10	20301.	0.1	0.1	0.0284
9	281.00	12	4952.	0.0	0.0	0.0059
10	279.00	14	46506.	0.3	0.3	0.0051
11	274.00	6	962.	0.0	0.0	0.0013
12	273.00	6	599.	0.0	0.0	0.0009
13	269.00	10	6811.	0.1	0.1	0.0025
14	268.00	6	1150.	0.0	0.0	0.0016
15	267.00	12	21359.	0.2	0.2	0.0239
16	266.00	6	637.	0.0	0.0	0.0021
17	263.00	6	857.	0.0	0.0	0.0009
18	259.00	5	71488.	0.5	0.5	0.0012
19	258.00	35	666176.	82.3	82.3	*15.68*
20	257.00	51	11288192.	3.7	3.7	0.6972*
21	255.00	25	498064.	0.2	0.2	0.0349*
22	254.00	17	24945.	0.1	0.1	0.0101
23	253.00	10	7201.	0.0	0.0	0.0047
24	243.00	8	3352.	0.0	0.0	0.0409
25	242.00	12	29234.	0.2	0.2	0.0409
26	241.00	21	264064.	1.9	1.9	0.3696
27	238.00	8	505.	0.0	0.0	0.0077
28	237.00	17	142752.	1.0	1.0	0.1998*
29	236.00	10	3033.	0.0	0.0	0.0042
30	235.00	17	61972.	0.5	0.5	0.0867
31	231.00	8	5316.	0.0	0.0	0.0074
32	228.00	17	83196.	0.6	0.6	0.1165*
33	227.00	35	1448000.	10.6	10.6	2.0268*
34	226.00	8	4423.	0.0	0.0	0.0062
35	223.00	8	9559.	0.1	0.1	0.0134
36	221.00	6	1817.	0.0	0.0	0.0025
37	219.00	14	13898.	0.1	0.1	0.0195
38	217.00	12	1932.	0.0	0.0	0.0028
39	213.00	12	43880.	0.3	0.3	0.0614*
40	212.00	6	1374.	0.0	0.0	0.0019
41	210.00	10	4536.	0.0	0.0	0.0063*
42	209.00	17	99724.	0.7	0.7	0.1396
43	207.00	10	12182.	0.1	0.1	0.0171*
44	191.00	12	33455.	0.2	0.2	0.0468*
45	183.00	10	19842.	0.1	0.1	0.0278
46	181.00	12	40065.	0.3	0.3	0.0561
47	179.00	14	26407.	0.2	0.2	0.0370*
48	169.00	6	1594.	0.0	0.0	0.0022
49	163.00	17	89872.	0.7	0.7	0.1258
50	163.00	8	4239.	0.0	0.0	0.0059
51	162.00	6	2061.	0.0	0.0	0.0029
52	161.00	12	17390.	0.1	0.1	0.0243*
53	151.00	8	10913.	0.1	0.1	0.0153
54	150.00	10	6310.	0.0	0.0	0.0088
55						

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	57.00	43	5687232.	49.1	49.1	9.3603*
112	56.00	43	2292544.	16.8	16.8	3.2089*
113	55.00	43	3673408.	27.0	27.0	5.1418*
114	54.00	21	155360.	1.1	1.1	0.2175*
115	53.00	25	543408.	4.0	4.0	0.7606
116	52.00	17	68292.	0.5	0.5	0.0956*
117	51.00	35	1611904.	11.8	11.8	2.2562*
118	50.00	21	85784.	0.6	0.6	0.1201*
119	49.00	12	30836.	0.2	0.2	0.0432
120	48.00	8	2043.	0.0	0.0	0.0029
121	47.00	25	139364.	1.0	1.0	0.1951
122	46.00	8	7682.	0.1	0.1	0.0108
123	45.00	35	555968.	4.1	4.1	0.7702*
124	44.00	35	453168.	3.3	3.3	0.6343*
125	43.00	59	13621504.	100.0	100.0	*19.06*
126	42.00	35	733952.	5.4	5.4	1.0273*
127	41.00	43	6885120.	44.7	44.7	8.5175*
128	40.00	35	323904.	2.4	2.4	0.4534*
129	39.00	51	2336448.	17.2	17.2	3.2704*
130	38.00	25	148072.	1.1	1.1	0.2084*
131	37.00	17	55083.	0.4	0.4	0.0771*
132	36.00	21	128440.	0.9	0.9	0.1798*
133	35.00	14	27153.	0.2	0.2	0.0380

AG3AV.1 [TIC-169959426, 100% 30710784] EI

2-methylpentanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. RREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. RREF	% TOT. ION
1	355.00	6	1413.	0.0	0.0	0.0008	56	151.00	6	1785.	0.0	0.0	0.0011
2	299.00	12	83732.	0.3	0.1	0.0493	57	150.00	10	49899.	0.2	0.2	0.0294
3	298.00	8	36703.	0.1	0.0	0.0216	58	145.00	10	33507.	0.1	0.1	0.0197
4	297.00	10	8481.	0.0	0.0	0.0050	59	142.00	6	1947.	0.0	0.0	0.0011
5	284.00	10	41880.	0.1	0.1	0.0246	60	137.00	14	165292.	0.5	0.5	0.0973
6	283.00	21	581056.	1.9	1.9	0.3419	61	135.00	12	75856.	0.3	0.3	0.0452
7	281.00	8	11338.	0.0	0.0	0.0067	62	134.00	6	4558.	0.0	0.0	0.0027
8	280.00	8	3007.	0.0	0.0	0.0018	63	133.00	17	262192.	0.9	0.9	0.1543
9	279.00	14	108192.	0.4	0.4	0.0637	64	132.00	6	2416.	0.0	0.0	0.0014
10	271.00	8	25312.	0.1	0.1	0.0149	65	131.00	17	226848.	0.7	0.7	0.1335
11	270.00	21	368320.	1.2	1.2	0.2167	66	123.00	10	27381.	0.1	0.1	0.0161
12	269.00	35	4188928.	13.5	13.5	2.4647	67	122.00	6	2381.	0.0	0.0	0.0014
13	268.00	10	28690.	0.1	0.1	0.0150	68	121.00	8	1998.	0.0	0.0	0.0012
14	267.00	10	25468.	0.1	0.0	0.0007	69	120.00	12	13818.	0.0	0.0	0.0081
15	259.00	8	1190.	0.0	0.0	0.0010	70	119.00	25	1812480.	5.9	5.9	1.0664
16	258.00	17	154740.	0.5	0.5	0.0910	71	117.00	6	766.	0.0	0.0	0.0256
17	257.00	29	1690688.	5.5	5.5	0.9948	72	114.00	25	43453.	0.1	0.1	0.0598
18	256.00	51	22870016.	74.5	74.5	13.45	73	113.00	10	3062.	0.0	0.0	0.0018
19	255.00	35	2112192.	6.9	6.9	1.2428	74	112.00	8	17110.	0.1	0.1	0.0101
20	254.00	12	28260.	0.1	0.1	0.0166	75	111.00	17	239892.	0.8	0.8	0.1411
21	253.00	12	16542.	0.1	0.0	0.0097	76	109.00	10	27886.	0.1	0.1	0.0164
22	251.00	6	4137.	0.0	0.0	0.0024	77	103.00	10	74796.	0.2	0.2	0.0440
23	249.00	8	19990.	0.1	0.1	0.0118	78	101.00	14	1053248.	3.4	3.4	0.6197
24	243.00	8	2755.	0.0	0.0	0.0016	79	100.00	29	4807168.	15.7	15.7	2.8284
25	242.00	12	56044.	0.2	0.2	0.0389	80	99.00	29	75224.	0.3	0.3	0.0466
26	241.00	17	451376.	1.5	1.5	0.2656	81	98.00	12	51674.	0.2	0.2	0.0304
27	239.00	10	12302.	0.0	0.0	0.0072	82	97.00	12	32739.	0.1	0.1	0.0193
28	237.00	10	21202.	0.1	0.1	0.0125	83	96.00	10	1426752.	4.6	4.6	0.8395
29	236.00	10	7982.	0.0	0.0	0.0047	84	95.00	25	5756.	0.0	0.0	0.0034
30	235.00	14	114272.	0.4	0.4	0.0672	85	94.00	8	27563.	0.1	0.1	0.0162
31	234.00	8	1487.	0.0	0.0	0.0009	86	93.00	12	22880.	0.1	0.1	0.0135
32	231.00	8	7283.	0.0	0.0	0.0043	87	91.00	10	49988.	0.2	0.2	0.0294
33	229.00	10	5905.	0.0	0.0	0.0035	88	87.00	14	14489.	0.0	0.0	0.0085
34	228.00	10	77224.	0.3	0.3	0.0454	89	85.00	10	18817.	0.1	0.1	0.0111
35	227.00	21	1492608.	4.9	4.9	0.8782	90	84.00	25	762304.	2.5	2.5	0.4485
36	223.00	12	112448.	0.4	0.4	0.0662	91	83.00	17	120256.	0.4	0.4	0.0708
37	221.00	10	8678.	0.0	0.0	0.0051	92	82.00	25	514816.	1.7	1.7	0.3029
38	219.00	10	3896.	0.0	0.0	0.0023	93	81.00	10	22635.	0.1	0.1	0.0133
39	214.00	6	793.	0.0	0.0	0.0005	94	80.00	10	35101.	0.1	0.1	0.0207
40	213.00	14	116960.	0.4	0.4	0.0688	95	79.00	6	1215.	0.0	0.0	0.0007
41	210.00	8	9158.	0.0	0.0	0.0054	96	78.00	12	41325.	0.1	0.1	0.0243
42	209.00	17	457392.	1.5	1.5	0.2691	97	77.00	17	154744.	0.5	0.5	0.0910
43	208.00	6	709.	0.0	0.0	0.0004	98	75.00	10	51208.	0.2	0.2	0.0301
44	207.00	8	12990.	0.0	0.0	0.0076	99	74.00	21	375744.	1.2	1.2	0.2211
45	193.00	8	2489.	0.0	0.0	0.0015	100	73.00	10	727872.	2.4	2.4	0.4283
46	191.00	10	61817.	0.2	0.2	0.0364	101	72.00	21	14834688.	48.3	48.3	8.7284
47	183.00	12	52306.	0.2	0.2	0.0308	102	71.00	43	1490880.	4.9	4.9	0.8772
48	181.00	10	68932.	0.2	0.2	0.0406	103	70.00	35	9282304.	30.2	30.2	5.4615
49	180.00	6	1357.	0.0	0.0	0.0008	104	69.00	17	142328.	0.5	0.5	0.0843
50	179.00	10	69368.	0.2	0.2	0.0408	105	68.00	17	281216.	0.9	0.9	0.1655
51	172.00	6	2173.	0.0	0.0	0.0013	106	67.00	12	34662.	0.1	0.1	0.0204
52	169.00	14	162868.	0.5	0.5	0.0958	107	66.00	13	118524.	0.4	0.4	0.0697
53	164.00	8	4475.	0.0	0.0	0.0026	108	65.00	25	949984.	3.1	3.1	0.5589
54	163.00	8	18654.	0.1	0.1	0.0110	109	64.00	14	78632.	0.2	0.2	0.0451
55	161.00	10	79964.	0.3	0.3	0.0470	110	63.00	14				

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	62.00	8	11738.	0.0	0.0	0.0069
112	61.00	17	125616.	0.4	0.4	0.0745*
113	60.00	6	6066.	0.0	0.0	0.0036
114	59.00	21	381344.	1.2	1.2	0.2244*
115	58.00	25	736176.	2.4	2.4	0.4331*
116	57.00	35	12351488.	40.2	40.2	7.2673*
117	56.00	35	4407552.	14.4	14.4	2.5933*
118	55.00	35	7966464.	25.9	25.9	4.6873*
119	54.00	21	257216.	0.8	0.8	0.1513
120	53.00	25	1013328.	3.3	3.3	0.5962*
121	52.00	14	114960.	0.4	0.4	0.0676*
122	51.00	35	3839872.	12.5	12.5	2.2593*
123	50.00	17	205312.	0.7	0.7	0.1208*
124	49.00	10	52366.	0.2	0.2	0.0308*
125	47.00	21	278416.	0.9	0.9	0.1638*
126	46.00	6	1290.	0.0	0.0	0.0008
127	45.00	35	1422720.	4.6	4.6	0.8371*
128	44.00	35	1136320.	3.7	3.7	0.6686*
129	43.00	59	30710784.	100.0	150.0	*16.06*
130	42.00	35	5058048.	16.5	16.5	2.9760*
131	41.00	43	14007040.	45.6	45.6	8.2414*
132	40.00	35	1098496.	3.6	3.6	0.6463*
133	39.00	35	5813760.	18.9	18.9	3.4207*
134	38.00	25	307968.	1.0	1.0	0.1812*
135	37.00	17	86672.	0.3	0.3	0.0510*
136	36.00	14	116808.	0.4	0.4	0.0687*
137	35.00	10	14318.	0.0	0.0	0.0084*

AC3PK.1 [TIC-84312864, 188X-13678656] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	6	1624.	0.0	0.0	0.0019	56	99.00	35	4347136.	31.8	31.8	5.1560*
2	299.00	10	35964.	0.3	0.3	0.00427	57	98.00	10	44669.	0.3	0.3	0.00530
3	298.00	8	5181.	0.0	0.0	0.0061	58	97.00	17	97216.	0.7	0.7	0.1153*
4	297.00	6	2288.	0.0	0.0	0.0027	59	96.00	6	4229.	0.0	0.0	0.0050
5	284.00	6	5224.	0.0	0.0	0.0062	60	95.00	21	578768.	4.2	4.2	0.16865
6	283.00	17	146372.	1.1	1.1	0.1736	61	93.00	8	11518.	0.1	0.1	0.0137
7	282.00	8	984.	0.0	0.0	0.0011	62	91.00	8	1840.	0.0	0.0	0.0022
8	281.00	8	2309.	0.0	0.0	0.0027	63	89.00	14	3027.	0.0	0.0	0.0036*
9	279.00	8	36077.	0.3	0.3	0.0428	64	85.00	5	1266.	0.0	0.0	0.0015
10	271.00	8	8872.	0.1	0.1	0.0105	65	84.00	8	8424.	0.1	0.1	0.0100
11	270.00	17	170176.	1.2	1.2	0.2018*	66	83.00	25	752352.	5.5	5.5	0.0923
12	269.00	25	2085248.	15.3	15.3	2.4732*	67	82.00	12	37277.	0.3	0.3	0.0442*
13	268.00	14	29517.	0.2	0.2	0.0350*	68	81.00	17	50583.	0.4	0.4	0.0600*
14	256.00	10	42319.	0.3	0.3	0.0502	69	80.00	8	12765.	0.1	0.1	0.0151
15	255.00	17	379376.	2.8	2.8	0.4500*	70	79.00	6	690.	0.0	0.0	0.0008
16	253.00	10	29530.	0.2	0.2	0.0350	71	77.00	8	3279.	0.0	0.0	0.0039
17	249.00	8	2550.	0.0	0.0	0.0030	72	75.00	12	37025.	0.3	0.3	0.0435
18	244.00	14	89068.	0.7	0.7	0.1056*	73	74.00	6	1095.	0.0	0.0	0.0013
19	243.00	25	1335368.	9.8	9.8	1.5838*	74	73.00	21	212796.	1.6	1.6	0.2524
20	242.00	51	10652160.	77.9	77.9	*12.63*	75	72.00	17	116404.	0.9	0.9	0.1381*
21	241.00	25	652112.	4.8	4.8	0.7735*	76	71.00	35	2670016.	19.5	19.5	3.1668
22	240.00	14	111900.	0.8	0.8	0.1327*	77	70.00	29	840368.	6.1	6.1	0.9967*
23	239.00	8	8355.	0.1	0.1	0.0099	78	69.00	35	499936.	36.6	36.6	5.9303
24	235.00	12	7838.	0.1	0.1	0.0093	79	68.00	17	131380.	1.0	1.0	0.1558
25	229.00	8	1629.	0.0	0.0	0.0019	80	67.00	17	117548.	0.5	0.5	0.1394*
26	228.00	17	176432.	1.3	1.3	0.2093*	81	66.00	6	6965.	0.1	0.1	0.0083
27	227.00	29	2972864.	21.7	21.7	3.5260*	82	65.00	10	22438.	0.2	0.2	0.0266
28	226.00	17	71240.	0.5	0.5	0.0845*	83	64.00	21	391101.	2.9	2.9	0.4639*
29	221.00	17	124992.	0.9	0.9	0.1482	84	63.00	12	13243.	0.1	0.1	0.0157*
30	221.00	6	2246.	0.0	0.0	0.0027	85	62.00	6	2526.	0.0	0.0	0.0030
31	219.00	8	4238.	0.0	0.0	0.0051	86	61.00	17	129040.	0.9	0.9	0.1531*
32	213.00	14	99584.	0.7	0.7	0.1181	87	60.00	14	51339.	0.4	0.4	0.0609*
33	207.00	6	1709.	0.0	0.0	0.0020	88	59.00	21	115872.	0.8	0.8	0.1374*
34	183.00	10	18020.	0.1	0.1	0.0214	89	58.00	21	245080.	1.8	1.8	0.2907
35	181.00	10	32678.	0.2	0.2	0.0388	90	57.00	43	6456304.	47.3	47.3	7.6695*
36	179.00	8	22255.	0.2	0.2	0.0264	91	56.00	35	1923584.	14.1	14.1	2.2815
37	169.00	14	75156.	0.5	0.5	0.0891	92	55.00	35	4337920.	31.7	31.7	5.1451
38	163.00	6	2089.	0.0	0.0	0.0025	93	54.00	21	164472.	1.2	1.2	0.1951*
39	161.00	8	6368.	0.0	0.0	0.0076	94	53.00	25	477296.	3.5	3.5	0.5661
40	150.00	6	7178.	0.1	0.1	0.0085	95	52.00	12	52101.	0.4	0.4	0.0618*
41	145.00	6	956.	0.0	0.0	0.0011	96	51.00	29	2162752.	15.8	15.8	2.5652*
42	135.00	10	32072.	0.2	0.2	0.0380	97	50.00	17	99184.	0.7	0.7	0.1176*
43	133.00	17	119432.	0.9	0.9	0.1417	98	49.00	8	17389.	0.1	0.1	0.0206
44	131.00	17	131136.	1.0	1.0	0.1555	99	47.00	25	296256.	2.2	2.2	0.3514
45	123.00	17	180964.	1.3	1.3	0.2146	100	45.00	29	638592.	4.7	4.7	0.7574*
46	120.00	8	1909.	0.0	0.0	0.0023	101	44.00	35	946704.	6.9	6.9	1.1229*
47	119.00	21	962624.	6.6	6.6	1.0706	102	43.00	51	13670656.	100.0	100.0	*16.21*
48	114.00	12	21036.	0.2	0.2	0.0250	103	42.00	35	3312576.	24.2	24.2	3.9289
49	113.00	21	1054656.	7.7	7.7	1.2509	104	41.00	35	8075520.	59.1	59.1	9.5781*
50	111.00	8	14684.	0.1	0.1	0.0174	105	40.00	29	465808.	3.4	3.4	0.5525*
51	109.00	6	6861.	0.1	0.1	0.0081	106	39.00	29	2478400.	18.1	18.1	2.9396
52	108.00	6	1087.	0.0	0.0	0.0013	107	38.00	17	135788.	1.0	1.0	0.1611*
53	103.00	6	2707.	0.0	0.0	0.0032	108	37.00	8	10537.	0.1	0.1	0.0125
54	101.00	10	9666.	0.1	0.1	0.0115	109	36.00	12	27445.	0.2	0.2	0.0326*
55	100.00	29	556960.	4.1	4.1	0.6606*							

EXAV3.1 [TIC-198829824, 188X-33356888] EI

4-methylpentanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	300.00	6	5354.	0.0	0.0	0.0028	56	123.00	12	56056.	0.2	0.0	0.0348
2	299.00	12	123224.	0.4	0.4	0.0648	57	122.00	6	1261.	0.0	0.0	0.0007
3	298.00	6	1886.	0.0	0.0	0.0010	58	120.00	8	9510.	0.0	0.0	0.0050
4	297.00	10	50944.	0.2	0.2	0.0268	59	119.00	25	1602880.	4.8	4.8	0.8435
5	284.00	14	85068.	0.3	0.3	0.0448	60	114.00	10	34886.	0.1	0.1	0.0184
6	283.00	21	936736.	2.8	2.8	0.4929*	61	113.00	25	1569408.	4.7	4.7	0.8259*
7	282.00	8	35465.	0.1	0.1	0.0187	62	112.00	8	1433.	0.0	0.0	0.0008
8	279.00	12	83548.	0.3	0.3	0.0448	63	111.00	14	64863.	0.2	0.2	0.0341
9	271.00	8	90788.	0.0	0.0	0.0006	64	109.00	17	112780.	0.3	0.3	0.0593*
10	269.00	14	1039424.	0.3	0.3	0.0478	65	108.00	6	2011.	0.0	0.0	0.0011
11	268.00	21	1536.	0.0	0.0	0.0002	66	103.00	8	12815.	0.0	0.0	0.0067
12	267.00	6	3753.	0.0	0.0	0.0002	67	101.00	17	87868.	0.3	0.3	0.0462*
13	265.00	6	44403.	0.1	0.1	0.0234	68	99.00	35	1254528.	3.6	3.6	0.5682
14	258.00	10	613072.	1.0	1.0	0.3226*	69	98.00	43	2041600.	27.7	27.7	4.8632*
15	257.00	21	3775744.	11.3	11.3	1.9869*	70	97.00	21	363328.	1.1	1.1	0.1944*
16	256.00	35	5514496.	16.5	16.5	2.5019*	71	96.00	8	15049.	0.0	0.0	0.0079
17	255.00	43	37572.	0.1	0.1	0.0190*	72	95.00	25	1190592.	3.6	3.6	0.6307
18	254.00	12	12305.	0.0	0.0	0.0065	73	94.00	6	1965.	0.0	0.0	0.0010
19	253.00	8	24564.	0.1	0.1	0.0129	74	93.00	12	36886.	0.1	0.1	0.0194*
20	244.00	10	387968.	1.2	1.2	0.2042	75	91.00	8	20776.	0.1	0.1	0.0109
21	243.00	17	4704000.	14.1	14.1	2.4754*	76	89.00	6	2702.	0.0	0.0	0.0014
22	242.00	35	2570752.	7.7	7.7	1.3570*	77	87.00	10	23896.	0.1	0.1	0.0116
23	241.00	35	185140.	0.3	0.3	0.0553*	78	85.00	10	23896.	0.1	0.1	0.0116
24	239.00	17	11472.	0.1	0.1	0.0254	79	84.00	17	170860.	0.5	0.5	0.0541*
25	237.00	12	2111.	0.0	0.0	0.0066	80	83.00	35	4092160.	12.3	12.3	2.1534
26	236.00	8	99708.	0.0	0.0	0.0011	81	82.00	25	497504.	1.5	1.5	0.2618*
27	235.00	17	1787.	0.0	0.0	0.0025	82	81.00	35	6207232.	18.6	18.6	3.2655*
28	231.00	8	18121.	0.1	0.1	0.0095	83	79.00	12	56310.	0.2	0.2	0.0296*
29	228.00	8	422832.	1.3	1.3	0.2225	84	78.00	12	59568.	0.2	0.2	0.0366*
30	227.00	17	12907.	0.0	0.0	0.0068	85	77.00	14	1207.	0.0	0.0	0.0006
31	223.00	12	29060.	0.1	0.1	0.0153	86	75.00	17	73040.	0.2	0.2	0.0384*
32	219.00	6	1459.	0.0	0.0	0.0008	87	74.00	17	166652.	0.5	0.5	0.0877
33	217.00	6	10680.	0.0	0.0	0.0008	88	73.00	8	11691.	0.0	0.0	0.0062
34	214.00	10	504336.	1.5	1.5	0.2654	89	72.00	21	276120.	0.8	0.8	0.1453
35	213.00	17	1584.	0.6	0.6	0.0808	90	71.00	35	141924.	0.4	0.4	0.0747
36	209.00	8	1899.	0.0	0.0	0.0008	91	69.00	35	2753664.	8.3	8.3	1.4491
37	193.00	6	15742.	0.0	0.0	0.00196	92	68.00	21	8127232.	7.2	7.2	1.2687
38	191.00	8	37241.	0.1	0.1	0.0146	93	67.00	43	158988.	0.5	0.5	0.0837*
39	181.00	6	27791.	0.0	0.0	0.0008	94	66.00	21	258872.	0.0	0.0	0.1352*
40	180.00	6	1574.	0.0	0.0	0.00196	95	65.00	29	115992.	0.3	0.3	0.0610*
41	179.00	10	23337.	0.1	0.1	0.0123	96	64.00	17	96912.	0.3	0.3	0.0510*
42	169.00	14	113548.	0.3	0.3	0.0598	97	63.00	25	803504.	2.7	2.7	0.4755
43	161.00	8	12177.	0.0	0.0	0.0008	98	62.00	12	33384.	0.2	0.2	0.0439
44	158.00	14	74844.	0.2	0.2	0.0394*	99	61.00	10	17693.	0.1	0.1	0.0092
45	150.00	10	38026.	0.1	0.1	0.0200	100	60.00	21	278912.	0.8	0.8	0.1468
46	145.00	6	1155.	0.0	0.0	0.0006	101	59.00	14	73588.	0.2	0.2	0.0387
47	137.00	12	77516.	0.2	0.2	0.0408*	102	58.00	21	227804.	0.7	0.7	0.1199
48	135.00	8	7741.	0.0	0.0	0.0004	103	57.00	29	1234816.	3.7	3.7	0.6498
49	133.00	17	224612.	0.7	0.7	0.1182	104	56.00	43	28540528.	85.6	85.6	15.01*
50	131.00	17	200748.	0.6	0.6	0.1099	105	55.00	71	4331264.	13.0	13.0	2.2793*
51							106	54.00	25	20533248.	61.6	61.6	10.80*
52							107	53.00	29	1324352.	4.0	4.0	0.6969
53							108						
54							109						
55							110						

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	52.00	21	176652.	0.5	0.5	0.0930*
112	51.00	35	3491712.	10.5	10.5	1.8375
113	50.00	21	253568.	0.8	0.8	0.1334
114	49.00	14	75656.	0.2	0.2	0.0398*
115	48.00	10	58395.	0.2	0.2	0.0307
116	47.00	21	152180.	0.5	0.5	0.0801*
117	46.00	8	9138.	0.0	0.0	0.0048
118	45.00	35	806400.	2.4	2.4	0.4244
119	44.00	35	1464832.	4.4	4.4	0.7708*
120	43.00	71	33356800.	100.0	100.0	*17.55*
121	42.00	35	4634368.	13.9	13.9	2.4388*
122	41.00	43	16047872.	48.1	48.1	8.4449*
123	40.00	29	876784.	2.6	2.6	0.4614
124	39.00	51	5578752.	16.7	16.7	2.9357*
125	38.00	29	319040.	1.0	1.0	0.1679*
126	37.00	17	91984.	0.3	0.3	0.0484*
127	36.00	25	272528.	0.8	0.8	0.1434*
128	35.00	10	40264.	0.1	0.1	0.0212

AL4PA.1 (TIC=124665256, 100% = 26156#32) EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	299.00	14	115504.	0.4	0.4	0.0886	56	133.00	17	166304.	0.6	0.6	0.1334
2	298.00	14	138436.	0.5	0.5	0.1110	57	132.00	8	1560.	0.0	0.0	0.0013
3	297.00	8	4701.	0.0	0.0	0.0038	58	131.00	17	166188.	0.6	0.6	0.1333
4	283.00	8	15812.	0.1	0.1	0.0127	59	126.00	8	2593.	0.0	0.0	0.0021
5	281.00	10	9534.	0.0	0.0	0.0076	60	123.00	17	151684.	0.6	0.6	0.1217
6	280.00	10	17055.	0.1	0.1	0.0137	61	122.00	14	65063.	0.2	0.2	0.0522
7	279.00	14	159752.	0.6	0.6	0.1281	62	121.00	16	1191.	0.0	0.0	0.0010
8	271.00	8	8076.	0.0	0.0	0.0065	63	120.00	10	17962.	0.1	0.1	0.0144
9	270.00	14	155796.	0.6	0.6	0.1250	64	119.00	21	1146175.	4.4	4.4	0.9194
10	269.00	25	1747520.	6.7	6.7	1.4018*	65	114.00	12	44725.	0.2	0.2	0.0359
11	268.00	10	2960.	0.0	0.0	0.0024	66	113.00	25	1343552.	5.1	5.1	1.0777
12	265.00	6	8871.	0.0	0.0	0.0071	67	112.00	8	8367.	0.0	0.0	0.0067
13	257.00	12	72552.	0.3	0.3	0.0582	68	111.00	17	67184.	0.3	0.3	0.0539*
14	256.00	29	777408.	3.0	3.0	0.6236*	69	109.00	14	93324.	0.4	0.4	0.06749
15	255.00	43	6877952.	26.3	26.3	5.5171*	70	108.00	10	10911.	0.0	0.0	0.0088
16	254.00	25	38920.	0.1	0.1	0.0312*	71	103.00	6	1978.	0.0	0.0	0.0016
17	253.00	14	22169.	0.1	0.1	0.0178*	72	101.00	12	11050.	0.2	0.2	0.0329
18	252.00	6	1542.	0.0	0.0	0.0012	73	100.00	35	886409.	3.4	3.4	0.7110
19	251.00	8	18184.	0.1	0.1	0.0146	74	99.00	43	7898800.	30.2	30.2	6.3260*
20	245.00	6	1088.	0.0	0.0	0.0009	75	98.00	21	389654.	1.5	1.5	0.3126
21	244.00	21	110000.	0.4	0.4	0.0883*	76	97.00	21	194516.	0.7	0.7	0.1560
22	243.00	35	1203712.	4.6	4.6	0.9656*	77	96.00	8	18872.	0.1	0.1	0.0151
23	242.00	51	12247552.	46.8	46.8	9.8243*	78	95.00	21	855936.	3.3	3.3	0.6866
24	241.00	29	308832.	1.2	1.2	0.2477*	79	93.00	8	14863.	0.1	0.1	0.0119
25	240.00	14	49543.	0.2	0.2	0.0397*	80	91.00	10	11354.	0.0	0.0	0.0091
26	239.00	10	20176.	0.1	0.1	0.0162	81	89.00	8	9447.	0.0	0.0	0.0076
27	237.00	10	19042.	0.1	0.1	0.0153	82	87.00	6	1965.	0.0	0.0	0.0016
28	235.00	12	72400.	0.3	0.3	0.0581	83	85.00	10	37116.	0.1	0.1	0.0298
29	229.00	8	9599.	0.0	0.0	0.0077	84	84.00	10	12849.	0.0	0.0	0.0103
30	228.00	17	130612.	0.5	0.5	0.1048	85	83.00	25	558800.	2.1	2.1	0.4483
31	227.00	29	2369984.	9.1	9.1	1.9011*	86	82.00	17	59301.	0.2	0.2	0.0476
32	226.00	10	26084.	0.1	0.1	0.0209	87	81.00	25	352324.	1.3	1.3	0.2825*
33	223.00	8	14282.	0.1	0.1	0.0115	88	80.00	25	255108.	1.0	1.0	0.2046
34	222.00	10	15493.	0.1	0.1	0.0124	89	79.00	12	18500.	0.1	0.1	0.0148*
35	221.00	8	1545.	0.0	0.0	0.0012	90	78.00	6	2174.	0.0	0.0	0.0017
36	219.00	10	8928.	0.0	0.0	0.0072	91	77.00	17	76472.	0.3	0.3	0.0613
37	217.00	10	8445.	0.0	0.0	0.0058*	92	76.00	8	12911.	0.0	0.0	0.0104
38	213.00	14	112404.	0.4	0.4	0.0902	93	75.00	17	110104.	0.4	0.4	0.0803*
39	209.00	10	20441.	0.5	0.5	0.0950	94	74.00	10	14099.	0.1	0.1	0.0113*
40	207.00	10	2326.	0.1	0.1	0.0164	95	73.00	21	236004.	0.9	0.9	0.1853
41	191.00	10	35541.	0.0	0.0	0.0019	96	72.00	21	197060.	0.8	0.8	0.1581
42	183.00	10	27839.	0.1	0.1	0.0285	97	71.00	35	3700280.	14.1	14.1	2.9682
43	181.00	12	1689.	0.1	0.1	0.0223	98	70.00	35	2518848.	9.6	9.6	2.0205
44	180.00	12	127764.	0.0	0.0	0.0014	99	69.00	35	5732096.	1.9	1.9	0.4500
45	179.00	17	77124.	0.5	0.5	0.1025	100	68.00	25	237160.	0.3	0.3	0.0622
46	169.00	12	17561.	0.3	0.3	0.0619	101	67.00	21	200048.	0.9	0.9	0.1685*
47	163.00	8	40278.	0.1	0.1	0.0141	102	66.00	10	19699.	0.1	0.1	0.0158*
48	161.00	10	17682.	0.2	0.2	0.0323	103	65.00	17	82836.	0.3	0.3	0.0664*
49	158.00	10	2339.	0.1	0.1	0.0142	104	64.00	21	620752.	2.4	2.4	0.4979
50	151.00	10	21092.	0.0	0.0	0.0019	105	63.00	17	83592.	0.3	0.3	0.0671*
51	150.00	12	1993.	0.1	0.1	0.0169	106	62.00	8	19386.	0.1	0.1	0.0156
52	145.00	6	1733.	0.0	0.0	0.0016	107	61.00	17	128128.	0.5	0.5	0.1028
53	137.00	6	1146.	0.0	0.0	0.0014	108	60.00	21	134636.	0.5	0.5	0.1080
54	135.00	6	1579.	0.0	0.0	0.0009	109	59.00	17	123476.	0.5	0.5	0.0990
55	134.00	8		0.0	0.0	0.0013	110	58.00	25	192880.	0.7	0.7	0.1547

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	57.00	35	3622592.	13.8	13.8	2.9058
112	56.00	35	1642752.	6.3	6.3	1.3177*
113	55.00	43	8168192.	31.2	31.2	6.5521*
114	54.00	21	262400.	1.0	1.0	0.2105
115	53.00	25	571792.	2.2	2.2	0.4587
116	52.00	21	93452.	0.4	0.4	0.0750
117	51.00	43	2892928.	11.1	11.1	2.3205*
118	50.00	21	133756.	0.5	0.5	0.1073*
119	49.00	12	30051.	0.1	0.1	0.0241*
120	48.00	17	106468.	0.4	0.4	0.0854
121	47.00	21	234312.	0.9	0.9	0.1880
122	46.00	10	10100.	0.0	0.0	0.0001
123	45.00	35	836448.	3.2	3.2	0.6710
124	44.00	35	1797888.	6.9	6.9	1.4422
125	43.00	71	26156032.	100.0	100.0	*20.98*
126	42.00	43	7032320.	26.9	26.9	5.6409*
127	41.00	43	9559296.	36.5	36.5	7.6679*
128	40.00	25	725920.	2.8	2.8	0.5823
129	39.00	43	3620928.	13.8	13.8	2.9045*
130	38.00	25	197192.	0.8	0.8	0.1582*
131	37.00	14	42051.	0.2	0.2	0.0337*
132	36.00	21	129244.	0.5	0.5	0.1037
133	35.00	10	15889.	0.1	0.1	0.0127*

AG4AV.1 [TIC=153694200, 100X=22801200] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	355.00	6	1041.	0.0	0.0	0.0057	56	163.00	8	16224.	0.1	0.1	0.0106
2	314.00	8	1262.	0.0	0.0	0.0008	57	161.00	10	48726.	0.2	0.2	0.0317
3	311.00	8	2431.	0.0	0.0	0.0016	58	1768.	6	1768.	0.0	0.0	0.0012
4	313.00	12	91404.	0.4	0.4	0.0595	59	150.00	10	36504.	0.2	0.2	0.0238
5	312.00	12	149564.	0.7	0.7	0.0973	60	145.00	8	18916.	0.1	0.1	0.0123
6	298.00	6	6151.	0.0	0.0	0.0040	61	143.00	6	1654.	0.0	0.0	0.0011
7	297.00	14	192004.	0.8	0.8	0.1249	62	137.00	17	160236.	0.7	0.7	0.1042
8	294.00	8	6691.	0.0	0.0	0.0044	63	136.00	10	55415.	0.2	0.2	0.0361*
9	293.00	12	91748.	0.4	0.4	0.0597	64	135.00	10	18911.	0.1	0.1	0.0123
10	284.00	10	66328.	0.3	0.3	0.0432	65	133.00	14	176100.	0.8	0.8	0.1146
11	283.00	17	863456.	3.8	3.8	0.5618*	66	131.00	17	186220.	0.8	0.8	0.1212
12	282.00	8	3936.	0.0	0.0	0.0026	67	123.00	10	3066.	0.0	0.0	0.0020
13	281.00	6	1622.	0.0	0.0	0.0011	68	122.00	8	5506.	0.0	0.0	0.0036
14	279.00	8	3640.	0.0	0.0	0.0324	69	120.00	8	9661.	0.0	0.0	0.0063
15	271.00	12	61855.	0.3	0.3	0.0402	70	119.00	21	1310336.	5.7	5.7	0.8526
16	270.00	21	668096.	2.9	2.9	0.4347*	71	114.00	17	232160.	1.0	1.0	0.1511*
17	269.00	35	6659072.	29.1	29.1	4.3327*	72	113.00	35	4394456.	19.2	19.2	2.8592*
18	268.00	12	19208.	0.1	0.1	0.0125*	73	112.00	17	163092.	0.7	0.7	0.1061
19	267.00	10	39753.	0.2	0.2	0.0259*	74	111.00	14	75320.	0.3	0.3	0.0490*
20	265.00	10	6834.	0.0	0.0	0.0044	75	109.00	17	153172.	0.7	0.7	0.0997*
21	259.00	6	1229.	0.0	0.0	0.0008	76	103.00	8	18462.	0.1	0.1	0.0120
22	258.00	14	137140.	0.6	0.6	0.0892*	77	101.00	8	9266.	0.0	0.0	0.0060
23	257.00	25	1630016.	7.1	7.1	0.0606*	78	100.00	21	455808.	2.0	2.0	0.2966
24	256.00	51	22881280.	100.0	100.0	*14.88*	79	99.00	10	8522.	0.0	0.0	0.0055
25	255.00	35	30797.	8.4	8.4	1.2531*	80	97.00	14	142056.	0.6	0.6	0.0924*
26	254.00	10	18870.	0.1	0.1	0.0200*	81	96.00	14	45118.	0.2	0.2	0.0294*
27	253.00	12	17425.	0.1	0.1	0.0123*	82	95.00	29	1476288.	6.5	6.5	0.9605*
28	251.00	10	35493.	0.1	0.1	0.0113	83	94.00	12	41092.	0.2	0.2	0.0267*
29	249.00	8	94080.	0.2	0.2	0.0231	84	93.00	12	27296.	0.1	0.1	0.0178
30	242.00	12	687680.	0.4	0.4	0.0612*	85	91.00	12	27426.	0.1	0.1	0.0178
31	241.00	17	5294.	3.0	3.0	0.4474	86	87.00	12	71908.	0.3	0.3	0.0466*
32	240.00	8	11101.	0.0	0.0	0.0034	87	86.00	21	455456.	2.0	2.0	0.2963
33	239.00	10	13665.	0.0	0.0	0.0072	88	85.00	35	8273920.	36.2	36.2	5.3834*
34	237.00	8	25810.	0.1	0.1	0.0089	89	84.00	21	629632.	2.8	2.8	0.4097
35	236.00	8	118688.	0.5	0.5	0.0168	90	83.00	29	1147136.	5.0	5.0	0.7464
36	235.00	14	1728.	0.0	0.0	0.0772*	91	82.00	14	95260.	0.4	0.4	0.0620
37	233.00	6	5550.	0.0	0.0	0.0011	92	81.00	17	144052.	0.6	0.6	0.0937*
38	231.00	6	27053.	0.1	0.1	0.0036	93	80.00	8	16825.	0.1	0.1	0.0109
39	229.00	10	111416.	0.5	0.5	0.0176	94	79.00	12	55943.	0.2	0.2	0.0364
40	228.00	12	2071808.	9.1	9.1	0.0725	95	78.00	8	6381.	0.0	0.0	0.0042
41	227.00	21	41495.	0.2	0.2	1.3480	96	77.00	14	75604.	0.3	0.3	0.0492*
42	223.00	10	5449.	0.0	0.0	0.0270	97	76.00	10	2803.	0.0	0.0	0.0018
43	217.00	17	5265.	0.0	0.0	0.0035	98	75.00	14	98284.	0.4	0.4	0.0639*
44	214.00	8	189364.	0.8	0.8	0.0034	99	74.00	10	46050.	0.2	0.2	0.0306*
45	213.00	14	255648.	1.1	1.1	0.1232	100	73.00	21	306832.	1.3	1.3	0.1996
46	210.00	6	2176.	0.0	0.0	0.0014	101	72.00	10	6133.	0.0	0.0	0.0040
47	209.00	17	14676.	0.1	0.1	0.0663	102	71.00	17	248240.	1.1	1.1	0.1615
48	207.00	10	61582.	0.3	0.3	0.0095	103	70.00	25	1299200.	5.7	5.7	0.8453*
49	193.00	12	68340.	0.3	0.3	0.0441*	104	69.00	43	7500800.	32.8	32.8	4.8602*
50	191.00	10	62472.	0.3	0.3	0.0445*	105	68.00	17	229880.	1.0	1.0	0.1496
51	183.00	12	45364.	0.2	0.2	0.0406	106	67.00	21	397775.	1.7	1.7	0.2588*
52	181.00	10	6635.	0.0	0.0	0.0295	107	66.00	8	17042.	0.1	0.1	0.0111
53	172.00	6	88992.	0.4	0.4	0.0043	108	65.00	17	128036.	0.6	0.6	0.0833
54	169.00	12	4632.	0.0	0.0	0.0579*	109	64.00	25	690400.	3.0	3.0	0.4492*
55	164.00	8		0.0	0.0	0.0030	110	63.00	17	54164.	0.2	0.2	0.0352

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	62.00	6	2956.	0.0	0.0	0.0019
112	61.00	12	86168.	0.4	0.4	0.0561*
113	60.00	8	2514.	0.0	0.0	0.0016
114	59.00	21	262416.	1.1	1.1	0.1707*
115	58.00	25	806384.	3.5	3.5	0.5247*
116	57.00	43	14470656.	63.2	63.2	9.4152*
117	56.00	35	5939456.	26.0	26.0	3.8645*
118	55.00	35	8827904.	38.6	38.6	5.7438*
119	54.00	21	324528.	1.4	1.4	0.2112*
120	53.00	25	1001568.	4.4	4.4	0.6517
121	52.00	17	116176.	0.5	0.5	0.0756*
122	51.00	29	3209024.	14.0	14.0	2.0879
123	50.00	17	146052.	0.6	0.6	0.0950*
124	49.00	10	31215.	0.1	0.1	0.0203
125	47.00	21	269696.	1.2	1.2	0.1755*
126	45.00	35	969008.	4.2	4.2	0.6305
127	44.00	35	812464.	3.6	3.6	0.5286*
128	43.00	51	21382144.	93.4	93.4	*13.91*
129	42.00	35	3479296.	15.2	15.2	2.2638*
130	41.00	35	14582016.	63.7	63.7	9.4877*
131	40.00	29	927472.	4.1	4.1	0.6035*
132	39.00	35	4744960.	20.7	20.7	3.0873*
133	38.00	21	195852.	0.9	0.9	0.1274*
134	37.00	12	44652.	0.2	0.2	0.0291*
135	36.00	14	94756.	0.4	0.4	0.0617*
136	35.00	8	5345.	0.0	0.0	0.0035

EV29K.1 [TIC-91664384, 180X-18257920] EI

5-methylhexanoic acid,

2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	381.00	6	1363.	0.0	0.0	0.0015	56	169.00	17	70712.	0.4	0.4	0.0771*
2	315.00	6	987.	0.0	0.0	0.0010	57	164.00	8	3661.	0.0	0.0	0.0040
3	313.00	12	42817.	0.2	0.2	0.0467*	58	163.00	8	5778.	0.0	0.0	0.0063
4	312.00	8	15353.	0.1	0.1	0.0167	59	161.00	12	27575.	0.2	0.2	0.0301
5	311.00	8	7291.	0.0	0.0	0.0080	60	158.00	6	2458.	0.0	0.0	0.0027
6	298.00	10	7053.	0.0	0.0	0.0077*	61	150.00	10	19370.	0.1	0.1	0.0211
7	297.00	17	114520.	0.6	0.6	0.1249	62	149.00	8	4517.	0.0	0.0	0.0049
8	295.00	10	16608.	0.1	0.1	0.0181	63	145.00	8	2051.	0.0	0.0	0.0022
9	294.00	17	176408.	1.0	1.0	0.1924	64	133.00	21	81364.	0.4	0.4	0.0888*
10	293.00	8	1874.	0.0	0.0	0.0020	65	131.00	17	94124.	0.5	0.5	0.1027*
11	284.00	8	3834.	0.0	0.0	0.0042	66	124.00	8	2412.	0.0	0.0	0.0026
12	281.00	10	8367.	0.0	0.0	0.0091	67	122.00	14	60162.	0.3	0.3	0.0656*
13	280.00	8	3128.	0.0	0.0	0.0034	68	120.00	10	24094.	0.1	0.1	0.0263
14	279.00	17	77744.	0.4	0.4	0.0848	69	120.00	8	6919.	0.0	0.0	0.0075
15	272.00	12	13908.	0.1	0.1	0.0152*	70	119.00	29	640352.	3.5	3.5	0.6986
16	271.00	21	230572.	1.3	1.3	0.2515	71	115.00	8	2862.	0.0	0.0	0.0032
17	270.00	25	274800.	1.5	1.5	0.2998*	72	114.00	25	142984.	0.8	0.8	0.1560*
18	269.00	35	2650240.	0.1	0.1	0.0062	73	113.00	43	2311488.	12.7	12.7	2.5217*
19	268.00	12	21436.	0.0	0.0	0.0034*	74	112.00	25	275568.	1.5	1.5	0.3006*
20	267.00	12	5715.	0.0	0.0	0.0062	75	111.00	25	189436.	1.0	1.0	0.2067*
21	266.00	6	490.	0.0	0.0	0.0005	76	109.00	17	58526.	0.3	0.3	0.0638*
22	265.00	6	849.	0.0	0.0	0.0009	77	108.00	10	6596.	0.0	0.0	0.0072
23	263.00	6	982.	0.0	0.0	0.0011	78	103.00	8	925.	0.0	0.0	0.0010
24	257.00	10	18987.	0.1	0.1	0.0207	79	101.00	10	7619.	0.0	0.0	0.0083
25	256.00	25	200012.	1.1	1.1	0.2269*	80	99.00	21	225076.	1.2	1.2	0.2455
26	255.00	35	1859328.	10.2	10.2	2.0284*	81	98.00	6	2764.	0.0	0.0	0.0030
27	254.00	10	10978.	0.1	0.1	0.0120*	82	98.00	21	100388.	0.5	0.5	0.1095
28	253.00	17	50156.	0.3	0.3	0.0547*	83	97.00	35	1603456.	8.8	8.8	1.7493
29	251.00	10	7275.	0.0	0.0	0.0079*	84	96.00	25	294864.	1.6	1.6	0.3217
30	244.00	12	37156.	0.2	0.2	0.0405*	85	95.00	43	4372736.	23.9	23.9	4.7704*
31	243.00	29	436304.	2.4	2.4	0.4760*	86	94.00	35	722928.	4.0	4.0	0.7887*
32	242.00	43	5896192.	32.3	32.3	6.4324*	87	93.00	12	34733.	0.2	0.2	0.0379*
33	241.00	17	64082.	0.4	0.4	0.0699*	88	91.00	10	7100.	0.0	0.0	0.0077*
34	240.00	10	21589.	0.1	0.1	0.0236*	89	89.00	8	8070.	0.0	0.0	0.0088
35	239.00	8	7735.	0.0	0.0	0.0004	90	87.00	6	5577.	0.0	0.0	0.0051
36	237.00	6	1868.	0.0	0.0	0.0020	91	86.00	10	3738.	0.0	0.0	0.0041
37	235.00	14	18311.	0.1	0.1	0.0200	92	85.00	29	212232.	1.2	1.2	0.2315*
38	229.00	6	2502.	0.0	0.0	0.0027	93	84.00	25	218984.	1.2	1.2	0.2388*
39	228.00	17	65481.	0.4	0.4	0.0714*	94	83.00	35	470720.	2.6	2.6	0.5135
40	227.00	35	1164672.	6.4	6.4	1.2706*	95	82.00	17	80892.	0.4	0.4	0.0882*
41	226.00	10	12598.	0.1	0.1	0.0137	96	81.00	21	115580.	0.6	0.6	0.1261*
42	222.00	8	10835.	0.1	0.1	0.0118	97	80.00	35	121552.	0.7	0.7	0.1326*
43	219.00	12	27933.	0.2	0.2	0.0305	98	79.00	25	142228.	0.8	0.8	0.1552*
44	217.00	8	1675.	0.0	0.0	0.0018	99	78.00	10	10905.	0.1	0.1	0.0119*
45	214.00	6	1641.	0.0	0.0	0.0018	100	77.00	17	58798.	0.3	0.3	0.0541*
46	213.00	17	99116.	0.5	0.5	0.1081	101	76.00	8	1841.	0.0	0.0	0.0020
47	209.00	14	56766.	0.3	0.3	0.0619*	102	75.00	17	73096.	0.4	0.4	0.0797*
48	207.00	8	2032.	0.0	0.0	0.0022	103	74.00	14	13768.	0.1	0.1	0.0150*
49	199.00	6	1470.	0.0	0.0	0.0016	104	73.00	21	86372.	0.5	0.5	0.0942*
50	193.00	10	2236.	0.0	0.0	0.0024	105	72.00	25	182004.	1.0	1.0	0.1986
51	192.00	8	2971.	0.0	0.0	0.0032	106	71.00	35	405388.	22.2	22.2	4.4225
52	191.00	8	6208.	0.0	0.0	0.0068*	107	70.00	35	976720.	5.3	5.3	1.0655
53	183.00	12	4487.	0.0	0.0	0.0049	108	69.00	35	11071488.	60.6	60.6	12.07*
54	181.00	8	23391.	0.1	0.1	0.0255	109	68.00	35	476352.	2.6	2.6	0.5197*
55	179.00	8	3004.	0.0	0.0	0.0033	110	67.00	29	368064.	2.0	2.0	0.4015

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	66.00	12	35558.	0.2	0.2	0.0388*
112	65.00	21	86592.	0.5	0.5	0.0945*
113	64.00	25	337104.	1.8	1.8	0.3678
114	63.00	14	35792.	0.2	0.2	0.0390*
115	62.00	8	2696.	0.0	0.0	0.0029
116	61.00	21	90312.	0.5	0.5	0.0985*
117	60.00	17	69844.	0.4	0.4	0.0762*
118	59.00	17	53651.	0.3	0.3	0.0585*
119	58.00	17	75572.	0.4	0.4	0.0824*
120	57.00	35	1360320.	7.5	7.5	1.4840
121	56.00	35	1002432.	5.5	5.5	1.0936*
122	55.00	43	4212992.	23.1	23.1	4.5961*
123	54.00	25	164564.	0.9	0.9	0.1795*
124	53.00	35	505456.	2.8	2.8	0.5514*
125	52.00	21	58137.	0.3	0.3	0.0634*
126	51.00	35	1540352.	8.4	8.4	1.6804*
127	50.00	21	75896.	0.4	0.4	0.0828*
128	49.00	25	75104.	0.4	0.4	0.0819*
129	48.00	25	253992.	1.4	1.4	0.2771*
130	47.00	25	132928.	0.7	0.7	0.1450*
131	46.00	8	8925.	0.0	0.0	0.0097
132	45.00	35	406208.	2.2	2.2	0.4431
133	44.00	43	937440.	5.1	5.1	1.0227*
134	43.00	71	18257920.	100.0	100.0	*19.91*
135	42.00	51	4828416.	26.4	26.4	5.2675*
136	41.00	59	9267200.	50.8	50.8	*10.10*
137	40.00	35	610320.	3.3	3.3	0.6658*
138	39.00	59	2872704.	15.7	15.7	3.1339*
139	38.00	35	159440.	0.9	0.9	0.1739*
140	37.00	14	29712.	0.2	0.2	0.0324*
141	36.00	21	127256.	0.7	0.7	0.1388*
142	35.00	14	30010.	0.2	0.2	0.0327*

AL-PA-1 [TIC=122269696, 100X-24558592] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	ABSOLUTE INTENSITY	NO. POINTS	MEASURED MASS	PEAK NO.	% INT. BASE	% INT. NREF	% TOT. ION
1	314.00	10	6528.	0.0	0.0	0.0053	17807.	10	181.00	56	0.1	0.1	0.0146
2	313.00	14	142216.	0.6	0.6	0.1163	5586.	8	179.00	57	0.0	0.0	0.0046
3	312.00	17	466992.	1.9	1.9	0.3819	60500.	12	169.00	58	0.2	0.2	0.0495
4	297.00	10	34454.	0.1	0.1	0.0282	5046.	8	163.00	59	0.0	0.0	0.0041
5	294.00	6	9291.	0.0	0.0	0.0076	49260.	12	161.00	60	0.2	0.2	0.0403
6	293.00	14	120256.	0.5	0.5	0.0984*	18044.	10	158.00	61	0.1	0.1	0.0148*
7	285.00	8	1632.	0.0	0.0	0.0013	18535.	10	150.00	62	0.1	0.1	0.0152
8	284.00	14	100704.	0.4	0.4	0.0824	1944.	8	145.00	63	0.0	0.0	0.0016
9	283.00	17	894080.	3.6	3.6	0.7312	48695.	10	135.00	64	0.2	0.2	0.0398
10	282.00	6	1554.	0.0	0.0	0.0013	150232.	17	133.00	65	0.6	0.6	0.1229
11	281.00	8	4445.	0.0	0.0	0.0036	115608.	14	131.00	66	0.5	0.5	0.0946
12	271.00	10	28890.	0.1	0.1	0.0236	155216.	17	123.00	67	0.6	0.6	0.1269
13	270.00	17	255812.	1.0	1.0	0.2092*	5078.	10	122.00	68	0.0	0.0	0.0074
14	269.00	35	3237888.	13.2	13.2	2.6482	7354.	8	120.00	69	0.0	0.0	0.0060
15	268.00	14	7587.	0.0	0.0	0.0062*	1012992.	21	119.00	70	4.1	4.1	0.8285
16	265.00	12	10092.	0.0	0.0	0.0083	25423.	12	115.00	71	0.1	0.1	0.0208*
17	258.00	6	1762.	0.0	0.0	0.0014	465168.	25	114.00	72	1.9	1.9	0.3804*
18	257.00	12	65544.	0.3	0.3	0.0536	7274496.	43	113.00	73	29.6	29.6	5.9495*
19	256.00	25	666704.	2.7	2.7	0.5453*	79096.	14	112.00	74	0.3	0.3	0.0653
20	255.00	43	7189504.	29.3	29.3	5.8800*	150936.	21	111.00	75	0.6	0.6	0.1234
21	254.00	14	29562.	0.1	0.1	0.0242*	69500.	17	109.00	76	0.3	0.3	0.0568
22	253.00	10	14722.	0.1	0.1	0.0120*	2550.	8	108.00	77	0.0	0.0	0.0021
23	252.00	16	3446.	0.0	0.0	0.0028	1682.	8	107.00	78	0.0	0.0	0.0014
24	251.00	10	24473.	0.1	0.1	0.0200	872.	6	103.00	79	0.0	0.0	0.0007
25	249.00	6	3663.	0.0	0.0	0.0030	16595.	10	101.00	80	0.1	0.1	0.0136
26	245.00	6	3862.	0.0	0.0	0.0032	278336.	17	100.00	81	1.1	1.1	0.2276
27	244.00	17	103860.	0.4	0.4	0.0849*	4795.	8	99.00	82	0.0	0.0	0.0039
28	243.00	35	1409472.	5.7	5.7	1.1528*	3369.	6	98.00	83	0.0	0.0	0.0028
29	242.00	51	11783424.	48.0	48.0	9.6372*	172884.	17	97.00	84	0.7	0.7	0.1414
30	241.00	25	523792.	2.1	2.1	0.4284*	37220.	14	96.00	85	0.2	0.2	0.0304*
31	240.00	10	52150.	0.2	0.2	0.0427	1219712.	35	95.00	86	5.0	5.0	0.9976
32	239.00	12	40506.	0.2	0.2	0.0331	119900.	17	94.00	87	0.5	0.5	0.0981*
33	237.00	8	12901.	0.1	0.1	0.0106	12454.	12	93.00	88	0.1	0.1	0.0102
34	236.00	6	2746.	0.0	0.0	0.0022	16442.	8	91.00	89	0.1	0.1	0.0134
35	235.00	14	137712.	0.6	0.6	0.1126	4464.	8	89.00	90	0.0	0.0	0.0037
36	233.00	8	1400.	0.0	0.0	0.0011	3176.	8	87.00	91	0.0	0.0	0.0026
37	232.00	10	16593.	0.1	0.1	0.0136*	89756.	17	86.00	92	0.4	0.4	0.0734
38	231.00	8	2538.	0.0	0.0	0.0021	1630720.	29	85.00	93	6.6	6.6	1.3337*
39	228.00	12	88640.	0.4	0.4	0.0725	2001600.	25	84.00	94	8.2	8.2	1.6370*
40	227.00	25	1450432.	5.9	5.9	1.1863*	1297536.	35	83.00	95	5.3	5.3	1.0612*
41	226.00	8	6356.	0.0	0.0	0.0052	74776.	17	82.00	96	0.3	0.3	0.0612*
42	223.00	8	13902.	0.1	0.1	0.0114	123644.	21	81.00	97	0.5	0.5	0.1011
43	222.00	8	4316.	0.0	0.0	0.0035	62881.	17	80.00	98	0.3	0.3	0.0514
44	221.00	8	2361.	0.0	0.0	0.0019	58955.	14	79.00	99	0.2	0.2	0.0482
45	219.00	8	9859.	0.0	0.0	0.0081	2696.	10	78.00	100	0.0	0.0	0.0022
46	217.00	8	6796.	0.0	0.0	0.0056	67888.	17	77.00	101	0.3	0.3	0.0549
47	216.00	6	1601.	0.0	0.0	0.0013	5223.	8	76.00	102	0.0	0.0	0.0043
48	213.00	14	159660.	0.7	0.7	0.1306	76032.	17	75.00	103	0.3	0.3	0.0622
49	209.00	10	86944.	0.4	0.4	0.0711	3679.	8	74.00	104	0.0	0.0	0.0030
50	207.00	10	6590.	0.0	0.0	0.0054	179236.	17	73.00	105	0.7	0.7	0.1466
51	199.00	8	1849.	0.0	0.0	0.0015	117316.	17	72.00	106	0.5	0.5	0.0959
52	194.00	8	4445.	0.0	0.0	0.0036	2407744.	25	71.00	107	9.8	9.8	1.9692
53	193.00	14	87272.	0.4	0.4	0.0714	1514176.	29	70.00	108	6.2	6.2	1.2384
54	191.00	6	1528.	0.0	0.0	0.0012	5853440.	43	69.00	109	23.8	23.8	4.7873*
55	183.00	12	40165.	0.2	0.2	0.0328	968176.	25	68.00	110	3.9	3.9	0.7918

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	67.00	21	366720.	1.5	1.5	0.2999*
112	66.00	12	30870.	0.1	0.1	0.0252
113	65.00	17	86404.	0.4	0.4	0.0707*
114	64.00	29	463328.	1.9	1.9	0.3789*
115	63.00	14	38430.	0.2	0.2	0.0314*
116	61.00	17	127928.	0.5	0.5	0.1046
117	60.00	17	87176.	0.4	0.4	0.0713*
118	59.00	21	109772.	0.4	0.4	0.0898
119	58.00	21	137512.	0.6	0.6	0.1125*
120	57.00	35	2646848.	10.8	10.8	2.1648
121	56.00	35	2041728.	8.3	8.3	1.6699
122	55.00	43	10193664.	41.5	41.5	8.3370*
123	54.00	21	374240.	1.5	1.5	0.3061
124	53.00	21	575648.	2.3	2.3	0.4708
125	52.00	14	79924.	0.3	0.3	0.0654
126	51.00	29	2327048.	9.5	9.5	1.9032
127	50.00	17	97148.	0.4	0.4	0.0795
128	49.00	8	9351.	0.0	0.0	0.0076
129	48.00	14	68292.	0.3	0.3	0.0559*
130	47.00	21	143116.	0.6	0.6	0.1170
131	46.00	10	7089.	0.0	0.0	0.0058
132	45.00	29	612336.	2.5	2.5	0.5000*
133	44.00	35	1532608.	6.2	6.2	1.2535
134	43.00	71	24558592.	100.0	100.0	*20.00*
135	42.00	35	3961920.	16.1	16.1	3.2403
136	41.00	35	10149632.	41.3	41.3	8.3010*
137	40.00	25	578432.	2.4	2.4	0.4731
138	39.00	35	3017792.	12.3	12.3	2.4681*
139	38.00	25	140400.	0.6	0.6	0.1148*
140	37.00	14	24823.	0.1	0.1	0.0203*
141	36.00	21	118036.	0.5	0.5	0.0965*
142	35.00	8	6498.	0.0	0.0	0.0053

AL6PA.1 [TIC-148918592, 188X-23447552] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	328.00	8	11946.	0.1	0.1	0.0085	56	217.00	17	11492.	0.0	0.0	0.0082*
2	327.00	17	214548.	0.9	0.9	0.1523*	57	216.00	8	3184.	0.0	0.0	0.0023
3	326.00	21	978064.	4.2	4.2	0.6941*	58	213.00	17	175728.	0.7	0.7	0.1247
4	325.00	8	1676.	0.0	0.0	0.0012	59	209.00	12	88824.	0.4	0.4	0.0630
5	312.00	8	6879.	0.0	0.0	0.0019	60	207.00	17	93508.	0.4	0.4	0.0664
6	311.00	12	87260.	0.4	0.4	0.0619	61	183.00	10	24229.	0.1	0.1	0.0172
7	308.00	8	15496.	0.1	0.1	0.0110	62	181.00	10	25196.	0.1	0.1	0.0179
8	307.00	17	111836.	0.5	0.5	0.08794	63	169.00	12	65948.	0.3	0.3	0.0468
9	299.00	6	1468.	0.0	0.0	0.0010	64	164.00	6	1685.	0.0	0.0	0.0012
10	298.00	12	115832.	0.5	0.5	0.0822	65	163.00	3	15620.	0.1	0.1	0.0111
11	297.00	21	1053376.	4.5	4.5	0.7475*	66	161.00	10	36564.	0.2	0.2	0.0259
12	296.00	6	1062.	0.0	0.0	0.0008	67	158.00	10	4915.	0.0	0.0	0.0035
13	285.00	8	28693.	0.1	0.1	0.0204	68	150.00	10	28310.	0.1	0.1	0.0201
14	284.00	17	268816.	1.1	1.1	0.1908	69	145.00	8	3567.	0.0	0.0	0.0025
15	283.00	29	2817984.	12.0	12.0	1.9998*	70	135.00	12	62150.	0.3	0.3	0.0441*
16	282.00	12	5568.	0.0	0.0	0.0040	71	134.00	6	2135.	0.0	0.0	0.0015
17	281.00	8	13994.	0.1	0.1	0.0099	72	133.00	17	139428.	0.6	0.6	0.0989
18	279.00	10	3201.	0.0	0.0	0.0023	73	131.00	17	113596.	0.5	0.5	0.0806
19	271.00	6	6572.	0.0	0.0	0.00347	74	129.00	10	4444.	0.0	0.0	0.0032
20	270.00	14	135124.	0.6	0.6	0.0959	75	128.00	17	450368.	1.9	1.9	0.3196*
21	269.00	21	1357760.	5.8	5.8	0.9636	76	127.00	32	550816.	23.6	23.6	3.9307*
22	268.00	10	28338.	0.1	0.1	0.0201	77	126.00	10	26022.	0.1	0.1	0.0185
23	266.00	8	1565.	0.0	0.0	0.0011	78	125.00	17	84500.	0.4	0.4	0.0500
24	265.00	10	37075.	0.2	0.2	0.0263	79	124.00	8	5948.	0.0	0.0	0.0042
25	258.00	6	827.	0.0	0.0	0.0006	80	123.00	17	160808.	0.7	0.7	0.1141
26	257.00	14	67708.	0.3	0.3	0.0481*	81	122.00	8	10305.	0.0	0.0	0.0073
27	256.00	25	813232.	3.5	3.5	0.5771*	82	121.00	5	1941.	0.0	0.0	0.0014
28	255.00	43	9554176.	40.7	40.7	6.7803*	83	120.00	8	2576.	0.0	0.0	0.0018
29	254.00	14	34655.	0.1	0.1	0.0246*	84	119.00	21	892224.	3.8	3.8	0.6332
30	253.00	12	48676.	0.2	0.2	0.0345	85	115.00	6	1985.	0.0	0.0	0.0014
31	252.00	8	2464.	0.0	0.0	0.0017	86	114.00	10	16452.	0.1	0.1	0.0117
32	251.00	10	17317.	0.1	0.1	0.0123	87	113.00	21	1109504.	4.7	4.7	0.7874
33	249.00	8	2404.	0.0	0.0	0.0017	88	111.00	21	134648.	0.6	0.6	0.0956
34	248.00	8	1783.	0.0	0.0	0.0013	89	110.00	8	33770.	0.1	0.1	0.0240
35	246.00	12	17127.	0.1	0.1	0.0122*	90	109.00	25	524544.	2.2	2.2	0.3723
36	245.00	10	12126.	0.1	0.1	0.0086*	91	108.00	17	108208.	0.5	0.5	0.0768*
37	244.00	17	114008.	0.5	0.5	0.0609*	92	107.00	8	15049.	0.1	0.1	0.0107
38	243.00	35	1679296.	7.2	7.2	1.1917*	93	101.00	8	8817.	0.0	0.0	0.0063
39	242.00	51	12221440.	52.1	52.1	8.6732*	94	100.00	17	252228.	1.1	1.1	0.1790
40	241.00	25	463936.	2.0	2.0	0.3292*	95	99.00	17	69308.	0.3	0.3	0.0492
41	240.00	14	57734.	0.2	0.2	0.0410*	96	98.00	21	797280.	3.4	3.4	0.5658
42	239.00	12	49435.	0.2	0.2	0.0351	97	97.00	25	596304.	2.5	2.5	0.4232
43	237.00	8	6275.	0.0	0.0	0.0045	98	96.00	12	32975.	0.1	0.1	0.0234
44	236.00	8	6738.	0.0	0.0	0.0048	99	95.00	21	688460.	2.9	2.9	0.4885
45	235.00	17	158768.	0.7	0.7	0.1127	100	94.00	8	3648.	0.0	0.0	0.0326
46	231.00	8	3928.	0.0	0.0	0.0028	101	93.00	14	54355.	0.2	0.2	0.0386*
47	229.00	8	4227.	0.0	0.0	0.0020	102	91.00	10	11215.	0.0	0.0	0.0080
48	228.00	12	79796.	0.3	0.3	0.0566	103	89.00	8	2253.	0.0	0.0	0.0016
49	227.00	21	1227456.	5.2	5.2	0.8711	104	87.00	12	13251.	0.1	0.1	0.0094
50	226.00	8	11192.	0.0	0.0	0.0079	105	86.00	17	195232.	9.8	9.8	0.1386
51	223.00	10	4960.	0.0	0.0	0.0035	106	85.00	35	3805632.	16.2	16.2	2.7007*
52	222.00	10	13307.	0.1	0.1	0.0094*	107	84.00	35	2795840.	11.9	11.9	1.9841
53	221.00	6	1784.	0.0	0.0	0.0013	108	83.00	35	2044096.	8.7	8.7	1.4506
54	219.00	10	8925.	0.0	0.0	0.0063	109	82.00	25	1063232.	4.5	4.5	0.7545
55	218.00	6	1521.	0.0	0.0	0.0011	110	81.00	21	268336.	1.1	1.1	0.1904

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	80.00	21	181184.	0.8	0.8	0.1286*
112	79.00	17	155864.	0.7	0.7	0.1106
113	78.00	12	21062.	0.1	0.1	0.0149
114	77.00	17	91200.	0.4	0.4	0.0647
115	75.00	12	52197.	0.2	0.2	0.0370
116	74.00	8	13098.	0.1	0.1	0.0093
117	73.00	17	183460.	0.8	0.8	0.1302
118	72.00	6	8259.	0.0	0.0	0.0059
119	71.00	21	285856.	1.2	1.2	0.2029
120	70.00	25	731552.	3.1	3.1	0.5192
121	69.00	43	6826436.	29.1	29.1	4.8446*
122	68.00	21	361744.	1.5	1.5	0.2567
123	67.00	25	989712.	4.2	4.2	0.7024
124	66.00	10	29638.	0.1	0.1	0.0210
125	65.00	17	106244.	0.5	0.5	0.0754*
126	64.00	21	384272.	1.6	1.6	0.2727
127	63.00	10	28668.	0.1	0.1	0.0203*
128	62.00	8	11873.	0.1	0.1	0.0084
129	61.00	17	132788.	0.6	0.6	0.0942
130	60.00	17	86956.	0.4	0.4	0.0617
131	59.00	21	166024.	0.7	0.7	0.1178
132	58.00	25	368016.	1.6	1.6	0.2617
133	57.00	43	8862208.	37.8	37.8	6.2892*
134	56.00	35	1973824.	8.4	8.4	1.4008
135	55.00	51	12568064.	53.6	53.6	8.9192*
136	54.00	21	532128.	2.3	2.3	0.3776
137	53.00	25	697328.	3.0	3.0	0.4949
138	52.00	17	79700.	0.3	0.3	0.0566
139	51.00	29	2315392.	9.9	9.9	1.6432
140	50.00	17	84816.	0.4	0.4	0.0602
141	49.00	10	15946.	0.1	0.1	0.0113*
142	48.00	12	34275.	0.1	0.1	0.0243*
143	47.00	21	161744.	0.7	0.7	0.1148
144	46.00	29	12488.	0.1	0.1	0.0089*
145	45.00	20	516640.	2.2	2.2	0.3666
146	44.00	35	1441984.	6.1	6.1	1.0233
147	43.00	59	23447552.	100.0	100.0	*16.64*
148	42.00	35	4633088.	19.8	19.8	3.2880*
149	41.00	43	11422464.	48.7	48.7	8.1062*
150	40.00	29	702784.	3.0	3.0	0.4987*
151	39.00	35	3186816.	13.6	13.6	2.2616*
152	38.00	21	122844.	0.5	0.5	0.0872*
153	37.00	17	25316.	0.1	0.1	0.0102*
154	36.00	21	140828.	0.6	0.6	0.0909*
155	35.00	10	3511.	0.0	0.0	0.0025

AL7PA.1 [TIC=139883776, 189X-22312968] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	342.00	8	24187.	0.1	0.1	0.0174	56	221.00	14	82564.	0.4	0.4	0.0594*
2	341.00	17	253600.	1.1	1.1	0.1823*	57	219.00	10	7079.	0.0	0.0	0.0051
3	340.00	21	121172.	5.4	5.4	0.8712*	58	218.00	6	1475.	0.0	0.0	0.0011
4	339.00	14	3510.	0.0	0.0	0.0025	59	217.00	14	12566.	0.1	0.1	0.0090*
5	325.00	8	7134.	0.0	0.0	0.0051	60	216.00	6	2401.	0.0	0.0	0.0017
6	322.00	8	13225.	0.1	0.1	0.0095	61	214.00	10	2147.	0.0	0.0	0.0015
7	321.00	12	108588.	0.5	0.5	0.0781	62	213.00	17	132764.	0.6	0.6	0.0955
8	314.00	6	1940.	0.0	0.0	0.0014	63	209.00	12	74648.	0.3	0.3	0.0537
9	313.00	8	4637.	0.0	0.0	0.0033	64	207.00	8	3706.	0.0	0.0	0.0027
10	312.00	17	226068.	1.0	1.0	0.1625	65	191.00	6	785.	0.0	0.0	0.0006
11	311.00	29	1933056.	8.7	8.7	1.3899	66	183.00	10	36604.	0.2	0.2	0.0263
12	299.00	10	30220.	0.1	0.1	0.0217	67	181.00	8	12139.	0.1	0.1	0.0087
13	298.00	17	250888.	1.1	1.1	0.1804*	68	169.00	12	45222.	0.2	0.2	0.0325
14	297.00	29	2294720.	10.3	10.3	1.5499*	69	163.00	8	2246.	0.0	0.0	0.0016
15	296.00	10	3200.	0.0	0.0	0.0023	70	161.00	12	25381.	0.1	0.1	0.0182
16	294.00	6	1073.	0.0	0.0	0.0008	71	158.00	8	9662.	0.0	0.0	0.0069
17	285.00	10	19995.	0.1	0.1	0.0144*	72	151.00	6	1366.	0.0	0.0	0.0010
18	284.00	14	74936.	0.3	0.3	0.0539	73	150.00	8	19473.	0.1	0.1	0.0140
19	283.00	17	441328.	2.0	2.0	0.3173	74	149.00	8	1141.	0.0	0.0	0.0008
20	281.00	8	18547.	0.1	0.1	0.0133	75	143.00	8	19226.	0.1	0.1	0.0138
21	280.00	8	1599.	0.0	0.0	0.0011	76	142.00	21	379568.	1.7	1.7	0.2729*
22	279.00	10	11650.	0.1	0.1	0.0084	77	141.00	35	4489216.	20.1	20.1	3.2277*
23	271.00	8	7786.	0.0	0.0	0.0056	78	140.00	8	19791.	0.1	0.1	0.0142
24	270.00	14	106208.	0.5	0.5	0.0764	79	139.00	14	74360.	0.3	0.3	0.0535
25	269.00	21	1062464.	4.8	4.8	0.7639	80	135.00	12	51681.	0.2	0.2	0.0372
26	268.00	10	29037.	0.1	0.1	0.0209*	81	133.00	17	116852.	0.5	0.5	0.0840
27	267.00	8	6004.	0.0	0.0	0.0043	82	131.00	14	99628.	0.4	0.4	0.0716
28	266.00	10	6452.	0.0	0.0	0.0046	83	125.00	10	37212.	0.2	0.2	0.0268
29	265.00	10	34415.	0.2	0.2	0.0247	84	124.00	8	6843.	0.0	0.0	0.0049
30	261.00	8	1633.	0.0	0.0	0.0012	85	123.00	25	326176.	1.5	1.5	0.2345*
31	260.00	12	6379.	0.0	0.0	0.0046*	86	122.00	17	118084.	0.5	0.5	0.0849
32	259.00	10	5111.	0.0	0.0	0.0037*	87	121.00	10	20937.	0.1	0.1	0.0151*
33	257.00	12	65904.	0.3	0.3	0.0474	88	119.00	21	725568.	3.3	3.3	0.5217
34	256.00	29	828928.	3.7	3.7	0.5960*	89	114.00	10	24508.	0.1	0.1	0.0176
35	255.00	43	9246720.	41.4	41.4	6.6483*	90	113.00	25	940272.	4.2	4.2	0.6760
36	254.00	14	52964.	0.2	0.2	0.0381*	91	112.00	21	257876.	1.2	1.2	0.1854
37	253.00	12	51023.	0.2	0.2	0.0367	92	111.00	21	226332.	1.0	1.0	0.1627*
38	252.00	10	12309.	0.1	0.1	0.0089*	93	110.00	6	2789.	0.0	0.0	0.0020
39	251.00	10	4399.	0.0	0.0	0.0032	94	109.00	14	59775.	0.3	0.3	0.0430
40	245.00	6	1893.	0.0	0.0	0.0014	95	108.00	8	9682.	0.0	0.0	0.0070
41	244.00	21	127628.	0.6	0.6	0.0918*	96	107.00	8	16637.	0.1	0.1	0.0120*
42	243.00	29	1587776.	7.1	7.1	1.1416*	97	101.00	10	5985.	0.0	0.0	0.0043*
43	242.00	51	10437632.	46.8	46.8	7.5046*	98	100.00	21	220788.	1.0	1.0	0.1587*
44	241.00	21	33319.	1.7	1.7	0.2667*	99	99.00	21	592992.	2.7	2.7	0.4264*
45	240.00	10	37312.	0.1	0.1	0.0240	100	98.00	25	1680064.	7.5	7.5	1.2080
46	239.00	12	42885.	0.2	0.2	0.0308	101	97.00	25	1035808.	4.6	4.6	0.7447
47	237.00	8	5578.	0.0	0.0	0.0040	102	96.00	25	1156672.	5.2	5.2	0.8316
48	236.00	8	9858.	0.0	0.0	0.0071	103	95.00	25	681488.	3.1	3.1	0.4900
49	235.00	14	142572.	0.6	0.6	0.1025	104	94.00	17	106468.	0.5	0.5	0.0765*
50	232.00	8	2337.	0.0	0.0	0.0017	105	93.00	17	77700.	0.3	0.3	0.0559*
51	228.00	10	54518.	0.2	0.2	0.0392	106	91.00	17	32629.	0.1	0.1	0.0235*
52	227.00	21	967296.	4.3	4.3	0.6955	107	86.00	8	1859.	0.0	0.0	0.0013
53	226.00	8	9484.	0.0	0.0	0.0068	108	85.00	25	171736.	0.8	0.8	0.1235
54	223.00	8	9763.	0.0	0.0	0.0070	109	84.00	25	1282816.	5.7	5.7	0.9223
55	222.00	8	1639.	0.0	0.0	0.0012	110	83.00	35	1946880.	8.7	8.7	1.3990

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	82.00	21	176888.	0.8	0.8	0.1272
112	81.00	25	982160.	4.4	4.4	0.7062
113	80.00	17	96696.	0.4	0.4	0.0695
114	79.00	17	147716.	0.7	0.7	0.1062
115	78.00	10	14356.	0.1	0.1	0.0103
116	77.00	17	91432.	0.4	0.4	0.0657
117	75.00	12	61985.	0.3	0.3	0.0446*
118	74.00	8	1810.	0.0	0.0	0.0013
119	73.00	21	184764.	0.8	0.8	0.1328*
120	72.00	17	128508.	0.6	0.6	0.0924
121	71.00	25	2285312.	10.2	10.2	1.6431*
122	70.00	25	1003136.	4.5	4.5	0.7212
123	69.00	43	7126784.	31.9	31.9	5.1241*
124	68.00	21	887696.	4.0	4.0	0.6382
125	67.00	21	916000.	4.1	4.1	0.6587
126	66.00	14	39792.	0.2	0.2	0.0286
127	65.00	17	106132.	0.5	0.5	0.0763
128	64.00	17	276784.	1.2	1.2	0.1990
129	63.00	12	30229.	0.1	0.1	0.0217
130	61.00	17	110720.	0.5	0.5	0.0796
131	60.00	12	72652.	0.3	0.3	0.0522*
132	59.00	21	134200.	0.6	0.6	0.0936
133	58.00	25	530192.	2.4	2.4	0.3812
134	57.00	51	12577200.	56.4	56.4	9.0430*
135	56.00	35	2294528.	10.3	10.3	1.6497
136	55.00	43	12250368.	54.9	54.9	8.8079*
137	54.00	25	804560.	3.6	3.6	0.5785
138	53.00	25	685168.	3.1	3.1	0.4926
139	52.00	17	75740.	0.3	0.3	0.0545
140	51.00	29	2001152.	9.0	9.0	1.4388
141	50.00	17	61110.	0.3	0.3	0.0439*
142	49.00	10	16571.	0.1	0.1	0.0119
143	48.00	12	17190.	0.1	0.1	0.0124
144	47.00	21	154944.	0.7	0.7	0.1114*
145	46.00	6	2062.	0.0	0.0	0.0015
146	45.00	29	439536.	2.0	2.0	0.3160
147	44.00	35	1199104.	5.4	5.4	0.8621
148	43.00	59	22312960.	100.0	100.0	*16.04*
149	42.00	35	3879488.	17.4	17.4	2.7893
150	41.00	35	11696896.	52.4	52.4	8.4100
151	40.00	25	563408.	2.5	2.5	0.4051
152	39.00	35	2657984.	11.9	11.9	1.9111*
153	38.00	21	87112.	0.4	0.4	0.0626*
154	37.00	8	12329.	0.1	0.1	0.0089
155	36.00	21	130776.	0.6	0.6	0.0940*
156	35.00	8	1972.	0.0	0.0	0.0014

Decanoic acid,

2,2,3,3,4,4,4-heptafluorobutyl ester

 $\text{CH}_3(\text{CH}_2)_8\text{COOCH}_2\text{C}_3\text{F}_7$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	356.00	8	19455.	0.1	0.1	0.0159	56	223.00	8	9180.	0.0	0.0	0.0075
2	355.00	17	292176.	1.5	1.5	0.2391*	57	222.00	6	3894.	0.0	0.0	0.0032
3	354.00	25	1577664.	8.0	8.0	1.2909*	58	221.00	10	3192.	0.0	0.0	0.0026
4	353.00	6	1136.	0.0	0.0	0.0009	59	219.00	8	4338.	0.0	0.0	0.0035
5	337.00	6	1034.	0.0	0.0	0.0008	60	217.00	10	11817.	0.1	0.1	0.0097*
6	336.00	8	17767.	0.1	0.1	0.0145	61	216.00	8	1945.	0.0	0.0	0.0016
7	335.00	12	103400.	0.5	0.5	0.0846	62	213.00	14	115860.	0.6	0.6	0.0948
8	326.00	10	54174.	0.3	0.3	0.0443	63	209.00	12	49218.	0.2	0.2	0.0403
9	325.00	17	377664.	1.9	1.9	0.3090	64	204.00	8	1241.	0.0	0.0	0.0010
10	313.00	10	30604.	0.2	0.2	0.0250	65	183.00	10	25523.	0.1	0.1	0.0209
11	312.00	17	358064.	1.8	1.8	0.2930*	66	181.00	8	15170.	0.1	0.1	0.0124
12	311.00	29	3011264.	15.3	15.3	2.4639*	67	169.00	12	38545.	0.2	0.2	0.0315
13	310.00	12	5888.	0.0	0.0	0.0048	68	161.00	10	20464.	0.1	0.1	0.0167
14	300.00	6	1629.	0.0	0.0	0.0013	69	158.00	6	1626.	0.0	0.0	0.0013
15	299.00	10	7240.	0.0	0.0	0.0059	70	157.00	12	12880.	0.1	0.1	0.0105
16	298.00	14	101240.	0.5	0.5	0.0828	71	156.00	21	327696.	1.7	1.7	0.2681*
17	297.00	17	767824.	3.9	3.9	0.6282*	72	155.00	35	3226048.	16.4	16.4	2.6396*
18	285.00	6	1656.	0.0	0.0	0.0014	73	154.00	8	4094.	0.0	0.0	0.0033
19	284.00	12	60661.	0.3	0.3	0.0496	74	153.00	8	32065.	0.2	0.2	0.0262
20	283.00	17	323376.	1.6	1.6	0.2646	75	150.00	8	6715.	0.0	0.0	0.0055
21	282.00	8	5766.	0.0	0.0	0.0047	76	145.00	10	2765.	0.0	0.0	0.0023
22	281.00	10	19519.	0.1	0.1	0.0160	77	143.00	10	17419.	0.1	0.1	0.0143
23	280.00	8	9407.	0.0	0.0	0.0077	78	139.00	8	8716.	0.0	0.0	0.0071
24	279.00	8	2733.	0.0	0.0	0.0022	79	137.00	14	81276.	0.4	0.4	0.0665*
25	275.00	8	2273.	0.0	0.0	0.0019	80	136.00	17	100420.	0.5	0.5	0.0822
26	274.00	10	13645.	0.1	0.1	0.0112*	81	135.00	17	82188.	0.4	0.4	0.0672*
27	273.00	8	7673.	0.0	0.0	0.0063	82	133.00	17	88308.	0.4	0.4	0.0723
28	271.00	8	9238.	0.0	0.0	0.0076	83	131.00	14	69608.	0.4	0.4	0.0570*
29	270.00	14	113696.	0.6	0.6	0.0930	84	127.00	8	2422.	0.0	0.0	0.0020
30	269.00	21	1143808.	5.8	5.8	0.9359	85	126.00	14	29223.	0.1	0.1	0.0239
31	268.00	10	44261.	0.2	0.2	0.0362	86	125.00	14	76056.	0.4	0.4	0.0622
32	267.00	6	3621.	0.0	0.0	0.0030	87	123.00	14	112604.	0.6	0.6	0.0921
33	266.00	8	9214.	0.0	0.0	0.0075	88	122.00	8	19837.	0.1	0.1	0.0162
34	265.00	8	13812.	0.1	0.1	0.0113	89	121.00	10	36687.	0.2	0.2	0.0300
35	256.00	12	62561.	0.3	0.3	0.0512*	90	120.00	8	4419.	0.0	0.0	0.0036
36	255.00	25	805504.	4.1	4.1	0.6591*	91	119.00	21	508992.	2.6	2.6	0.4165
37	254.00	43	8119808.	41.2	41.2	6.6438*	92	116.00	6	1469.	0.0	0.0	0.0012
38	254.00	14	24101.	0.1	0.1	0.0197*	93	115.00	10	30416.	0.2	0.2	0.0249
39	253.00	10	47629.	0.2	0.2	0.0390	94	114.00	14	38642.	0.2	0.2	0.0316*
40	252.00	8	13184.	0.1	0.1	0.0108	95	113.00	35	1139392.	5.8	5.8	0.9323
41	251.00	10	2111.	0.0	0.0	0.0017	96	112.00	25	751728.	3.8	3.8	0.6151
42	249.00	10	12912.	0.1	0.1	0.0106*	97	111.00	21	336448.	1.7	1.7	0.2753
43	245.00	10	3161.	0.0	0.0	0.0026	98	110.00	21	974256.	4.9	4.9	0.7972
44	244.00	17	105180.	0.5	0.5	0.0861*	99	109.00	17	79884.	0.4	0.4	0.0554*
45	243.00	35	1516160.	7.7	7.7	1.2406*	100	108.00	14	27616.	0.1	0.1	0.0226*
46	242.00	43	8734720.	44.4	44.4	7.1469*	101	107.00	12	58326.	0.3	0.3	0.0477*
47	241.00	21	284640.	1.4	1.4	0.2329*	102	101.00	8	5256.	0.0	0.0	0.0043
48	240.00	12	72672.	0.4	0.4	0.0595	103	100.00	17	152080.	0.8	0.8	0.1244
49	239.00	12	50844.	0.3	0.3	0.0416	104	99.00	17	60331.	0.3	0.3	0.0494
50	236.00	12	5623.	0.0	0.0	0.0046*	105	98.00	21	708640.	3.6	3.6	0.5796
51	235.00	17	190368.	1.0	1.0	0.1558	106	97.00	25	877776.	4.5	4.5	0.7182
52	229.00	8	13269.	0.1	0.1	0.0109	107	96.00	17	112700.	0.6	0.6	0.0922
53	228.00	12	45879.	0.2	0.2	0.0375	108	95.00	29	1016256.	5.2	5.2	0.8315
54	227.00	21	801952.	4.1	4.1	0.6562*	109	94.00	14	50510.	0.3	0.3	0.0413
55	226.00	10	2388.	0.0	0.0	0.0020	110	93.00	14	84980.	0.4	0.4	0.0695

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	91.00	10	22930.	0.1	0.1	0.0188
112	89.00	10	3268.	0.0	0.0	0.0027
113	87.00	10	4603.	0.0	0.0	0.0038
114	86.00	14	51836.	0.3	0.3	0.0424*
115	85.00	25	858944.	4.4	4.4	0.7028*
116	84.00	25	1252224.	6.4	6.4	1.0246*
117	83.00	35	2328384.	11.8	11.8	1.9051*
118	82.00	21	398864.	2.0	2.0	0.3264
119	81.00	25	862800.	4.4	4.4	0.7060
120	80.00	25	90956.	0.5	0.5	0.0744*
121	79.00	21	174560.	0.9	0.9	0.1428
122	78.00	8	18134.	0.1	0.1	0.0148
123	77.00	14	69288.	0.4	0.4	0.0567*
124	75.00	12	27363.	0.1	0.1	0.0224*
125	74.00	8	3323.	0.0	0.0	0.0027
126	73.00	21	144388.	0.7	0.7	0.1181
127	72.00	21	251444.	1.3	1.3	0.2057
128	71.00	35	5139968.	26.1	26.1	4.2056*
129	70.00	25	948528.	4.8	4.8	0.7761
130	69.00	35	6032896.	30.6	30.6	4.9362*
131	68.00	25	844560.	4.3	4.3	0.6910
132	67.00	25	768816.	3.9	3.9	0.6291
133	66.00	14	52068.	0.3	0.3	0.0426
134	65.00	17	92836.	0.5	0.5	0.0760*
135	64.00	17	195576.	1.0	1.0	0.1600
136	63.00	12	32490.	0.2	0.2	0.0266*
137	61.00	12	56455.	0.3	0.3	0.0462*
138	60.00	14	46004.	0.2	0.2	0.0376*
139	59.00	14	81088.	0.4	0.4	0.0663
140	58.00	25	332064.	1.7	1.7	0.2717
141	57.00	43	7707648.	39.2	39.2	6.3066*
142	56.00	29	1860736.	9.5	9.5	1.5225
143	55.00	43	10283520.	52.2	52.2	8.4142*
144	54.00	25	670896.	3.4	3.4	0.5489
145	53.00	21	586064.	3.0	3.0	0.4795
146	52.00	12	60776.	0.3	0.3	0.0497*
147	51.00	25	1569792.	8.0	8.0	1.2844
148	50.00	10	35202.	0.2	0.2	0.0288*
149	49.00	12	7634.	0.0	0.0	0.0062
150	48.00	12	20481.	0.1	0.1	0.0158*
151	47.00	17	116876.	0.6	0.6	0.0956*
152	46.00	6	4872.	0.0	0.0	0.0040
153	45.00	29	330384.	1.7	1.7	0.2703*
154	44.00	35	1007232.	5.1	5.1	0.8241
155	43.00	51	19687424.	100.0	100.0	*16.10*
156	42.00	35	3103360.	15.8	15.8	2.5392
157	41.00	35	10147840.	51.5	51.5	8.3032*
158	40.00	29	487696.	2.5	2.5	0.3990
159	39.00	35	2059776.	10.5	10.5	1.6854*
160	38.00	17	62304.	0.3	0.3	0.0510*
161	37.00	10	13500.	0.1	0.1	0.0110*
162	36.00	21	113776.	0.6	0.6	0.0931*
163	35.00	12	8234.	0.0	0.0	0.0067

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	370.00	10	26000.	0.2	0.2	0.0256	56	227.00	17	611744.	3.8	3.8	0.5032
2	369.00	17	286528.	1.8	1.8	0.0285	57	223.00	10	7477.	0.0	0.0	0.0074
3	368.00	29	1631616.	10.2	10.2	1.6088*	58	218.00	6	1722.	0.0	0.0	0.0017
4	367.00	8	3324.	0.0	0.0	0.0033	59	217.00	8	693.	0.0	0.0	0.0007
5	350.00	12	12283.	0.1	0.1	0.0121	60	214.00	6	1446.	0.0	0.0	0.0014
6	349.00	12	99560.	0.6	0.6	0.0098	61	213.00	12	89456.	0.5	0.5	0.0793
7	340.00	12	45485.	0.3	0.3	0.0448	62	209.00	10	34548.	0.2	0.2	0.0341
8	339.00	14	252668.	1.6	1.6	0.2491	63	207.00	8	1559.	0.0	0.0	0.0015
9	327.00	8	10017.	0.1	0.1	0.0099	64	183.00	8	5896.	0.0	0.0	0.0058
10	326.00	14	158284.	1.0	1.0	0.1561	65	181.00	10	3689.	0.0	0.0	0.0036
11	325.00	25	1190592.	7.4	7.4	1.1740*	66	180.00	8	1482.	0.0	0.0	0.0015
12	313.00	10	19190.	0.1	0.1	0.0189	67	171.00	10	10404.	0.1	0.1	0.0103
13	312.00	17	182564.	1.1	1.1	0.1800*	68	170.00	17	241956.	1.5	1.5	0.2386*
14	311.00	21	1466944.	9.1	9.1	1.4464	69	169.00	29	2409472.	15.0	15.0	2.3758*
15	310.00	8	2230.	0.0	0.0	0.0022	70	168.00	8	2457.	0.0	0.0	0.0024
16	298.00	12	83876.	0.5	0.5	0.0827	71	167.00	10	1453.	0.1	0.1	0.0143
17	297.00	17	569088.	3.5	3.5	0.5611	72	164.00	8	2707.	0.0	0.0	0.0027
18	293.00	8	3050.	0.0	0.0	0.0030	73	161.00	8	6753.	0.0	0.0	0.0067
19	288.00	12	1784.	0.0	0.0	0.0018	74	158.00	6	3279.	0.0	0.0	0.0032
20	287.00	10	3558.	0.0	0.0	0.0035	75	153.00	12	10509.	0.1	0.1	0.0104
21	284.00	12	77740.	0.5	0.5	0.0767	76	151.00	12	30665.	0.2	0.2	0.0302
22	283.00	17	428384.	2.7	2.7	0.4224	77	150.00	17	88468.	0.6	0.6	0.0872*
23	282.00	8	9699.	0.1	0.1	0.0096	78	149.00	8	17774.	0.1	0.1	0.0175
24	281.00	8	11549.	0.1	0.1	0.0114	79	143.00	6	1704.	0.0	0.0	0.0017
25	280.00	8	10083.	0.1	0.1	0.0099	80	141.00	6	2446.	0.0	0.0	0.0024
26	279.00	8	10455.	0.1	0.1	0.0103	81	139.00	12	42089.	0.3	0.3	0.0415*
27	271.00	8	11325.	0.1	0.1	0.0112	82	135.00	12	40457.	0.3	0.3	0.0399*
28	270.00	17	154400.	1.0	1.0	0.1522	83	133.00	14	70660.	0.4	0.4	0.0697
29	269.00	21	975632.	6.1	6.1	0.9620	84	131.00	12	73144.	0.5	0.5	0.0721
30	268.00	12	26800.	0.2	0.2	0.0264	85	128.00	9	6173.	0.0	0.0	0.0061
31	267.00	10	5634.	0.0	0.0	0.0056	86	127.00	21	225748.	1.4	1.4	0.2226
32	266.00	10	12977.	0.1	0.1	0.0126	87	126.00	21	350128.	2.2	2.2	0.3452
33	265.00	10	9943.	0.1	0.1	0.0098	88	125.00	17	159572.	1.0	1.0	0.1573
34	263.00	10	4383.	0.0	0.0	0.0043*	89	124.00	21	663648.	4.1	4.1	0.6544
35	258.00	6	1906.	0.0	0.0	0.0019	90	123.00	17	92204.	0.6	0.6	0.0909
36	257.00	14	68520.	0.4	0.4	0.0676*	91	122.00	10	30755.	0.2	0.2	0.0304*
37	256.00	29	767872.	4.8	4.8	0.7571*	92	121.00	14	77168.	0.5	0.5	0.0761
38	255.00	35	6807552.	42.4	42.4	6.7124*	93	119.00	17	380896.	2.4	2.4	0.3756
39	254.00	10	6211.	0.0	0.0	0.0061*	94	114.00	12	4724.	0.0	0.0	0.0047
40	253.00	12	37448.	0.2	0.2	0.0369	95	113.00	21	547648.	3.4	3.4	0.5400*
41	252.00	8	6800.	0.0	0.0	0.0067	96	112.00	17	110124.	0.7	0.7	0.1086
42	250.00	10	5041.	0.0	0.0	0.0050	97	111.00	21	228240.	1.4	1.4	0.2251
43	249.00	12	62803.	0.4	0.4	0.0619	98	109.00	14	49755.	0.3	0.3	0.0491*
44	245.00	8	5594.	0.0	0.0	0.0055	99	108.00	21	201736.	1.3	1.3	0.1989
45	244.00	17	90512.	0.6	0.6	0.0892*	100	108.00	8	7116.	0.0	0.0	0.0070
46	243.00	25	1365568.	8.5	8.5	1.3465*	101	107.00	12	56097.	0.3	0.3	0.0553*
47	242.00	43	7026944.	43.8	43.8	6.9288*	102	101.00	8	1696.	0.0	0.0	0.0017
48	241.00	21	283312.	1.8	1.8	0.2794*	103	100.00	17	115248.	0.7	0.7	0.1136*
49	240.00	12	30805.	0.2	0.2	0.0304*	104	99.00	17	137800.	0.9	0.9	0.1359
50	239.00	10	43564.	0.3	0.3	0.0430	105	98.00	21	802128.	5.0	5.0	0.7909
51	236.00	6	2043.	0.0	0.0	0.0020	106	97.00	25	1086464.	6.8	6.8	1.0713
52	235.00	12	100332.	0.6	0.6	0.0989	107	96.00	21	276704.	1.7	1.7	0.2728
53	231.00	6	1972.	0.0	0.0	0.0019	108	95.00	25	905232.	5.6	5.6	0.8926
54	229.00	6	1994.	0.0	0.0	0.0020	109	94.00	10	41061.	0.3	0.3	0.0405*
55	228.00	12	31163.	0.2	0.2	0.0307	110	93.00	17	102400.	0.6	0.6	0.1010

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	91.00	10	12346.	0.1	0.1	0.0122
112	87.00	12	6543.	0.0	0.0	0.0065
113	86.00	17	138800.	0.9	0.9	0.1369
114	85.00	29	2334000.	14.6	14.6	2.3015*
115	84.00	25	1103744.	6.9	6.9	1.0883
116	83.00	35	2176192.	13.6	13.6	2.1458
117	82.00	21	502512.	3.1	3.1	0.4955
118	81.00	25	555104.	3.5	3.5	0.5473
119	80.00	14	66048.	0.4	0.4	0.0651*
120	79.00	17	153692.	1.0	1.0	0.1515
121	78.00	8	11209.	0.1	0.1	0.0111
122	77.00	17	69176.	0.4	0.4	0.0682*
123	75.00	10	26413.	0.2	0.2	0.0260*
124	74.00	8	5756.	0.0	0.0	0.0057
125	73.00	17	105892.	0.7	0.7	0.1044
126	72.00	21	192916.	1.2	1.2	0.1902
127	71.00	35	3766976.	23.5	23.5	3.7143
128	70.00	25	792800.	4.9	4.9	0.7818
129	69.00	35	4855552.	30.3	30.3	4.7877*
130	68.00	21	638192.	4.0	4.0	0.6293
131	67.00	21	651712.	4.1	4.1	0.6426
132	66.00	12	42805.	0.3	0.3	0.0422*
133	65.00	12	47476.	0.3	0.3	0.0468*
134	64.00	17	123244.	0.8	0.8	0.1215
135	63.00	8	7481.	0.0	0.0	0.0074
136	62.00	10	1921.	0.0	0.0	0.0019
137	61.00	12	44132.	0.3	0.3	0.0435*
138	60.00	12	33999.	0.2	0.2	0.0335*
139	59.00	17	65956.	0.4	0.4	0.0650*
140	58.00	25	259130.	1.6	1.6	0.2556
141	57.00	35	5870000.	36.6	36.6	5.7881
142	56.00	35	1581120.	9.9	9.9	1.5590
143	55.00	43	8518400.	53.1	53.1	8.3994*
144	54.00	25	573360.	3.6	3.6	0.5653*
145	53.00	21	436128.	2.7	2.7	0.4300
146	52.00	14	46437.	0.3	0.3	0.0458*
147	51.00	25	1110528.	6.9	6.9	1.0950
148	50.00	10	27331.	0.2	0.2	0.0269
149	49.00	10	4106.	0.0	0.0	0.0040
150	48.00	6	3798.	0.0	0.0	0.0037
151	47.00	17	69156.	0.4	0.4	0.0682*
152	45.00	25	247408.	1.5	1.5	0.2440*
153	44.00	35	701104.	4.4	4.4	0.6913
154	43.00	43	16040192.	100.0	100.0	*15.81*
155	42.00	35	2424512.	15.1	15.1	2.3906*
156	41.00	35	8032512.	50.1	50.1	7.9203*
157	40.00	25	296272.	1.8	1.8	0.2921*
158	39.00	35	1474368.	9.2	9.2	1.4538*
159	38.00	17	44143.	0.3	0.3	0.0435*
160	36.00	17	95852.	0.6	0.6	0.0945*
161	35.00	12	4550.	0.0	0.0	0.0045*

AL10PA.1 [TIC=128864736, 100X=19495936] EI

Dodecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester
 $\text{CH}_3(\text{CH}_2)_{10}\text{COOCH}_2\text{C}_3\text{F}_7$

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	384.00	12	46072.	0.2	0.2	0.357	56	242.00	43	8722176.	44.7	44.7	6.7674*
2	383.00	17	46016.	2.4	2.4	0.3616*	57	241.00	21	313472.	1.6	1.6	0.2432
3	382.00	35	260064.	13.3	13.3	2.0174*	58	240.00	10	32631.	0.2	0.2	0.0253
4	381.00	8	2876.	0.0	0.0	0.0022	59	239.00	12	56083.	0.3	0.3	0.0435
5	367.00	8	5619.	0.1	0.1	0.0044	60	237.00	6	1084.	0.0	0.0	0.0008
6	364.00	10	27089.	0.1	0.1	0.0210	61	236.00	8	2119.	0.0	0.0	0.0016
7	363.00	14	130916.	0.7	0.7	0.1016	62	235.00	14	121168.	0.6	0.6	0.0940
8	354.00	12	74220.	0.4	0.4	0.0576	63	233.00	8	1328.	0.0	0.0	0.0010
9	353.00	17	454400.	2.3	2.3	0.3526	64	231.00	8	1849.	0.0	0.0	0.0014
10	341.00	10	8491.	0.0	0.0	0.0055	65	229.00	8	8396.	0.0	0.0	0.0065*
11	340.00	14	190488.	1.0	1.0	0.1478	66	228.00	10	49588.	0.3	0.3	0.0385
12	339.00	21	1408064.	7.2	7.2	1.0925*	67	227.00	17	762400.	3.9	3.9	0.5915
13	327.00	8	6028.	0.0	0.0	0.0047	68	226.00	6	1200.	0.0	0.0	0.0009
14	326.00	12	57689.	0.3	0.3	0.0448	69	223.00	8	5560.	0.0	0.0	0.0043
15	325.00	17	323952.	1.7	1.7	0.2514	70	222.00	8	2031.	0.0	0.0	0.0016
16	313.00	8	10280.	0.1	0.1	0.0080	71	217.00	8	4660.	0.0	0.0	0.0036
17	312.00	17	264432.	1.4	1.4	0.2052*	72	216.00	6	1555.	0.0	0.0	0.0012
18	311.00	25	2014272.	10.3	10.3	1.5628*	73	213.00	14	93488.	0.5	0.5	0.0725
19	307.00	6	3052.	0.0	0.0	0.0024	74	212.00	8	1431.	0.0	0.0	0.0011
20	302.00	6	2061.	0.0	0.0	0.0016	75	209.00	10	28559.	0.1	0.1	0.0222
21	301.00	8	3567.	0.0	0.0	0.0028	76	207.00	8	1341.	0.0	0.0	0.0010
22	299.00	8	8656.	0.0	0.0	0.0057	77	185.00	10	21089.	0.1	0.1	0.0164
23	298.00	14	150296.	0.8	0.8	0.1166*	78	184.00	21	319376.	1.6	1.6	0.2478*
24	297.00	21	977008.	5.0	5.0	0.71580*	79	183.00	29	2710208.	13.9	13.9	2.1028*
25	296.00	8	1173.	0.0	0.0	0.0009	80	182.00	8	7593.	0.0	0.0	0.0059
26	295.00	6	1663.	0.0	0.0	0.0013	81	181.00	12	23610.	0.1	0.1	0.0183*
27	293.00	6	7573.	0.0	0.0	0.0059	82	171.00	6	1732.	0.0	0.0	0.0013
28	285.00	12	8262.	0.0	0.0	0.0064	83	169.00	14	27808.	0.1	0.1	0.0216
29	284.00	8	147928.	0.8	0.8	0.1148	84	165.00	10	20690.	0.1	0.1	0.0161
30	283.00	17	665248.	3.4	3.4	0.5162	85	164.00	17	101836.	0.5	0.5	0.0790
31	282.00	10	12698.	0.1	0.1	0.0099	86	163.00	10	27718.	0.1	0.1	0.0215
32	281.00	8	20096.	0.1	0.1	0.0156	87	161.00	12	17062.	0.1	0.1	0.0132
33	280.00	10	13828.	0.1	0.1	0.0107	88	153.00	10	20148.	0.1	0.1	0.0156
34	279.00	8	16103.	0.1	0.1	0.0125	89	150.00	10	8896.	0.0	0.0	0.0069
35	277.00	8	8108.	0.0	0.0	0.0063	90	149.00	8	16192.	0.1	0.1	0.0126
36	271.00	8	6613.	0.0	0.0	0.0051	91	147.00	8	8131.	0.0	0.0	0.0063
37	270.00	17	180100.	0.9	0.9	0.1397	92	143.00	6	2645.	0.0	0.0	0.0021
38	269.00	21	977056.	5.0	5.0	0.7581	93	142.00	10	8873.	0.0	0.0	0.0069
39	268.00	10	36958.	0.2	0.2	0.0287	94	141.00	17	229288.	1.2	1.2	0.1779
40	267.00	10	11426.	0.1	0.1	0.0089	95	140.00	17	325872.	1.7	1.7	0.2528*
41	266.00	8	9713.	0.0	0.0	0.0075	96	139.00	17	128864.	0.7	0.7	0.1000
42	265.00	10	27944.	0.1	0.1	0.0217	97	138.00	21	817392.	4.2	4.2	0.6342
43	264.00	6	1913.	0.0	0.0	0.0015	98	137.00	10	5456.	0.0	0.0	0.0042
44	263.00	12	61714.	0.3	0.3	0.0479	99	136.00	6	1657.	0.0	0.0	0.0013
45	257.00	14	71240.	0.4	0.4	0.0553*	100	135.00	17	97936.	0.5	0.5	0.0760*
46	256.00	25	875600.	4.5	4.5	0.6794*	101	133.00	12	61329.	0.3	0.3	0.0476
47	255.00	43	8454656.	43.4	43.4	6.5599*	102	131.00	12	62242.	0.3	0.3	0.0483*
48	254.00	17	35023.	0.2	0.2	0.0272*	103	127.00	6	1999.	0.0	0.0	0.0016
49	253.00	14	62592.	0.3	0.3	0.0486*	104	126.00	12	33122.	0.2	0.2	0.0257*
50	252.00	10	17794.	0.1	0.1	0.0138	105	125.00	17	13696.	0.7	0.7	0.1022
51	251.00	6	1345.	0.0	0.0	0.0010	106	124.00	10	23456.	0.1	0.1	0.0182
52	246.00	6	834.	0.0	0.0	0.0006	107	123.00	21	138348.	0.7	0.7	0.1073*
53	245.00	8	5438.	0.0	0.0	0.0042	108	122.00	10	20244.	0.1	0.1	0.0157
54	244.00	17	134264.	0.7	0.7	0.1042*	109	121.00	14	95148.	0.5	0.5	0.0738
55	243.00	29	1837184.	9.4	9.4	1.4254*	110	119.00	21	418000.	2.1	2.1	0.3243

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	115.00	6	2886.	0.0	0.0	0.0022	166	50.00	10	32144.	0.2	0.2	0.0249
112	114.00	12	16131.	0.1	0.1	0.0125*	167	49.00	8	4842.	0.0	0.0	0.0038
113	113.00	25	616304.	3.2	3.2	0.4782*	168	48.00	6	4105.	0.0	0.0	0.0032
114	112.00	17	255272.	1.3	1.3	0.1981	169	47.00	17	84212.	0.4	0.4	0.0653
115	111.00	25	570672.	2.9	2.9	0.4428*	170	46.00	6	1250.	0.0	0.0	0.0010
116	110.00	17	249760.	1.3	1.3	0.1938	171	45.00	25	249176.	1.3	1.3	0.1933
117	109.00	21	361329.	0.1	0.1	0.0146*	172	44.00	35	945264.	4.8	4.8	0.7334*
118	108.00	10	18789.	0.4	0.4	0.0592	173	43.00	51	19495936.	100.0	100.0	*15.12*
119	107.00	17	76320.	0.0	0.0	0.0025	174	42.00	35	2744000.	14.1	14.1	2.1290*
120	105.00	8	2181.	0.0	0.0	0.0060*	175	41.00	35	9895424.	50.8	50.8	7.6777*
121	101.00	12	7733.	0.0	0.0	0.0060*	176	40.00	29	341840.	1.8	1.8	0.2652*
122	100.00	25	173276.	0.9	0.9	0.1344*	177	39.00	35	1644992.	8.4	8.4	1.2763*
123	99.00	21	716928.	3.7	3.7	0.5563	178	38.00	14	44736.	0.2	0.2	0.0347*
124	98.00	25	1066560.	5.5	5.5	0.8275	179	37.00	12	7875.	0.0	0.0	0.0061*
125	97.00	29	1670464.	8.6	8.6	1.2961*	180	36.00	21	118592.	0.6	0.6	0.0920*
126	96.00	21	46048.	2.4	2.4	0.3573	181	35.00	8	2796.	0.0	0.0	0.0022
127	95.00	29	1026944.	5.3	5.3	0.7968							
128	94.00	14	59249.	0.3	0.3	0.0460*							
129	93.00	17	114328.	0.6	0.6	0.0887							
130	91.00	12	38645.	0.2	0.2	0.0300							
131	89.00	6	1117.	0.0	0.0	0.0009							
132	86.00	17	189328.	1.0	1.0	0.1469*							
133	85.00	29	3138800.	16.1	16.1	2.4354							
134	84.00	25	1321160.	6.8	6.8	1.0274*							
135	83.00	35	2791744.	14.3	14.3	2.1661*							
136	82.00	25	498336.	2.6	2.6	0.3867*							
137	81.00	21	694480.	3.6	3.6	0.5388							
138	80.00	17	109576.	0.6	0.6	0.0850*							
139	79.00	17	189796.	1.0	1.0	0.1473							
140	78.00	8	20157.	0.1	0.1	0.0156							
141	77.00	17	70416.	0.4	0.4	0.0546*							
142	75.00	8	9439.	0.0	0.0	0.0073							
143	74.00	8	2914.	0.0	0.0	0.0023							
144	73.00	17	138876.	0.7	0.7	0.1078*							
145	72.00	17	195564.	1.0	1.0	0.1517							
146	71.00	29	3911680.	20.1	20.1	3.0350							
147	70.00	25	1042384.	5.3	5.3	0.8088							
148	69.00	35	6076416.	31.2	31.2	4.7146							
149	68.00	25	7840000.	4.0	4.0	0.6083							
150	67.00	25	910784.	4.7	4.7	0.7067							
151	66.00	17	59509.	0.3	0.3	0.0462*							
152	65.00	17	83016.	0.4	0.4	0.0644*							
153	64.00	17	151948.	0.8	0.8	0.1178							
154	63.00	12	19586.	0.1	0.1	0.0152							
155	61.00	14	55949.	0.3	0.3	0.0434*							
156	60.00	17	48600.	0.2	0.2	0.0377*							
157	59.00	17	82884.	0.4	0.4	0.0643							
158	58.00	25	363088.	1.9	1.9	0.2817							
159	57.00	43	8540672.	43.8	43.8	6.6266*							
160	56.00	35	2112192.	10.8	10.8	1.6388*							
161	55.00	35	10484992.	53.8	53.8	8.1352*							
162	54.00	25	741184.	3.8	3.8	0.5751*							
163	53.00	25	557136.	2.9	2.9	0.4323							
164	52.00	14	25553.	0.1	0.1	0.0198							
165	51.00	25	1241152.	6.4	6.4	0.9630*							

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
166	50.00	10	32144.	0.2	0.2	0.0249
167	49.00	8	4842.	0.0	0.0	0.0038
168	48.00	6	4105.	0.0	0.0	0.0032
169	47.00	17	84212.	0.4	0.4	0.0653
170	46.00	6	1250.	0.0	0.0	0.0010
171	45.00	25	249176.	1.3	1.3	0.1933
172	44.00	35	945264.	4.8	4.8	0.7334*
173	43.00	51	19495936.	100.0	100.0	*15.12*
174	42.00	35	2744000.	14.1	14.1	2.1290*
175	41.00	35	9895424.	50.8	50.8	7.6777*
176	40.00	29	341840.	1.8	1.8	0.2652*
177	39.00	35	1644992.	8.4	8.4	1.2763*
178	38.00	14	44736.	0.2	0.2	0.0347*
179	37.00	12	7875.	0.0	0.0	0.0061*
180	36.00	21	118592.	0.6	0.6	0.0920*
181	35.00	8	2796.	0.0	0.0	0.0022

AL11PA.1 [TIC=119242752, 100X=17783800] E1

Tridecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester
 $\text{CH}_3(\text{CH}_2)_{11}\text{COOCH}_2\text{C}_3\text{F}_7$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	398.00	12	67344.	0.4	0.4	0.0565	56	241.00	17	280304.	1.6	1.6	0.2351
2	397.00	21	545504.	3.1	3.1	0.4575	5	240.00	10	34770.	0.2	0.2	0.0292
3	396.00	29	2788992.	15.7	15.7	0.3389*	58	239.00	10	46264.	0.3	0.3	0.0388
4	381.00	8	1126.	0.0	0.0	0.0009	59	236.00	8	5457.	0.0	0.0	0.0046
5	379.00	8	2079.	0.0	0.0	0.0017	60	235.00	12	97672.	0.5	0.5	0.0819
6	378.00	8	21710.	0.1	0.1	0.0182	61	229.00	6	472.	0.0	0.0	0.0004
7	377.00	12	124772.	0.7	0.7	0.1046	62	228.00	10	29603.	0.2	0.2	0.0248*
8	368.00	12	66164.	0.4	0.4	0.0555	63	227.00	21	675424.	3.8	3.8	0.5664
9	367.00	17	404176.	2.3	2.3	0.3390	64	226.00	6	4915.	0.0	0.0	0.0041
10	359.00	6	911.	0.0	0.0	0.0008	65	224.00	6	1684.	0.0	0.0	0.0014
11	355.00	8	22616.	0.1	0.1	0.0190	66	223.00	8	6141.	0.0	0.0	0.0051
12	354.00	17	189196.	1.1	1.1	0.1587*	67	219.00	6	997.	0.0	0.0	0.0008
13	353.00	21	1325952.	7.5	7.5	1.1120	68	218.00	6	1296.	0.0	0.0	0.0011
14	341.00	12	5669.	0.0	0.0	0.0048	69	217.00	6	2925.	0.0	0.0	0.0025
15	340.00	10	54962.	0.3	0.3	0.0461	70	216.00	6	852.	0.0	0.0	0.0007
16	339.00	14	213068.	1.2	1.2	0.1787	71	213.00	12	78268.	0.4	0.4	0.0656
17	326.00	10	41896.	0.2	0.2	0.0351	72	209.00	10	30560.	0.2	0.2	0.0256
18	325.00	17	205724.	1.2	1.2	0.1725	73	207.00	8	10664.	0.1	0.1	0.0089
19	316.00	8	5913.	0.0	0.0	0.0050	74	202.00	6	1085.	0.0	0.0	0.0009
20	315.00	6	3525.	0.0	0.0	0.0030	75	199.00	10	39329.	0.2	0.2	0.0330
21	313.00	10	17310.	0.1	0.1	0.0145	76	198.00	17	483584.	2.7	2.7	0.4055*
22	312.00	17	229688.	1.3	1.3	0.1926*	77	197.00	25	1933248.	10.9	10.9	1.6213*
23	311.00	25	2075328.	11.7	11.7	1.7404	78	196.00	10	11671.	0.1	0.1	0.0098
24	299.00	8	21677.	0.1	0.1	0.0182	79	195.00	8	3478.	0.0	0.0	0.0029
25	298.00	17	218904.	1.2	1.2	0.1836*	80	191.00	8	1557.	0.0	0.0	0.0013
26	297.00	21	976096.	5.5	5.5	0.8186	81	183.00	8	7344.	0.0	0.0	0.0062
27	293.00	6	5495.	0.0	0.0	0.0046	82	181.00	6	3051.	0.0	0.0	0.0026
28	291.00	6	3535.	0.0	0.0	0.0030	83	179.00	10	22884.	0.1	0.1	0.0192
29	290.00	8	2234.	0.0	0.0	0.0019	84	178.00	14	66160.	0.4	0.4	0.0555
30	285.00	8	4923.	0.0	0.0	0.0041	85	170.00	10	9056.	0.1	0.1	0.0976
31	284.00	14	134652.	0.8	0.8	0.1129	86	169.00	10	29664.	0.2	0.2	0.0249
32	283.00	17	288320.	1.6	1.6	0.2418	87	167.00	10	15446.	0.1	0.1	0.0130
33	282.00	8	7046.	0.0	0.0	0.0059	88	163.00	8	6309.	0.0	0.0	0.0053
34	281.00	8	17322.	0.1	0.1	0.0145	89	161.00	12	13254.	0.1	0.1	0.0111
35	280.00	10	21714.	0.1	0.1	0.0182	90	156.00	8	13790.	0.1	0.1	0.0116
36	279.00	8	14669.	0.1	0.1	0.0123	91	155.00	17	188660.	1.1	1.1	0.1584
37	277.00	12	61542.	0.3	0.3	0.0516	92	154.00	17	235588.	1.3	1.3	0.1976
38	271.00	8	2747.	0.0	0.0	0.0023	93	153.00	17	100380.	0.6	0.6	0.0842
39	270.00	14	110644.	0.6	0.6	0.0928	94	152.00	17	555376.	3.1	3.1	0.4658
40	269.00	21	930464.	5.2	5.2	0.7803*	95	151.00	8	2118.	0.0	0.0	0.0018
41	268.00	8	28234.	0.2	0.2	0.0237	96	150.00	8	8026.	0.0	0.0	0.0074
42	267.00	6	14313.	0.1	0.1	0.0120	97	149.00	10	24659.	0.1	0.1	0.0207
43	266.00	10	13307.	0.1	0.1	0.0112	98	141.00	8	5371.	0.0	0.0	0.0045
44	265.00	10	18899.	0.1	0.1	0.0158	99	140.00	8	4337.	0.0	0.0	0.0036
45	263.00	6	852.	0.0	0.0	0.0007	100	139.00	12	63089.	0.4	0.4	0.0529
46	257.00	14	67348.	0.4	0.4	0.0565*	101	138.00	8	6282.	0.0	0.0	0.0053
47	256.00	25	857184.	4.8	4.8	0.7189*	102	136.00	10	29274.	0.2	0.2	0.0245
48	255.00	43	7594496.	42.7	42.7	6.3689*	103	135.00	10	3484.	0.0	0.0	0.0029
49	254.00	8	7725.	0.0	0.0	0.0065*	104	135.00	17	103592.	0.6	0.6	0.0869*
50	253.00	12	48395.	0.3	0.3	0.0406	105	131.00	14	63663.	0.4	0.4	0.0534
51	252.00	10	13449.	0.1	0.1	0.0113	106	131.00	12	45353.	0.3	0.3	0.0380
52	245.00	8	12322.	0.1	0.1	0.0103	107	127.00	10	15623.	0.1	0.1	0.0131
53	244.00	17	149528.	0.8	0.8	0.1254*	108	126.00	17	103332.	0.6	0.6	0.0867*
54	243.00	29	1879872.	10.6	10.6	1.5755*	109	125.00	21	243660.	1.4	1.4	0.2043*
55	242.00	35	8038400.	45.2	45.2	6.7412*	110	124.00	17	154600.	0.9	0.9	0.1297

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	123.00	17	180608.	1.0	1.0	0.1515*	166	53.00	21	480320.	2.7	2.7	0.4028
112	122.00	10	16139.	0.1	0.1	0.0135	167	52.00	12	32349.	0.2	0.2	0.0271*
113	121.00	17	90400.	0.5	0.5	0.0758	168	51.00	25	1003312.	5.6	5.6	0.8414
114	119.00	17	298864.	1.7	1.7	0.2506	169	50.00	12	28390.	0.2	0.2	0.0238*
115	115.00	8	5685.	0.0	0.0	0.0048	170	48.00	8	4441.	0.0	0.0	0.0037
116	114.00	10	20238.	0.1	0.1	0.0170	171	47.00	17	66484.	0.4	0.4	0.0558*
117	113.00	29	794752.	4.5	4.5	0.6665	172	46.00	8	1536.	0.0	0.0	0.0013
118	112.00	21	211380.	1.2	1.2	0.1773	173	45.00	21	218128.	1.2	1.2	0.1829*
119	111.00	25	590336.	3.3	3.3	0.4951	174	44.00	35	765424.	4.3	4.3	0.6419*
120	110.00	17	225240.	1.3	1.3	0.1889	175	43.00	51	17783808.	100.0	100.0	*14.91*
121	109.00	21	301360.	0.1	0.1	0.0212*	176	42.00	35	2341120.	13.2	13.2	1.9633
122	108.00	12	25331.	0.4	0.4	0.0667	177	41.00	35	8588288.	48.3	48.3	7.2024*
123	107.00	14	79516.	0.9	0.9	0.0813	178	40.00	21	295072.	1.7	1.7	0.2475*
124	106.00	6	1554.	0.0	0.0	0.1276*	179	39.00	29	1286336.	7.2	7.2	1.0788*
125	99.00	25	152212.	4.7	4.7	0.7079	180	38.00	17	36234.	0.2	0.2	0.0304*
126	98.00	21	844112.	5.6	5.6	0.8281	181	37.00	12	4557.	0.0	0.0	0.0038*
127	97.00	25	987440.	9.6	9.6	1.4334*	182	35.00	17	109536.	0.6	0.6	0.0919*
128	96.00	21	1709248.	2.4	2.4	0.3522	183	35.00	6	1825.	0.0	0.0	0.0015
129	95.00	25	419920.	4.8	4.8	0.7228							
130	94.00	14	861072.	0.5	0.5	0.0743*							
131	93.00	17	88568.	0.6	0.6	0.0961							
132	91.00	12	114536.	0.1	0.1	0.0139*							
133	89.00	6	16521.	0.0	0.0	0.0020							
134	87.00	8	2440.	0.1	0.1	0.0080							
135	86.00	17	9597.	0.8	0.8	0.1218							
136	85.00	25	145276.	13.8	13.8	2.0541							
137	84.00	25	2449344.	7.0	7.0	1.0429							
138	83.00	35	1243584.	14.3	14.3	2.1392							
139	82.00	21	2550848.	2.9	2.9	0.4253							
140	81.00	25	507120.	3.9	3.9	0.5754							
141	80.00	17	686128.	0.5	0.5	0.0697*							
142	79.00	17	83072.	1.1	1.1	0.1698							
143	78.00	17	202452.	0.1	0.1	0.0167							
144	77.00	10	19915.	0.4	0.4	0.0657*							
145	76.00	8	13712.	0.5	0.5	0.0810							
146	75.00	17	78336.	0.1	0.1	0.0115							
147	74.00	21	96564.	1.0	1.0	0.0810							
148	73.00	21	176964.	20.8	20.8	3.1020							
149	72.00	35	3698880.	6.0	6.0	0.8910							
150	71.00	25	1062464.	33.0	33.0	4.9194*							
151	70.00	43	5865984.	4.5	4.5	0.6712							
152	69.00	21	800368.	5.1	5.1	0.7589*							
153	68.00	25	904896.	0.3	0.3	0.0424*							
154	67.00	14	50515.	0.4	0.4	0.0590*							
155	66.00	14	70344.	0.7	0.7	0.1033*							
156	65.00	17	123176.	0.0	0.0	0.0045							
157	64.00	8	5366.	0.2	0.2	0.0231							
158	63.00	10	27574.	0.2	0.2	0.0372							
159	62.00	12	44304.	0.3	0.3	0.0520*							
160	61.00	14	62034.	2.2	2.2	0.3260							
161	60.00	25	388768.	49.1	49.1	7.3292*							
162	59.00	35	8739584.	11.1	11.1	1.6506							
163	58.00	35	1968192.	53.5	53.5	7.9727*							
164	57.00	43	9506816.	3.8	3.8	0.5599							
165	56.00	25	667664.										

CS2553.1 [TIC=378816, 188X-41195] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	410.00	10	2657.	6.4	6.4	0.7181	56	51.00	2584.	6.3	6.3	0.6983
2	392.00	8	1819.	4.4	4.4	0.4916	57	45.00	5256.	12.8	12.8	1.4205
3	325.00	12	4147.	10.1	10.1	1.1208	58	43.00	37494.	91.0	91.0	*10.13
4	319.00	6	969.	2.4	2.4	0.2619	59	42.00	9701.	23.5	23.5	2.6218
5	298.00	6	1304.	3.2	3.2	0.3524	60	41.00	7557.	18.3	18.3	2.0423
6	297.00	14	4350.	10.6	10.6	1.1756	61	40.00	137.	0.3	0.3	0.0370
7	283.00	8	638.	1.5	1.5	0.1724						
8	269.00	14	5105.	12.4	12.4	1.3797						
9	257.00	10	3235.	7.9	7.9	0.8743						
10	256.00	21	38299.	93.0	93.0	*10.35						
11	255.00	14	4084.	9.9	9.9	1.1037						
12	239.00	6	801.	1.9	1.9	0.2165						
13	227.00	10	6327.	15.4	15.4	1.7099						
14	211.00	10	1835.	4.5	4.5	0.4959						
15	209.00	8	1104.	2.7	2.7	0.2984						
16	208.00	8	1802.	4.4	4.4	0.4870						
17	191.00	8	1339.	3.3	3.3	0.3619						
18	181.00	8	1433.	3.5	3.5	0.3873						
19	179.00	10	249.	0.6	0.6	0.0673						
20	177.00	12	458.	1.1	1.1	0.1238						
21	169.00	8	1629.	4.0	4.0	0.4403						
22	167.00	10	1695.	4.1	4.1	0.4581						
23	164.00	14	4245.	10.3	10.3	1.1472						
24	155.00	8	1292.	3.1	3.1	0.3492						
25	153.00	14	3830.	9.3	9.3	1.0351						
26	152.00	21	18031.	43.8	43.8	4.8730						
27	139.00	17	2551.	6.2	6.2	0.6894						
28	136.00	12	697.	1.7	1.7	0.1884						
29	127.00	8	1746.	4.2	4.2	0.4719						
30	126.00	12	3378.	8.2	8.2	0.9129						
31	125.00	17	5530.	13.4	13.4	1.4945						
32	124.00	12	1079.	2.6	2.6	0.2916						
33	122.00	14	1980.	4.8	4.8	0.5351						
34	115.00	6	1141.	2.8	2.8	0.3084						
35	113.00	14	6353.	15.4	15.4	1.7170*						
36	111.00	10	2459.	6.0	6.0	0.6646						
37	110.00	8	2129.	5.2	5.2	0.5754						
38	108.00	17	296.	0.7	0.7	0.0800						
39	100.00	8	1284.	3.1	3.1	0.3470						
40	98.00	14	3239.	7.9	7.9	0.8754*						
41	97.00	21	16914.	41.1	41.1	4.5712						
42	91.00	14	1223.	3.0	3.0	0.3305						
43	85.00	17	930.	2.3	2.3	0.2513						
44	80.00	17	5266.	12.8	12.8	1.4232						
45	71.00	21	21101.	51.2	51.2	5.7027						
46	70.00	17	4753.	11.6	11.6	1.2953						
47	66.00	8	139.	0.3	0.3	0.0376						
48	65.00	14	3420.	8.3	8.3	0.9243*						
49	64.00	17	3354.	8.1	8.1	0.9064						
50	58.00	8	3291.	8.0	8.0	0.8894						
51	57.00	25	41195.	100.0	100.0	*11.13						
52	56.00	21	4999.	12.1	12.1	1.3510						
53	55.00	29	19601.	47.6	47.6	5.2973						
54	54.00	17	3373.	8.2	8.2	0.9116						
55	53.00	21	7214.	17.5	17.5	1.9496						

AL12PA.1 [TIC-128622592, 180X-18941952] EI

Tetradecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester
 $\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}_2\text{CF}_3$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	413.00	10	3714.	0.0	0.0	0.0029	56	255.00	35	781388.	41.3	41.3	6.0751
2	412.00	14	85140.	0.4	0.4	0.0662	57	254.00	10	17167.	0.1	0.1	0.0133*
3	411.00	21	695168.	3.7	3.7	0.5405*	58	253.00	12	252.00	0.2	0.2	0.0349*
4	410.00	35	3470720.	18.3	18.3	2.6984*	59	252.00	10	10973.	0.1	0.1	0.0085
5	409.00	10	10623.	0.1	0.1	0.0083*	60	249.00	6	1623.	0.0	0.0	0.0013
6	408.00	6	1787.	0.0	0.0	0.0014	61	244.00	17	138016.	0.7	0.7	0.1073*
7	392.00	10	40837.	0.2	0.2	0.0317	62	243.00	29	2174336.	11.5	11.5	1.5905*
8	391.00	12	147608.	0.8	0.8	0.1148	63	242.00	43	8271104.	43.7	43.7	6.4305*
9	382.00	17	56901.	0.3	0.3	0.0442*	64	241.00	21	288800.	1.5	1.5	0.2245*
10	381.00	12	221172.	1.2	1.2	0.1720	65	240.00	10	31165.	0.2	0.2	0.0242
11	369.00	8	21729.	0.1	0.1	0.0169	66	239.00	10	39314.	0.2	0.2	0.0306
12	368.00	17	235744.	1.2	1.2	0.1833*	67	237.00	10	2708.	0.0	0.0	0.0021*
13	367.00	21	1412032.	7.5	7.5	1.0978	68	236.00	8	7109.	0.0	0.0	0.0055
14	366.00	6	1464.	0.0	0.0	0.0011	69	235.00	12	91260.	0.5	0.5	0.0710
15	355.00	10	13704.	0.1	0.1	0.0107	70	229.00	8	4006.	0.0	0.0	0.0031
16	354.00	14	90592.	0.5	0.5	0.0704	71	228.00	10	30013.	0.2	0.2	0.0233
17	353.00	17	391760.	2.1	2.1	0.3046	72	227.00	17	636656.	3.4	3.4	0.4950
18	341.00	6	1969.	0.0	0.0	0.0015	73	226.00	6	2229.	0.0	0.0	0.0017
19	340.00	10	37274.	0.2	0.2	0.0290	74	223.00	8	6545.	0.0	0.0	0.0051
20	339.00	12	150312.	0.8	0.8	0.1169	75	219.00	8	3476.	0.0	0.0	0.0027
21	330.00	6	1130.	0.0	0.0	0.0009	76	218.00	6	733.	0.0	0.0	0.0006
22	329.00	10	3709.	0.0	0.0	0.0029	77	217.00	8	5667.	0.0	0.0	0.0044
23	328.00	6	986.	0.0	0.0	0.0008	78	213.00	21	180096.	1.0	1.0	0.1400*
24	327.00	8	5120.	0.0	0.0	0.0040	79	212.00	21	727008.	3.8	3.8	0.5652*
25	326.00	10	62144.	0.3	0.3	0.0483	80	211.00	21	1526976.	8.1	8.1	1.1872
26	325.00	17	442032.	2.3	2.3	0.3437	81	210.00	10	7868.	0.0	0.0	0.0061
27	319.00	6	2041.	0.0	0.0	0.0016	82	209.00	12	35010.	0.2	0.2	0.0272*
28	318.00	8	2184.	0.0	0.0	0.0017	83	207.00	10	13245.	0.1	0.1	0.0103
29	313.00	10	29708.	0.2	0.2	0.0231	84	194.00	6	1113.	0.0	0.0	0.0009
30	312.00	17	355136.	1.9	1.9	0.2761	85	193.00	12	33082.	0.2	0.2	0.0257
31	311.00	25	2368384.	12.5	12.5	1.8413	86	192.00	14	67392.	0.4	0.4	0.0524
32	309.00	6	1359.	0.0	0.0	0.0011	87	191.00	10	8059.	0.0	0.0	0.0063
33	303.00	6	1570.	0.0	0.0	0.0012	88	183.00	8	8492.	0.0	0.0	0.0066
34	299.00	8	23359.	0.1	0.1	0.0182	89	182.00	6	1257.	0.0	0.0	0.0010
35	298.00	17	299104.	1.6	1.6	0.2325	90	181.00	10	18357.	0.1	0.1	0.0143
36	297.00	17	670976.	3.5	3.5	0.5217	91	170.00	14	30984.	0.2	0.2	0.0241*
37	293.00	8	5233.	0.0	0.0	0.0041	92	169.00	21	184924.	1.0	1.0	0.1438*
38	292.00	10	22270.	0.1	0.1	0.0173	93	168.00	17	172460.	0.9	0.9	0.1341*
39	291.00	12	49310.	0.3	0.3	0.0383	94	167.00	17	164140.	0.9	0.9	0.1276*
40	284.00	12	106264.	0.6	0.6	0.0826	95	166.00	17	414784.	2.2	2.2	0.3225
41	283.00	17	337712.	1.8	1.8	0.2626	96	164.00	6	2856.	0.0	0.0	0.0022
42	282.00	8	14354.	0.1	0.1	0.0112	97	163.00	12	14476.	0.1	0.1	0.0113
43	281.00	10	28221.	0.1	0.1	0.0219	98	161.00	8	18132.	0.1	0.1	0.0141
44	280.00	10	30558.	0.2	0.2	0.0238	99	158.00	6	2325.	0.0	0.0	0.0018
45	279.00	8	19861.	0.1	0.1	0.0154	100	154.00	6	2325.	0.0	0.0	0.0014
46	271.00	8	10224.	0.1	0.1	0.0079	101	153.00	10	38548.	0.2	0.2	0.0300
47	270.00	14	125004.	0.7	0.7	0.0972	102	152.00	10	7050.	0.0	0.0	0.0055
48	269.00	21	1021584.	5.4	5.4	0.7942	103	151.00	8	8413.	0.0	0.0	0.0065
49	268.00	8	22829.	0.1	0.1	0.0177	104	150.00	10	8252.	0.0	0.0	0.0064
50	267.00	10	11456.	0.1	0.1	0.0089	105	149.00	12	30095.	0.2	0.2	0.0234
51	266.00	8	18418.	0.1	0.1	0.0143	106	145.00	8	1835.	0.0	0.0	0.0014
52	265.00	10	9353.	0.0	0.0	0.0073	107	145.00	6	2585.	0.0	0.0	0.0020
53	258.00	6	2173.	0.0	0.0	0.0017	108	141.00	10	13716.	0.1	0.1	0.0107
54	257.00	14	76964.	0.4	0.4	0.0598	109	140.00	14	82092.	0.4	0.4	0.0638
55	256.00	21	915280.	4.8	4.8	0.7116*	110	139.00	17	147588.	0.8	0.8	0.1147

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	138.00	17	133060.	0.7	0.7	0.1034	166	66.00	12	59227.	0.3	0.3	0.0460*
112	137.00	14	74920.	0.4	0.4	0.0582	167	65.00	17	78924.	0.4	0.4	0.0614*
113	136.00	10	6689.	0.0	0.0	0.0052	168	64.00	17	108672.	0.6	0.6	0.0845*
114	135.00	17	118532.	0.6	0.6	0.0922	169	63.00	8	5130.	0.2	0.0	0.0040
115	133.00	10	61828.	0.3	0.3	0.0481	170	61.00	14	52178.	0.3	0.3	0.0406
116	131.00	12	30672.	0.2	0.2	0.0238	171	60.00	17	20599.	0.1	0.1	0.0160
117	128.00	10	19198.	0.1	0.1	0.0149	172	59.00	12	77032.	0.4	0.4	0.0599
118	127.00	17	196784.	1.0	1.0	0.1530	173	58.00	25	462160.	2.4	2.4	0.3593*
119	126.00	17	83136.	0.4	0.4	0.0646	174	57.00	43	10011904.	52.9	52.9	7.7839*
120	125.00	21	279904.	1.5	1.5	0.1276	175	56.00	35	2058560.	10.9	10.9	1.6005
121	124.00	17	160116.	0.8	0.8	0.1245	176	55.00	35	9653248.	51.0	51.0	7.5051*
122	123.00	21	209368.	1.1	1.1	0.1628	177	54.00	21	685488.	3.6	3.6	0.5329
123	122.00	10	23749.	0.1	0.1	0.0185	178	53.00	21	488176.	2.6	2.6	0.3795
124	121.00	17	113800.	0.6	0.6	0.0885*	179	52.00	10	17129.	0.1	0.1	0.0133
125	120.00	10	2719.	0.0	0.0	0.0021	180	51.00	25	967152.	5.1	5.1	0.7519
126	119.00	17	292320.	1.5	1.5	0.2273	181	50.00	14	19995.	0.1	0.1	0.0155
127	114.00	12	46874.	0.2	0.2	0.0364*	182	48.00	6	2611.	0.0	0.0	0.0020
128	113.00	35	1004016.	5.3	5.3	0.7806	183	47.00	17	65980.	0.3	0.3	0.0513*
129	112.00	21	269840.	1.4	1.4	0.2098	184	45.00	21	223292.	1.2	1.2	0.1736
130	111.00	25	774464.	4.1	4.1	0.6021	185	44.00	35	863312.	4.6	4.6	0.6712
131	110.00	17	220656.	1.2	1.2	0.1716	186	43.00	43	18941952.	100.0	100.0	*14.72*
132	109.00	21	336304.	1.8	1.8	0.2615	187	42.00	35	2470272.	13.0	13.0	1.9206
133	108.00	12	32627.	0.2	0.2	0.0254	188	41.00	35	9054720.	47.8	47.8	7.0398*
134	107.00	17	92636.	0.5	0.5	0.0720*	189	40.00	25	279152.	1.5	1.5	0.2170
135	105.00	6	2473.	0.0	0.0	0.0019	190	39.00	35	1297280.	6.8	6.8	1.0086*
136	100.00	25	146276.	0.8	0.8	0.1137*	191	38.00	12	41213.	0.2	0.2	0.0320*
137	99.00	21	817248.	4.3	4.3	0.6354	192	36.00	17	92096.	0.5	0.5	0.0716*
138	98.00	25	1000192.	5.7	5.7	0.8398	193	35.00	8	5294.	0.0	0.0	0.0041
139	97.00	25	1834048.	9.7	9.7	1.4259*							
140	96.00	21	481184.	2.5	2.5	0.3741							
141	95.00	25	860576.	4.5	4.5	0.6691							
142	94.00	17	81588.	0.4	0.4	0.0634							
143	93.00	17	151524.	0.8	0.8	0.1178							
144	92.00	8	2295.	0.0	0.0	0.0018							
145	91.00	12	36300.	0.2	0.2	0.0282*							
146	87.00	8	5103.	0.0	0.0	0.0040							
147	86.00	17	161396.	0.9	0.9	0.1255*							
148	85.00	29	2530948.	13.4	13.4	1.9670							
149	84.00	25	1399424.	7.4	7.4	1.0880							
150	83.00	35	2922176.	15.4	15.4	2.2719*							
151	82.00	25	623456.	3.3	3.3	0.4847*							
152	81.00	21	760640.	4.0	4.0	0.5914							
153	80.00	17	107300.	0.6	0.6	0.0834*							
154	79.00	17	212256.	1.1	1.1	0.1650							
155	78.00	10	23659.	0.1	0.1	0.0184*							
156	77.00	17	74664.	0.4	0.4	0.0580*							
157	76.00	6	1442.	0.0	0.0	0.0011							
158	75.00	10	9243.	0.0	0.0	0.0072							
159	73.00	17	104764.	0.6	0.6	0.0815*							
160	72.00	17	211888.	1.1	1.1	0.1647							
161	71.00	35	4340736.	22.9	22.9	3.3748*							
162	70.00	29	1093952.	5.8	5.8	0.8505							
163	69.00	35	6299136.	33.3	33.3	4.8974							
164	68.00	21	802544.	4.2	4.2	0.6240							
165	67.00	21	975040.	5.1	5.1	0.7581							

CS2813.1 [TIC-1472512, 188X-211888] EI

3,7,11-trimethyldodecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	427.00	8	758.	0.4	0.4	0.0515
2	424.00	12	6313.	3.0	3.0	0.4287
3	422.00	6	21.9	0.0	0.0	0.0006
4	409.00	8	21.9	0.1	0.0	0.0146
5	406.00	17	3268.	1.5	1.5	0.2219
6	405.00	6	1719.	0.8	0.8	0.1167
7	362.00	6	1365.	0.6	0.6	0.0927
8	340.00	12	2023.	1.0	1.0	0.1374
9	339.00	17	1364.	6.3	6.3	0.9076
10	336.00	8	898.	0.4	0.4	0.0610
11	334.00	6	152.	0.1	0.1	0.0103
12	327.00	6	752.	0.4	0.4	0.0511
13	321.00	6	256.	0.1	0.1	0.0174
14	313.00	8	788.	0.4	0.4	0.0535
15	312.00	12	2393.	1.1	1.1	0.1625
16	311.00	14	7285.	3.4	3.4	0.4947
17	308.00	8	870.	0.4	0.4	0.0591
18	297.00	14	3327.	1.5	1.5	0.2259
19	296.00	10	1002.	0.5	0.5	0.0680
20	295.00	8	1254.	0.6	0.6	0.0852
21	293.00	8	751.	0.4	0.4	0.0510
22	284.00	6	910.	0.4	0.4	0.0618
23	283.00	12	1581.	0.7	0.7	0.1074
24	280.00	10	2972.	1.4	1.4	0.2018
25	279.00	6	1715.	0.8	0.8	0.1165
26	271.00	8	2027.	0.9	0.9	0.1363
27	270.00	17	13224.	6.2	6.2	0.8981
28	269.00	29	101236.	47.8	47.8	6.8751
29	267.00	12	2288.	1.1	1.1	0.1554
30	265.00	6	1194.	0.6	0.6	0.0811
31	255.00	14	802.	0.4	0.4	0.0545
32	254.00	8	1541.	0.7	0.7	0.1047
33	244.00	6	1327.	0.6	0.6	0.0901
34	243.00	17	7740.	3.7	3.7	0.5256
35	242.00	17	17754.	8.4	8.4	1.2057
36	241.00	14	8468.	4.0	4.0	0.5751
37	227.00	21	8888.	4.2	4.2	0.6036
38	225.00	10	2234.	1.1	1.1	0.1517
39	224.00	8	3514.	1.7	1.7	0.2386
40	221.00	12	572.	0.3	0.3	0.0388*
41	208.00	10	129.	0.1	0.1	0.0088
42	206.00	17	9350.	4.4	4.4	0.6350
43	203.00	6	1927.	0.9	0.9	0.1309
44	195.00	6	1586.	0.7	0.7	0.1077
45	192.00	10	301.	0.1	0.1	0.0204
46	190.00	8	2752.	1.3	1.3	0.1876
47	189.00	6	1181.	0.6	0.6	0.0802
48	183.00	17	6049.	2.9	2.9	0.4108
49	182.00	8	2151.	1.0	1.0	0.1451
50	181.00	12	2284.	1.1	1.1	0.1551
51	180.00	17	13480.	6.4	6.4	0.9154
52	167.00	14	2070.	1.0	1.0	0.1406
53	153.00	10	843.	0.4	0.4	0.0572
54	152.00	17	4002.	1.9	1.9	0.2718
55	151.00	21	2315.	1.1	1.1	0.1572

CS3183.1 [TIC=1728384, 188X=278976] EI

Pentadecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	443.00	12	2961.	1.1	1.1	0.1713	56	250.00	6	1287.	0.5	0.5	0.0745
2	434.00	10	446.	0.2	0.2	0.0258	57	245.00	6	972.	0.4	0.4	0.0562
3	431.00	8	1702.	0.6	0.6	0.0985	58	244.00	12	4201.	1.6	1.5	0.2431
4	430.00	10	1850.	0.7	0.7	0.1070	59	243.00	17	35843.	13.2	13.2	2.0738
5	426.00	10	1590.	0.6	0.6	0.0920	60	242.00	35	125620.	46.4	46.4	7.2681*
6	425.00	21	20526.	7.6	7.6	0.43518*	61	241.00	12	4954.	1.8	1.8	0.2866
7	424.00	25	75216.	27.8	27.8	4.3518*	62	237.00	8	1850.	0.7	0.7	0.1070
8	423.00	6	1197.	0.4	0.4	0.0693	63	235.00	21	2244.	0.8	0.8	0.1298
9	419.00	10	784.	0.3	0.3	0.0454	64	231.00	8	27.	0.0	0.0	0.0016
10	405.00	14	249.	0.1	0.1	0.0144	65	228.00	6	1083.	0.4	0.4	0.0627
11	400.00	8	836.	0.3	0.3	0.0484	66	227.00	21	13345.	4.9	4.9	0.7721
12	395.00	10	4588.	1.7	1.7	0.2655	67	226.00	12	3507.	1.3	1.3	0.2029
13	389.00	10	370.	0.1	0.1	0.0214	68	225.00	17	35842.	13.2	13.2	2.0737
14	382.00	17	3108.	1.1	1.1	0.1798*	69	215.00	6	1216.	0.4	0.4	0.0704
15	381.00	25	24738.	9.1	9.1	1.4313	70	214.00	6	1879.	0.7	0.7	0.1087
16	379.00	10	2239.	0.8	0.8	0.1295	71	213.00	10	1879.	0.7	0.7	0.1087
17	376.00	6	258.	0.1	0.1	0.0149	72	206.00	17	104.	0.0	0.0	0.0060
18	368.00	12	3551.	1.3	1.3	0.2055	73	188.00	14	2183.	0.8	0.8	0.1263
19	367.00	14	11968.	4.4	4.4	0.6924	74	185.00	10	757.	0.3	0.3	0.0438
20	361.00	8	768.	0.3	0.3	0.0444	75	183.00	10	2881.	1.1	1.1	0.1667
21	359.00	8	1994.	0.7	0.7	0.1154	76	182.00	6	2546.	0.9	0.9	0.1473
22	354.00	14	1681.	0.6	0.6	0.0973*	77	180.00	17	3338.	1.2	1.2	0.1931
23	353.00	14	7314.	2.7	2.7	0.4232	78	176.00	14	2507.	0.9	0.9	0.1450*
24	350.00	8	1185.	0.4	0.4	0.0686	79	173.00	6	924.	0.3	0.3	0.0535
25	340.00	14	1052.	0.4	0.4	0.0609	80	172.00	10	1073.	0.4	0.4	0.0621
26	339.00	12	5121.	1.9	1.9	0.2963	81	169.00	8	1257.	0.5	0.5	0.0727
27	334.00	8	801.	0.3	0.3	0.0463	82	167.00	12	2832.	1.0	1.0	0.1639
28	332.00	6	415.	0.2	0.2	0.0240	83	152.00	17	4016.	1.5	1.5	0.2324
29	327.00	8	1542.	0.6	0.6	0.0892	84	139.00	17	890.	0.3	0.3	0.0515
30	326.00	8	2565.	0.9	0.9	0.1484	85	134.00	12	3277.	1.2	1.2	0.1896
31	325.00	17	16267.	6.0	6.0	0.9412	86	127.00	17	5000.	1.8	1.8	0.2893
32	319.00	6	957.	0.4	0.4	0.0554	87	113.00	35	11834.	4.4	4.4	0.6847
33	313.00	8	1305.	0.5	0.5	0.0755	88	112.00	21	5010.	1.8	1.8	0.2899
34	311.00	10	6289.	2.3	2.3	0.3639	89	111.00	25	6649.	2.5	2.5	0.3847
35	309.00	21	38878.	14.3	14.3	2.2494	90	104.00	6	1534.	0.6	0.6	0.0888
36	308.00	8	842.	0.3	0.3	0.0487	91	103.00	8	1287.	0.5	0.5	0.0745
37	305.00	8	1198.	0.4	0.4	0.0693	92	100.00	10	1789.	0.7	0.7	0.1035
38	299.00	8	805.	0.3	0.3	0.0466	93	100.00	14	5644.	2.1	2.1	0.3265
39	298.00	8	1451.	0.5	0.5	0.0840	94	99.00	17	5644.	4.8	4.8	0.7465
40	297.00	12	4370.	1.6	1.6	0.2528	95	98.00	17	12902.	6.0	6.0	0.9446
41	296.00	14	7625.	2.8	2.8	0.4412	96	97.00	29	16326.	2.7	2.7	0.4254
42	296.00	6	3.	0.0	0.0	0.0002	97	89.00	6	7353.	0.2	0.2	0.0377
43	295.00	12	2234.	0.8	0.8	0.1293	98	86.00	12	652.	0.2	0.2	0.0377
44	284.00	14	3803.	1.4	1.4	0.2200	99	85.00	25	3296.	1.2	1.2	0.1907
45	283.00	21	4125.	1.5	1.5	0.2387	100	84.00	21	23460.	8.7	8.7	1.3573
46	282.00	6	226.	0.1	0.1	0.0131	101	83.00	35	16113.	5.9	5.9	0.9323
47	271.00	12	2263.	0.8	0.8	0.1309*	102	78.00	21	22668.	8.4	8.4	1.3115
48	270.00	17	5939.	2.2	2.2	0.3436	103	72.00	17	2697.	1.0	1.0	0.1560
49	269.00	17	13194.	4.9	4.9	0.7634	104	71.00	29	5630.	2.1	2.1	0.3257
50	265.00	6	626.	0.2	0.2	0.0362	105	70.00	29	68736.	25.4	25.4	3.9769
51	257.00	8	483.	0.2	0.2	0.0279	106	69.00	35	5768.	2.1	2.1	0.3337
52	256.00	25	8675.	3.2	3.2	0.5019*	107	68.00	21	37320.	13.8	13.8	2.1592
53	255.00	29	104975.	38.7	38.7	6.0737	108	66.00	17	15555.	5.7	5.7	0.9000
54	254.00	6	772.	0.3	0.3	0.0447	109	64.00	8	2958.	1.1	1.1	0.1711*
55							110	58.00	21	368.	0.1	0.1	0.0213
										7962.	2.9	2.9	0.4607

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	57.00	29	156972.	57.9	57.9	9.0820
112	56.00	29	14431.	5.3	5.3	0.8349
113	55.00	43	100684.	37.2	37.2	5.8253*
114	54.00	21	1160.	0.4	0.4	0.0671
115	52.00	8	772.	0.3	0.3	0.0447
116	51.00	21	12288.	4.5	4.5	0.7110
117	50.00	14	1461.	0.5	0.5	0.0845
118	49.00	17	2341.	0.9	0.9	0.1354
119	44.00	35	5007.	1.8	1.8	0.2897*
120	43.00	35	270976.	100.0	100.0	*15.67
121	42.00	25	22215.	8.2	8.2	1.2853
122	41.00	25	93508.	34.5	34.5	5.4101
123	39.00	25	13231.	4.9	4.9	0.7655
124	38.00	14	728.	0.3	0.3	0.0421
125	35.00	17	1308.	0.5	0.5	0.0757

CS3#53.1 [TIC-836296, 16#X-134144] E1

4,8,12-trimethyltridecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PAGE 1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	438.00	17	3977.	3.0	3.0	0.4761
2	436.00	6	1161.	0.9	0.9	0.1390
3	462.00	8	553.	0.4	0.4	0.0662
4	395.00	6	599.	0.4	0.4	0.0717
5	389.00	10	1081.	0.8	0.8	0.1294
6	382.00	6	1960.	1.5	1.5	0.2346
7	381.00	14	7939.	5.9	5.9	0.9504
8	354.00	10	1742.	1.3	1.3	0.2085
9	353.00	12	5443.	4.1	4.1	0.6516
10	352.00	6	626.	0.5	0.5	0.0749
11	328.00	6	515.	0.4	0.4	0.0617
12	326.00	12	3638.	2.7	2.7	0.4355
13	325.00	17	9052.	6.7	6.7	1.0837
14	324.00	6	1353.	1.0	1.0	0.1620
15	311.00	14	5547.	4.1	4.1	0.6641
16	298.00	8	2469.	1.8	1.8	0.2956
17	297.00	14	5495.	4.1	4.1	0.6579
18	294.00	10	3614.	2.7	2.7	0.4327
19	283.00	14	1192.	0.9	0.9	0.1427
20	267.00	17	3397.	2.5	2.5	0.4067
21	265.00	10	1985.	1.5	1.5	0.2376
22	256.00	14	3053.	2.3	2.3	0.3555
23	255.00	17	31928.	23.8	23.8	3.8224
24	243.00	14	3348.	7.5	7.5	0.4008
25	242.00	21	10110.	7.5	7.5	1.2103
26	241.00	17	1704.	1.3	1.3	0.2040
27	233.00	6	2268.	1.7	1.7	0.2715
28	227.00	17	4606.	3.4	3.4	0.5514
29	223.00	8	2532.	1.9	1.9	0.3031
30	219.00	12	1556.	1.2	1.2	0.1863
31	218.00	10	1410.	1.1	1.1	0.1688
32	213.00	10	572.	0.4	0.4	0.0685
33	206.00	8	131.	0.1	0.1	0.0157
34	203.00	8	1250.	0.9	0.9	0.1496
35	198.00	6	1484.	1.1	1.1	0.1777
36	197.00	14	5479.	4.1	4.1	0.6559
37	196.00	10	783.	0.6	0.6	0.0937
38	195.00	10	1746.	1.3	1.3	0.2090
39	175.00	8	1476.	1.1	1.1	0.1767
40	173.00	8	235.	0.2	0.2	0.0281
41	169.00	6	1653.	1.2	1.2	0.1979
42	167.00	14	1359.	1.0	1.0	0.1627
43	153.00	17	19219.	14.3	14.3	2.3009
44	148.00	8	529.	0.4	0.4	0.0633
45	146.00	6	632.	0.5	0.5	0.0757
46	145.00	17	1978.	1.5	1.5	0.2366
47	141.00	17	13906.	10.4	10.4	1.6648
48	140.00	12	3938.	2.9	2.9	0.4714
49	128.00	12	419.	0.3	0.3	0.0502
50	127.00	17	13266.	9.9	9.9	1.5882
51	126.00	21	8907.	6.6	6.6	1.0663
52	115.00	14	1005.	0.7	0.7	0.1203
53	113.00	35	21217.	15.8	15.8	2.5401
54	111.00	25	19203.	14.3	14.3	2.2989
55	106.00	14	3124.	2.3	2.3	0.3740

PAGE 2

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
56	101.00	6	1716.	1.3	1.3	0.2054
57	99.00	17	22660.	16.9	16.9	2.7128
58	86.00	21	3303.	2.5	2.5	0.3954
59	85.00	25	30730.	22.9	22.9	3.6789
60	84.00	21	93.	0.1	0.1	0.0111
61	83.00	25	32735.	24.4	24.4	3.9190
62	74.00	17	3185.	2.4	2.4	0.3813*
63	73.00	21	1095.	0.8	0.8	0.1311
64	72.00	21	7927.	5.9	5.9	0.9490
65	71.00	35	111540.	83.1	83.1	*13.35*
66	70.00	21	5557.	4.1	4.1	0.6653
67	69.00	35	23080.	17.2	17.2	2.7631
68	66.00	21	4564.	3.4	3.4	0.5464
69	61.00	8	1487.	1.1	1.1	0.1780
70	58.00	17	2911.	2.2	2.2	0.3485
71	57.00	29	134144.	100.0	100.0	*16.05
72	56.00	29	11662.	8.7	8.7	1.3962
73	55.00	25	30100.	22.4	22.4	3.6035
74	52.00	6	2257.	1.7	1.7	0.2702
75	50.00	10	3047.	2.3	2.3	0.3648
76	45.00	10	1235.	0.9	0.9	0.1479
77	43.00	43	97212.	72.5	72.5	*11.03*
78	42.00	25	6062.	4.5	4.5	0.7257
79	41.00	25	37976.	28.3	28.3	4.5464

LA13PA.1 [TIC-133365768, 188X-19726336] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	169.00	10	30646.	0.2	0.2	0.0230*	166	95.00	29	877376.	4.4	4.4	0.5579
112	168.00	10	36850.	0.2	0.2	0.0276	167	94.00	14	62945.	0.3	0.3	0.0472*
113	167.00	14	65356.	0.3	0.3	0.0490*	168	93.00	17	150852.	0.8	0.8	0.1131
114	166.00	17	92600.	0.5	0.5	0.0694	169	91.00	10	17056.	0.1	0.1	0.0128
115	165.00	17	347904.	1.8	1.8	0.2609*	170	89.00	8	3042.	0.0	0.0	0.0023
116	164.00	12	31408.	0.2	0.2	0.0236	171	87.00	8	12810.	0.1	0.1	0.0096
117	163.00	17	86754.	0.4	0.4	0.0651*	172	86.00	17	181832.	0.9	0.9	0.1363*
118	162.00	6	1833.	0.0	0.0	0.0014	173	85.00	29	2710400.	13.7	13.7	2.0323
119	161.00	10	21124.	0.1	0.1	0.0158	174	84.00	29	1385472.	7.0	7.0	1.0389*
120	156.00	10	35038.	0.2	0.2	0.0262	175	83.00	29	3425344.	17.4	17.4	2.5684
121	155.00	14	68888.	0.3	0.3	0.0517*	176	82.00	21	639168.	3.2	3.2	0.4793
122	154.00	14	39018.	0.2	0.2	0.0293*	177	81.00	21	794016.	4.0	4.0	0.5954
123	153.00	17	116340.	0.6	0.6	0.0872*	178	80.00	14	78316.	0.4	0.4	0.0587*
124	152.00	12	75940.	0.4	0.4	0.0569	179	79.00	17	222620.	1.1	1.1	0.1669*
125	151.00	10	21271.	0.1	0.1	0.0159	180	78.00	12	24064.	0.1	0.1	0.0180
126	150.00	8	9057.	0.0	0.0	0.0068*	181	77.00	14	36732.	0.2	0.2	0.0275
127	149.00	12	58996.	0.3	0.3	0.0442	182	75.00	10	17895.	0.1	0.1	0.0134
128	147.00	10	3065.	0.0	0.0	0.0023	183	74.00	8	5062.	0.0	0.0	0.0038
129	144.00	12	40964.	0.2	0.2	0.0307	184	73.00	17	138640.	0.7	0.7	0.1040*
130	142.00	10	15630.	0.1	0.1	0.0117	185	72.00	21	273760.	1.4	1.4	0.2053
131	141.00	17	208748.	1.1	1.1	0.1565*	186	71.00	35	4960512.	25.1	25.1	3.7195*
132	140.00	10	55200.	0.3	0.3	0.0414*	187	70.00	25	1253120.	6.4	6.4	0.9396
133	139.00	21	205868.	1.0	1.0	0.1544	188	69.00	35	6364416.	32.3	32.3	4.7722
134	138.00	17	121328.	0.6	0.6	0.0910*	189	68.00	25	878192.	4.5	4.5	0.6585*
135	137.00	12	71132.	0.4	0.4	0.0533	190	67.00	25	1010400.	5.1	5.1	0.7576
136	136.00	8	6135.	0.0	0.0	0.0046	191	66.00	10	38384.	0.2	0.2	0.0288
137	135.00	17	118580.	0.6	0.6	0.0889*	192	65.00	12	51694.	0.3	0.3	0.0463*
138	133.00	14	57759.	0.3	0.3	0.0433*	193	64.00	17	78700.	0.4	0.4	0.0590*
139	131.00	12	32274.	0.2	0.2	0.0242	194	63.00	10	19378.	0.1	0.1	0.0145
140	129.00	6	1020.	0.0	0.0	0.0008	195	62.00	6	1619.	0.0	0.0	0.0012
141	128.00	8	26228.	0.1	0.1	0.0197	196	61.00	8	14742.	0.1	0.1	0.0111
142	127.00	21	323712.	1.6	1.6	0.2427	197	60.00	14	25969.	0.4	0.4	0.0195*
143	126.00	17	119392.	0.6	0.6	0.0895*	198	59.00	14	83712.	0.4	0.4	0.0628*
144	125.00	17	369008.	1.9	1.9	0.2767	199	58.00	25	546768.	2.8	2.8	0.4100*
145	124.00	17	140240.	0.7	0.7	0.1052	200	57.00	35	10985216.	55.7	55.7	8.2369*
146	123.00	21	210648.	1.1	1.1	0.1579*	201	56.00	29	2264768.	11.5	11.5	1.6982
147	122.00	10	24326.	0.1	0.1	0.0182*	202	55.00	35	9844992.	49.9	49.9	7.3819*
148	121.00	17	144484.	0.7	0.7	0.1083*	203	54.00	21	712656.	3.6	3.6	0.5344
149	120.00	6	1359.	0.0	0.0	0.0010	204	53.00	21	397888.	2.0	2.0	0.2983
150	119.00	17	234144.	1.2	1.2	0.1756	205	52.00	10	19104.	0.1	0.1	0.0143
151	115.00	12	22904.	0.1	0.1	0.0172	206	51.00	25	756944.	3.8	3.8	0.5676
152	114.00	12	38749.	0.2	0.2	0.0291*	207	50.00	10	20803.	0.1	0.1	0.0156
153	113.00	35	834624.	4.2	4.2	0.6258	208	47.00	17	45531.	0.2	0.2	0.0341*
154	112.00	17	318272.	1.6	1.6	0.2386	209	45.00	17	184212.	0.9	0.9	0.1381
155	111.00	25	870032.	4.4	4.4	0.6524	210	44.00	35	835120.	4.2	4.2	0.6262*
156	109.00	17	231692.	1.2	1.2	0.1737	211	43.00	43	19726336.	100.0	100.0	*14.79*
157	109.00	21	339840.	1.7	1.7	0.2548	212	42.00	35	2281792.	11.6	11.6	1.7109
158	108.00	14	34385.	0.2	0.2	0.0258*	213	41.00	35	8802816.	44.6	44.6	6.6005
159	107.00	17	93240.	0.5	0.5	0.0699*	214	40.00	21	244760.	1.2	1.2	0.1835*
160	101.00	6	844.	0.0	0.0	0.0006	215	39.00	29	1085568.	5.5	5.5	0.8140*
161	100.00	21	157188.	0.8	0.8	0.1179*	216	38.00	10	27034.	0.1	0.1	0.0203*
162	99.00	25	756352.	3.8	3.8	0.5671	217	37.00	6	6798.	0.0	0.0	0.0051
163	98.00	25	1111616.	5.6	5.6	0.8335	218	36.00	17	118712.	0.6	0.6	0.0890*
164	97.00	25	2190336.	11.1	11.1	1.6424	219	35.00	8	1506.	0.0	0.0	0.0011
165	96.00	21	562448.	2.9	2.9	0.4217							

CS3278.1 [TIC=1136384, 16.2-222744] EI

5,9,13-trimethyltetradecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	452.00	17	11785.	5.3	5.3	1.0371	56	227.00	17	5386.	2.4	2.4	0.4740
2	458.00	6	1056.	0.5	0.5	0.0929	57	217.00	17	2753.	1.2	1.2	0.2423*
3	459.00	10	1739.	0.8	0.8	0.1530	58	217.00	12	298.	0.1	0.1	0.0262
4	464.00	12	396.	0.2	0.2	0.0348	59	216.00	8	917.	0.4	0.4	0.0807
5	431.00	12	2180.	1.0	1.0	0.1918	60	183.00	14	2762.	1.2	1.2	0.2431
6	428.00	6	653.	0.3	0.3	0.0575	61	183.00	8	2740.	1.2	1.2	0.2411
7	420.00	8	1267.	0.6	0.6	0.1115	62	180.00	17	4791.	2.2	2.2	0.4216
8	419.00	10	2006.	0.9	0.9	0.1765	63	169.00	12	2217.	1.0	1.0	0.1951
9	414.00	10	1927.	0.9	0.9	0.1696	64	168.00	8	6854.	2.7	2.7	0.5327
10	410.00	6	1577.	0.7	0.7	0.1388	65	167.00	17	18492.	8.3	8.3	1.6273
11	409.00	12	8180.	3.7	3.7	0.7198	66	154.00	12	1867.	0.8	0.8	0.1643
12	405.00	12	461.	0.2	0.2	0.0406	67	149.00	21	4502.	2.0	2.0	0.3962
13	395.00	12	1552.	0.7	0.7	0.1366	68	143.00	10	2604.	1.2	1.2	0.2291
14	389.00	10	954.	0.4	0.4	0.0840	69	141.00	17	4580.	2.1	2.1	0.4030
15	383.00	6	1611.	0.7	0.7	0.1418	70	139.00	17	1765.	0.8	0.8	0.1553
16	382.00	6	1834.	0.8	0.8	0.1614	71	130.00	6	1116.	0.5	0.5	0.0982
17	381.00	8	4082.	1.8	1.8	0.3592	72	127.00	21	18564.	8.3	8.3	1.6336
18	367.00	14	9716.	4.4	4.4	0.8550	73	125.00	21	5264.	2.4	2.4	0.4632
19	366.00	8	1708.	0.8	0.8	0.1503	74	116.00	10	317.	0.1	0.1	0.0279
20	356.00	6	1050.	0.5	0.5	0.0924	75	114.00	14	2695.	1.2	1.2	0.2372
21	355.00	12	469.	0.2	0.2	0.0413	76	113.00	35	17918.	8.0	8.0	1.5768
22	353.00	8	1413.	0.6	0.6	0.1243	77	112.00	29	12201.	5.5	5.5	1.0737*
23	352.00	8	675.	0.3	0.3	0.0594	78	111.00	21	5190.	2.3	2.3	0.4567
24	350.00	10	2180.	1.0	1.0	0.1918	79	100.00	12	262.	0.1	0.1	0.0231
25	347.00	8	1722.	0.8	0.8	0.1515	80	99.00	17	4880.	2.2	2.2	0.4294
26	346.00	5	930.	0.4	0.4	0.0818	81	98.00	25	13782.	6.2	6.2	1.2128
27	339.00	12	1976.	0.9	0.9	0.1739	82	97.00	25	40980.	18.4	18.4	3.6062
28	337.00	10	1425.	0.6	0.6	0.1254	83	87.00	6	917.	0.4	0.4	0.0807
29	329.00	8	1328.	0.6	0.6	0.1169	84	86.00	21	6980.	3.1	3.1	0.6142*
30	325.00	12	306.	0.1	0.1	0.0269	85	85.00	25	31212.	14.0	14.0	2.7466
31	322.00	6	854.	0.4	0.4	0.0752	86	84.00	21	7968.	3.6	3.6	0.7012
32	312.00	12	3613.	1.6	1.6	0.3179	87	83.00	29	33852.	15.2	15.2	2.9789
33	311.00	12	1079.	0.5	0.5	0.0950	88	72.00	17	11421.	5.1	5.1	1.0050
34	310.00	14	5757.	2.6	2.6	0.5066	89	71.00	25	137896.	61.9	61.9	*12.13
35	309.00	8	2621.	1.2	1.2	0.2306	90	70.00	35	10323.	4.6	4.6	0.9084
36	308.00	8	974.	0.4	0.4	0.0857	91	69.00	35	74896.	33.6	33.6	6.5907
37	307.00	6	1711.	0.8	0.8	0.1506	92	64.00	6	1546.	0.7	0.7	0.1360
38	298.00	14	4109.	1.8	1.8	0.3616	93	58.00	21	6154.	2.8	2.8	0.5415
39	297.00	17	27896.	12.5	12.5	2.4548	94	57.00	35	222744.	100.0	100.0	*19.60
40	296.00	8	1080.	0.5	0.5	0.0950	95	56.00	25	30658.	13.8	13.8	2.6979
41	295.00	10	1045.	0.5	0.5	0.0920	96	55.00	29	4924.	2.2	2.2	0.4333
42	293.00	12	2365.	1.1	1.1	0.2081	97	54.00	25	6334.	2.8	2.8	0.5574*
43	284.00	8	1131.	0.5	0.5	0.0995	98	50.00	8	543.	0.2	0.2	0.0478
44	270.00	12	1792.	0.8	0.8	0.1577	99	49.00	6	1034.	0.5	0.5	0.0910
45	269.00	17	3233.	1.5	1.5	0.2845	100	45.00	8	816.	0.4	0.4	0.0718
46	268.00	10	464.	0.2	0.2	0.0408	101	44.00	35	655.	0.3	0.3	0.0576*
47	263.00	6	846.	0.4	0.4	0.0744	102	43.00	35	124108.	55.7	55.7	*10.92
48	257.00	8	1417.	0.6	0.6	0.1247	103	41.00	35	28456.	12.8	12.8	2.5041
49	255.00	17	11935.	5.4	5.4	1.0503	104	40.00	17	6049.	2.7	2.7	0.5323
50	253.00	17	8165.	3.7	3.7	0.7185							
51	243.00	14	6159.	2.8	2.8	0.5420							
52	242.00	17	17731.	8.0	8.0	0.0744							
53	235.00	17	1051.	0.5	0.5	0.0925*							
54	234.00	17	5858.	2.6	2.6	0.5155							
55	228.00	6	931.	0.4	0.4	0.0819							

AL14PA.1 [TIC-118489688, 188X-16285824] EI

Heptadecanoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester
 $\text{CH}_3(\text{CH}_2)_{15}\text{COOCH}_2\text{C}_3\text{F}_7$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	455.00	10	4862.	0.0	0.0	0.0044	56	271.00	10	6091.	0.0	0.0	0.0055
2	454.00	17	115536.	0.7	0.7	0.1046	57	270.00	12	91028.	0.6	0.6	0.0024
3	453.00	25	1449216.	8.9	8.9	1.3116*	58	269.00	17	823520.	5.1	5.1	0.7453
4	452.00	35	3583040.	22.1	22.1	3.2429*	59	268.00	6	17545.	0.1	0.1	0.0159
5	451.00	10	17638.	0.1	0.1	0.0160*	60	267.00	8	5078.	0.0	0.0	0.0046
6	450.00	8	929.	0.0	0.0	0.0008	61	266.00	10	15373.	0.1	0.1	0.0139
7	436.00	8	1612.	0.0	0.0	0.0015	62	265.00	8	7180.	0.0	0.0	0.0065
8	435.00	8	3030.	0.0	0.0	0.0027	63	257.00	12	54632.	0.3	0.3	0.0494*
9	434.00	12	49109.	0.3	0.3	0.0444*	64	256.00	17	672304.	4.1	4.1	0.6085*
10	433.00	14	111240.	0.7	0.7	0.1007	65	255.00	51	6074112.	37.5	37.5	5.4975*
11	425.00	8	1574.	0.0	0.0	0.0014	66	254.00	29	1201024.	7.4	7.4	1.0870*
12	424.00	10	31373.	0.2	0.2	0.0284	67	253.00	12	203440.	1.3	1.3	0.1841
13	423.00	12	179856.	1.1	1.1	0.1628	68	252.00	12	19526.	0.1	0.1	0.0177*
14	411.00	8	21580.	0.1	0.1	0.0195	69	250.00	6	666.	0.0	0.0	0.0006
15	410.00	17	174452.	1.1	1.1	0.1579	70	245.00	10	2887.	0.0	0.0	0.0026
16	409.00	17	855632.	5.3	5.3	0.7744*	71	244.00	17	151712.	0.9	0.9	0.1373*
17	397.00	8	6111.	0.0	0.0	0.0055	72	243.00	35	2251648.	13.9	13.9	2.0379*
18	396.00	12	49278.	0.3	0.3	0.0446	73	242.00	35	6251008.	38.6	38.6	5.6576*
19	395.00	12	130740.	0.8	0.8	0.1183	74	241.00	17	201512.	1.2	1.2	0.1024
20	382.00	8	10627.	0.1	0.1	0.0096	75	239.00	8	19421.	0.1	0.1	0.0176
21	381.00	14	82628.	0.5	0.5	0.0748	76	236.00	6	3950.	0.0	0.0	0.0368
22	372.00	10	1027.	0.0	0.0	0.0009	77	235.00	25	135208.	0.8	0.8	0.0036
23	371.00	6	1192.	0.0	0.0	0.0011	78	234.00	25	13032.	0.1	0.1	0.1224*
24	369.00	6	4747.	0.0	0.0	0.0043	79	233.00	25	2800.	0.0	0.0	0.0118*
25	368.00	12	89188.	0.6	0.6	0.0807	80	229.00	8	3154.	0.0	0.0	0.0025
26	367.00	17	482640.	3.0	3.0	0.4368	81	228.00	10	23869.	0.1	0.1	0.0029
27	356.00	6	1508.	0.0	0.0	0.0014	82	227.00	17	404688.	2.5	2.5	0.3663
28	355.00	8	17636.	0.1	0.1	0.0160	83	226.00	6	1950.	0.0	0.0	0.0018
29	354.00	14	130924.	0.8	0.8	0.1185*	84	223.00	8	1289.	0.0	0.0	0.0012
30	353.00	17	537104.	3.3	3.3	0.4861	85	221.00	8	11509.	0.1	0.1	0.0104
31	341.00	8	4485.	0.0	0.0	0.0040	86	219.00	8	1164.	0.0	0.0	0.0011
32	340.00	12	70968.	0.4	0.4	0.0642	87	218.00	6	2865.	0.0	0.0	0.0026
33	339.00	12	109476.	0.7	0.7	0.0991	88	213.00	17	55647.	0.3	0.3	0.0504*
34	334.00	10	35443.	0.2	0.2	0.0321	89	212.00	14	61903.	0.4	0.4	0.0560
35	333.00	12	11272.	0.1	0.1	0.0102	90	211.00	17	91400.	0.6	0.6	0.0827*
36	326.00	10	31855.	0.2	0.2	0.0288	91	210.00	14	50402.	0.3	0.3	0.0456*
37	325.00	14	168388.	1.0	1.0	0.1524	92	209.00	21	159500.	1.0	1.0	0.1444*
38	321.00	8	1726.	0.0	0.0	0.0016	93	208.00	25	186228.	1.1	1.1	0.1685
39	313.00	8	11705.	0.1	0.1	0.0106	94	207.00	17	135288.	0.8	0.8	0.1224
40	312.00	17	226896.	1.4	1.4	0.2054	95	198.00	6	2181.	0.0	0.0	0.0020
41	311.00	21	1648256.	10.2	10.2	1.4918	96	197.00	6	2181.	0.0	0.0	0.0020
42	299.00	10	41174.	0.3	0.3	0.0373	97	196.00	8	4342.	0.0	0.0	0.0039
43	298.00	21	450832.	2.8	2.8	0.4080*	98	195.00	8	4431.	0.0	0.0	0.0040
44	297.00	17	578176.	3.6	3.6	0.5233	99	194.00	6	2381.	0.0	0.0	0.0022
45	295.00	8	2386.	0.0	0.0	0.0022	100	194.00	6	2175.	0.0	0.0	0.0020
46	293.00	6	2789.	0.0	0.0	0.0025	101	191.00	10	12290.	0.1	0.1	0.0111
47	285.00	8	7915.	0.0	0.0	0.0072	102	183.00	12	12487.	0.1	0.1	0.0113*
48	284.00	14	130180.	0.8	0.8	0.1178	103	182.00	10	25528.	0.2	0.2	0.0231
49	283.00	17	246368.	1.5	1.5	0.2230	104	181.00	12	34672.	0.2	0.2	0.0314
50	282.00	10	15837.	0.1	0.1	0.0143	105	180.00	12	34457.	0.2	0.2	0.0312
51	281.00	12	62276.	0.4	0.4	0.0564	106	179.00	8	3929.	0.0	0.0	0.0036
52	280.00	10	26410.	0.2	0.2	0.0239*	107	178.00	12	5929.	0.0	0.0	0.0054
53	279.00	10	14017.	0.1	0.1	0.0127	108	177.00	10	8614.	0.1	0.1	0.0078
54	278.00	10	1837.	0.0	0.0	0.0017	109	170.00	17	17683.	0.1	0.1	0.0160
55	276.00	8	1172.	0.0	0.0	0.0011	110	169.00	14	58190.	0.4	0.4	0.0527*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	168.00	10	21507.	0.1	0.1	0.0195	166	95.00	25	683392.	4.2	4.2	0.6185
112	167.00	12	50767.	0.3	0.3	0.0459	167	94.00	14	77660.	0.5	0.5	0.5703*
113	166.00	14	58821.	0.4	0.4	0.0532	168	93.00	17	115944.	0.7	0.7	0.1049
114	165.00	12	16992.	0.1	0.1	0.0154	169	92.00	6	2209.	0.0	0.0	0.0020
115	164.00	10	8627.	0.1	0.1	0.0078	170	91.00	10	23267.	0.1	0.1	0.0211
116	163.00	10	26228.	0.2	0.2	0.0237*	171	89.00	8	2441.	0.0	0.0	0.0022
117	161.00	8	5447.	0.0	0.0	0.0049	172	87.00	8	3757.	0.0	0.0	0.0034
118	156.00	12	35437.	0.2	0.2	0.0321	173	86.00	17	154672.	1.0	1.0	0.1400
119	155.00	14	110848.	0.7	0.7	0.1003	174	85.00	29	2361664.	14.6	14.6	2.1375
120	154.00	10	38833.	0.2	0.2	0.0351	175	84.00	25	1134976.	7.0	7.0	1.0272
121	153.00	17	92212.	0.6	0.6	0.0835	176	83.00	29	2840128.	17.5	17.5	2.5705
122	152.00	14	77316.	0.5	0.5	0.0700	177	82.00	21	559488.	3.5	3.5	0.5064
123	151.00	10	31188.	0.2	0.2	0.0282	178	81.00	21	670800.	4.1	4.1	0.6071
124	150.00	10	12807.	0.1	0.1	0.0116	179	80.00	17	97988.	0.6	0.6	0.0887
125	149.00	12	53327.	0.3	0.3	0.0483*	180	79.00	17	174444.	1.1	1.1	0.1579
126	147.00	14	4468.	0.0	0.0	0.0040	181	78.00	10	11421.	0.1	0.1	0.0103*
127	145.00	8	1985.	0.0	0.0	0.0018	182	77.00	14	45089.	0.3	0.3	0.0408
128	142.00	10	9120.	0.1	0.1	0.0083	183	75.00	10	24073.	0.1	0.1	0.0218*
129	141.00	21	210440.	1.3	1.3	0.1905*	184	74.00	8	3639.	0.0	0.0	0.0033
130	140.00	14	42322.	0.3	0.3	0.0383	185	73.00	17	125396.	0.8	0.8	0.1135
131	139.00	17	164088.	1.0	1.0	0.1485	186	72.00	21	190444.	1.2	1.2	0.1724
132	138.00	14	72752.	0.4	0.4	0.0658	187	71.00	29	4269312.	26.3	26.3	3.8640
133	137.00	17	74804.	0.5	0.5	0.0677	188	69.00	35	1065216.	6.6	6.6	0.9641
134	136.00	8	9583.	0.1	0.1	0.0087	189	68.00	25	5015064.	31.0	31.0	4.5399*
135	135.00	17	122948.	0.8	0.8	0.1113	190	67.00	21	748304.	4.6	4.6	0.6773
136	134.00	8	1573.	0.0	0.0	0.0014	191	66.00	25	791440.	4.9	4.9	0.7163
137	133.00	10	42712.	0.3	0.3	0.0387	192	66.00	12	38051.	0.2	0.2	0.0344*
138	131.00	10	17752.	0.1	0.1	0.0161	193	65.00	12	30648.	0.2	0.2	0.0277*
139	129.00	6	3213.	0.0	0.0	0.0029	194	64.00	12	59212.	0.4	0.4	0.0536
140	128.00	8	18292.	0.1	0.1	0.0166	195	63.00	14	6921.	0.0	0.0	0.0063*
141	127.00	17	259956.	1.6	1.6	0.2353	196	61.00	10	25391.	0.2	0.2	0.0238*
142	126.00	17	25750.	0.6	0.6	0.0818	197	60.00	12	18637.	0.1	0.1	0.0169*
143	125.00	21	337632.	2.1	2.1	0.3056	198	59.00	17	74040.	0.5	0.5	0.0670
144	124.00	17	121444.	0.7	0.7	0.1099	199	58.00	25	457600.	2.8	2.8	0.4142
145	123.00	17	167824.	1.0	1.0	0.1519	200	57.00	43	9286144.	57.3	57.3	8.4045*
146	122.00	10	25750.	0.2	0.2	0.0233*	201	56.00	29	1852352.	11.4	11.4	1.6765
147	121.00	17	120560.	0.7	0.7	0.1091	202	55.00	35	7958528.	49.1	49.1	7.2030*
148	120.00	6	2581.	0.0	0.0	0.0023	203	54.00	21	595520.	3.7	3.7	0.5390
149	119.00	17	194648.	1.2	1.2	0.1762	204	53.00	21	343312.	2.1	2.1	0.3107
150	115.00	10	2893.	0.0	0.0	0.0026	205	52.00	12	6923.	0.0	0.0	0.0063*
151	114.00	12	27923.	0.2	0.2	0.0253*	206	51.00	21	539440.	3.3	3.3	0.4882
152	113.00	35	628320.	3.5	3.5	0.5687	207	50.00	8	7287.	0.0	0.0	0.0066
153	112.00	21	248556.	1.5	1.5	0.2250	208	49.00	8	1930.	0.0	0.0	0.0017
154	111.00	21	770832.	4.8	4.8	0.6977	209	47.00	8	24971.	0.2	0.2	0.0226
155	110.00	17	194204.	1.2	1.2	0.1758	210	45.00	21	143456.	0.9	0.9	0.1298*
156	109.00	21	276192.	1.7	1.7	0.2500	211	44.00	35	672400.	4.1	4.1	0.6086
157	108.00	10	29151.	0.2	0.2	0.0264*	212	43.00	43	16205824.	100.0	100.0	*14.66*
158	107.00	17	89248.	0.6	0.6	0.0808*	213	42.00	35	1879360.	11.6	11.6	1.7009
159	105.00	6	1582.	0.0	0.0	0.0014	214	41.00	35	7071488.	43.6	43.6	6.4001*
160	101.00	6	1976.	0.0	0.0	0.0018	215	40.00	21	199800.	1.2	1.2	0.1808*
161	100.00	25	108668.	0.7	0.7	0.0984*	216	39.00	25	812400.	5.0	5.0	0.7353*
162	99.00	21	653104.	4.0	4.0	0.5911	217	38.00	12	26945.	0.2	0.2	0.0244*
163	98.00	25	869216.	5.4	5.4	0.7867	218	37.00	6	9360.	0.1	0.1	0.0085
164	97.00	25	2000512.	12.3	12.3	1.8106	219	36.00	17	80984.	0.5	0.5	0.0733*
165	96.00	25	474768.	2.9	2.9	0.4297*							

EXAV18.1 [TIC=186928968, 188X-25798656] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	469.00	8	14203.	0.1	0.1	0.0076	56	298.00	21	739584.	2.9	2.9	0.3957
2	468.00	17	219608.	0.9	0.9	0.1175	57	297.00	21	887584.	3.4	3.4	0.4748
3	467.00	25	1145856.	4.4	4.4	0.6130*	58	296.00	8	3270.	0.0	0.0	0.0017
4	466.00	43	6803456.	26.4	26.4	3.6398*	59	295.00	8	2494.	0.0	0.0	0.0013
5	465.00	14	36066.	0.1	0.1	0.0193*	60	293.00	8	6733.	0.0	0.0	0.0036
6	464.00	6	3810.	0.0	0.0	0.0020	61	292.00	8	1167.	0.0	0.0	0.0006
7	462.00	6	1005.	0.0	0.0	0.0005	62	290.00	8	3715.	0.0	0.0	0.0020
8	451.00	6	965.	0.0	0.0	0.0005	63	289.00	8	1564.	0.0	0.0	0.0008
9	449.00	8	1272.	0.0	0.0	0.0007	64	288.00	6	1964.	0.0	0.0	0.0011
10	448.00	12	57413.	0.2	0.2	0.0307	65	285.00	10	12532.	0.0	0.0	0.0067
11	447.00	14	193744.	0.8	0.8	0.1037	66	284.00	17	210728.	0.8	0.8	0.1127
12	439.00	8	2264.	0.0	0.0	0.0012	67	283.00	17	504640.	2.0	2.0	0.2700
13	438.00	12	64065.	0.2	0.2	0.0343	68	282.00	10	43645.	0.2	0.2	0.2733
14	437.00	17	259508.	1.0	1.0	0.1388	69	281.00	14	110504.	0.4	0.4	0.0591
15	425.00	10	31262.	0.1	0.1	0.0167	70	280.00	12	57897.	0.2	0.2	0.0310
16	424.00	17	340016.	1.3	1.3	0.1823	71	279.00	10	29711.	0.1	0.1	0.0159
17	423.00	21	156454.	6.1	6.1	0.8370	72	271.00	10	11424.	0.0	0.0	0.0061
18	422.00	6	1651.	0.0	0.0	0.0009	73	270.00	17	181356.	0.7	0.7	0.0970
19	411.00	6	2231.	0.0	0.0	0.0012	74	269.00	25	1502784.	5.8	5.8	0.8040
20	410.00	12	86012.	0.3	0.3	0.0464	75	268.00	25	403088.	1.6	1.6	0.2156*
21	409.00	17	283728.	1.1	1.1	0.1518	76	267.00	29	1946496.	7.5	7.5	1.0413*
22	401.00	6	2064.	0.0	0.0	0.0011	77	266.00	17	73328.	0.3	0.3	0.0392*
23	396.00	8	39768.	0.2	0.2	0.0213	78	265.00	10	31223.	0.1	0.1	0.0167*
24	395.00	14	148100.	0.6	0.6	0.0792	79	260.00	6	10085.	0.0	0.0	0.0006
25	385.00	6	3740.	0.0	0.0	0.0020	80	258.00	6	1821.	0.0	0.0	0.0010
26	384.00	6	594.	0.0	0.0	0.0003	81	257.00	14	87635.	0.3	0.3	0.0469
27	383.00	8	6049.	0.0	0.0	0.0032	82	256.00	25	1197760.	4.6	4.6	0.6400*
28	382.00	12	70724.	0.3	0.3	0.0378	83	255.00	43	10017280.	38.8	38.8	5.3591*
29	381.00	17	430480.	1.7	1.7	0.2303	84	254.00	12	16106.	0.1	0.1	0.0086*
30	369.00	8	20025.	0.1	0.1	0.0107	85	253.00	12	78948.	0.3	0.3	0.0422
31	368.00	17	223240.	0.9	0.9	0.1194	86	252.00	8	21501.	0.1	0.1	0.0115
32	367.00	21	1102784.	4.6	4.6	0.6328	87	249.00	12	32971.	0.1	0.1	0.0176*
33	366.00	8	3115.	0.0	0.0	0.0017	88	248.00	17	103928.	0.4	0.4	0.0556
34	360.00	6	1324.	0.0	0.0	0.0007	89	247.00	6	1619.	0.0	0.0	0.0009
35	359.00	6	1658.	0.0	0.0	0.0009	90	245.00	10	15412.	0.1	0.1	0.0082
36	356.00	6	1637.	0.0	0.0	0.0009	91	244.00	17	263152.	1.0	1.0	0.1400*
37	355.00	10	45929.	0.2	0.2	0.0246	92	243.00	35	4326912.	16.8	16.8	2.3148*
38	354.00	14	173284.	0.7	0.7	0.0927	93	242.00	43	11002496.	43.0	43.0	5.9290*
39	353.00	17	476000.	1.8	1.8	0.2547	94	241.00	21	371664.	1.4	1.4	0.1988*
40	349.00	6	1337.	0.0	0.0	0.0007	95	240.00	12	40838.	0.2	0.2	0.0218
41	348.00	6	10118.	0.0	0.0	0.0054	96	239.00	12	59772.	0.2	0.2	0.0320
42	347.00	12	76288.	0.3	0.3	0.0408	97	236.00	10	5330.	0.0	0.0	0.0029
43	343.00	8	983.	0.0	0.0	0.0005	98	235.00	17	101724.	0.4	0.4	0.0544*
44	341.00	8	7677.	0.0	0.0	0.0041	99	234.00	6	1552.	0.0	0.0	0.0008
45	340.00	12	91560.	0.4	0.4	0.0490	100	229.00	8	4909.	0.0	0.0	0.0026
46	339.00	14	190012.	0.7	0.7	0.1017	101	228.00	12	35439.	0.1	0.1	0.0190
47	327.00	6	1866.	0.0	0.0	0.0010	102	227.00	21	741904.	2.9	2.9	0.3969
48	326.00	12	85924.	0.3	0.3	0.0460	103	226.00	10	25716.	0.1	0.1	0.0138
49	325.00	17	400192.	1.6	1.6	0.2141	104	225.00	17	154304.	0.6	0.6	0.0826
50	314.00	8	3001.	0.0	0.0	0.0020	105	224.00	17	120180.	0.5	0.5	0.0643*
51	313.00	12	49524.	0.2	0.2	0.0265	106	223.00	17	99776.	0.4	0.4	0.0534*
52	312.00	21	512272.	2.0	2.0	0.2741*	107	222.00	21	441024.	1.7	1.7	0.2359
53	311.00	23	3006592.	11.7	11.7	1.6085*	108	221.00	12	10414.	0.0	0.0	0.0056*
54	310.00	6	1004.	0.0	0.0	0.0005	109	220.00	8	4434.	0.0	0.0	0.0024
55	299.00	14	81228.	0.3	0.3	0.0435	110	219.00	10	2287.	0.0	0.0	0.0012

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	213.00	17	90648.	0.4	0.4	0.485	166	125.00	25	618256.	2.4	2.4	0.3308
112	211.00	8	2165.	0.0	0.0	0.0012	167	124.00	21	197228.	0.8	0.8	0.1055*
113	209.00	21	87452.	0.3	0.3	0.0468*	168	123.00	25	302880.	1.2	1.2	0.1620
114	209.00	17	82952.	0.3	0.3	0.0444*	169	122.00	14	53357.	0.2	0.2	0.0285*
115	207.00	21	314944.	1.2	1.2	0.1685*	170	121.00	21	197176.	0.8	0.8	0.1055*
116	205.00	8	5284.	0.0	0.0	0.0028	171	120.00	6	1189.	0.0	0.0	0.0006
117	197.00	8	1256.	0.0	0.0	0.0007	172	119.00	21	254976.	1.0	1.0	0.1364
118	196.00	12	43751.	0.2	0.2	0.0234	173	114.00	12	58297.	0.2	0.2	0.0312*
119	195.00	10	22202.	0.1	0.1	0.0119	174	113.00	35	1017696.	3.9	3.9	0.5445
120	194.00	12	57334.	0.2	0.2	0.0307	175	112.00	21	433840.	1.7	1.7	0.2321
121	193.00	14	23325.	0.1	0.1	0.0125*	176	111.00	29	1362816.	5.3	5.3	0.7291
122	191.00	12	45106.	0.2	0.2	0.0241*	177	110.00	21	366336.	1.4	1.4	0.1960
123	190.00	6	682.	0.0	0.0	0.0004	178	109.00	25	447168.	1.7	1.7	0.2332
124	184.00	6	1587.	0.0	0.0	0.0008	179	108.00	14	52732.	0.2	0.2	0.0282
125	183.00	17	80516.	0.3	0.3	0.0431*	180	107.00	17	157244.	0.6	0.6	0.0841
126	182.00	14	26656.	0.1	0.1	0.0143	181	105.00	8	5821.	0.0	0.0	0.0036
127	181.00	14	71828.	0.3	0.3	0.0384	182	101.00	6	2879.	0.0	0.0	0.0015
128	180.00	17	140944.	0.5	0.5	0.0754	183	99.00	25	203848.	0.8	0.8	0.1091*
129	179.00	8	13624.	0.1	0.1	0.0073	184	98.00	25	1176256.	4.6	4.6	0.6293
130	177.00	10	30366.	0.1	0.1	0.0162*	185	98.00	25	1506672.	5.8	5.8	0.8071
131	172.00	8	2891.	0.0	0.0	0.0015	186	97.00	29	3451456.	13.4	13.4	1.8465
132	170.00	8	4594.	0.0	0.0	0.0025	187	96.00	29	879744.	3.4	3.4	0.4707*
133	169.00	21	153636.	0.6	0.6	0.0822*	188	95.00	29	1217856.	4.7	4.7	0.6515
134	168.00	12	45221.	0.2	0.2	0.0242	189	94.00	17	123224.	0.5	0.5	0.0659*
135	167.00	17	106052.	0.4	0.4	0.0567*	190	93.00	21	194120.	0.8	0.8	0.1039*
136	166.00	17	116736.	0.5	0.5	0.0625	191	92.00	6	2289.	0.0	0.0	0.0012
137	165.00	12	30860.	0.1	0.1	0.0165*	192	91.00	12	50319.	0.2	0.2	0.0269
138	164.00	6	1782.	0.0	0.0	0.0010	193	89.00	10	5312.	0.0	0.0	0.0028
139	163.00	14	58876.	0.2	0.2	0.0315*	194	87.00	10	9234.	0.0	0.0	0.0049*
140	161.00	10	13267.	0.1	0.1	0.0071	195	86.00	31	258776.	1.0	1.0	0.1384
141	158.00	8	1864.	0.0	0.0	0.0010	196	85.00	35	4207616.	16.3	16.3	2.2510*
142	156.00	8	8340.	0.0	0.0	0.0045	197	84.00	35	1946432.	7.5	7.5	1.0413
143	155.00	17	229884.	0.9	0.9	0.1230	198	83.00	35	4865280.	18.9	18.9	2.5029
144	154.00	14	80284.	0.3	0.3	0.0430	199	82.00	25	963568.	3.7	3.7	0.5155
145	153.00	17	151300.	0.6	0.6	0.0809*	200	81.00	29	1128064.	4.4	4.4	0.6035
146	152.00	17	87436.	0.3	0.3	0.0468	201	80.00	21	140424.	0.5	0.5	0.0751*
147	151.00	12	42157.	0.2	0.2	0.0226*	202	79.00	21	280496.	1.1	1.1	0.1501
148	150.00	10	11525.	0.0	0.0	0.0062*	203	78.00	12	26538.	0.1	0.1	0.0142
149	149.00	17	105088.	0.4	0.4	0.0562	204	77.00	17	84596.	0.3	0.3	0.0453*
150	147.00	10	17272.	0.1	0.1	0.0139	205	75.00	10	15915.	0.1	0.1	0.0085
151	142.00	12	25965.	0.1	0.1	0.0092*	206	74.00	8	5769.	0.0	0.0	0.0031
152	141.00	21	326112.	1.3	1.3	0.1745*	207	73.00	21	191488.	0.7	0.7	0.1024*
153	139.00	17	105112.	0.4	0.4	0.0562	208	72.00	25	385456.	1.5	1.5	0.2062*
154	138.00	21	318576.	1.2	1.2	0.1704	209	71.00	35	7485952.	29.0	29.0	4.0049
155	138.00	17	115480.	0.4	0.4	0.0618	210	70.00	29	1742912.	6.8	6.8	0.9324*
156	137.00	17	121804.	0.5	0.5	0.0652	211	69.00	35	8439040.	32.7	32.7	4.5148*
157	136.00	10	39076.	0.2	0.2	0.0209*	212	68.00	29	1254016.	4.9	4.9	0.6709*
158	135.00	21	216724.	0.8	0.8	0.1159	213	67.00	25	1307328.	5.1	5.1	0.6994
159	134.00	6	1775.	0.0	0.0	0.0009	214	66.00	14	68672.	0.3	0.3	0.0367*
160	133.00	14	77160.	0.3	0.3	0.0413*	215	65.00	17	100844.	0.4	0.4	0.0540*
161	132.00	6	1495.	0.0	0.0	0.0008	216	64.00	17	95096.	0.4	0.4	0.0509*
162	131.00	12	21119.	0.1	0.1	0.0113	217	63.00	12	4748.	0.0	0.0	0.0025
163	128.00	12	28615.	0.1	0.1	0.0153	218	62.00	6	1567.	0.0	0.0	0.0008
164	127.00	21	437456.	1.7	1.7	0.2340*	219	61.00	10	44781.	0.2	0.2	0.0240
165	126.00	21	171640.	0.7	0.7	0.0918*	220	60.00	10	27811.	0.1	0.1	0.0149

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
221	59.00	17	127164.	0.5	0.5	0.0680*
222	58.00	29	766400.	3.0	3.0	0.4100
223	57.00	43	15936256.	61.8	61.8	8.5257*
224	56.00	35	2991296.	11.6	11.6	1.6003
225	55.00	43	13051648.	50.6	50.6	6.9824
226	54.00	25	900144.	3.5	3.5	0.4816
227	53.00	25	545792.	2.1	2.1	0.2920
228	52.00	8	12397.	0.0	0.0	0.0066
229	51.00	29	817248.	3.2	3.2	0.4372
230	50.00	8	24063.	0.1	0.1	0.0129
231	49.00	8	2653.	0.0	0.0	0.0014
232	47.00	14	42574.	0.2	0.2	0.0228*
233	46.00	6	1416.	0.0	0.0	0.0008
234	45.00	21	210048.	0.8	0.8	0.1128*
235	44.00	35	1053504.	4.1	4.1	0.5636
236	43.00	51	25798556.	100.0	100.0	*13.80*
237	42.00	35	3046400.	11.8	11.8	1.6298
238	41.00	35	11140864.	43.2	43.2	5.9602*
239	40.00	21	310944.	1.2	1.2	0.1664*
240	39.00	29	1295744.	5.0	5.0	0.6932
241	38.00	21	90468.	0.4	0.4	0.0484*
242	37.00	6	7415.	0.0	0.0	0.0040
243	36.00	25	180112.	0.7	0.7	0.1006*
244	35.00	10	9357.	0.0	0.0	0.0050

$$\text{CH}_3\text{---}\underset{\text{CH}_3}{\overset{|}{\text{CH}}}\text{---}(\text{CH}_2)_3\text{---}\underset{\text{CH}_3}{\overset{|}{\text{CH}}}\text{---}(\text{CH}_2)_3\text{---}\underset{\text{CH}_3}{\overset{|}{\text{CH}}} \parallel \text{O}$$

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	481.00	12	4168.	1.6	1.6	0.2958	56	225.00	14	2071.	0.8	0.8	0.1470*
2	480.00	14	10309.	3.9	3.9	0.7315	57	224.00	6	721.	0.3	0.3	0.0512
3	472.00	10	2009.	0.8	0.8	0.1426	58	223.00	21	11847.	4.5	4.5	0.8407
4	465.00	12	4009.	1.5	1.5	0.2845	59	222.00	17	54119.	20.5	20.5	3.8404
5	449.00	6	1641.	0.6	0.6	0.1164	60	213.00	14	2468.	0.9	0.9	0.1751
6	442.00	8	262.	0.1	0.1	0.0186	61	210.00	8	793.	0.3	0.3	0.0563
7	435.00	6	599.	0.2	0.2	0.0425	62	197.00	14	2784.	1.1	1.1	0.1976
8	432.00	6	195.	0.1	0.1	0.0138	63	196.00	17	6937.	2.6	2.6	0.4923
9	425.00	10	1957.	0.7	0.7	0.1389	64	195.00	17	10661.	4.0	4.0	0.7585
10	423.00	8	1088.	0.4	0.4	0.0772	65	184.00	17	869.	0.3	0.3	0.0617
11	421.00	6	1179.	0.4	0.4	0.0745	66	181.00	17	8035.	3.0	3.0	0.5702
12	415.00	6	1179.	0.4	0.4	0.0837	67	173.00	8	1635.	0.6	0.6	0.1160
13	408.00	6	885.	0.3	0.3	0.0628	68	170.00	14	1910.	0.7	0.7	0.1355*
14	406.00	8	888.	0.3	0.3	0.0630	69	168.00	17	2034.	0.8	0.8	0.1443
15	402.00	10	1321.	0.5	0.5	0.0937	70	167.00	17	1381.	0.5	0.5	0.0980
16	401.00	6	1322.	0.5	0.5	0.0938	71	156.00	8	1591.	0.6	0.6	0.1129
17	395.00	8	164.	0.1	0.1	0.0116	72	154.00	10	1023.	0.4	0.4	0.0726
18	389.00	10	291.	0.1	0.1	0.0206	73	153.00	21	4643.	1.8	1.8	0.3295
19	381.00	12	2114.	0.8	0.8	0.1500	74	141.00	21	4604.	1.7	1.7	0.3267
20	366.00	8	991.	0.4	0.4	0.0703	75	139.00	17	469.	0.2	0.2	0.0933
21	364.00	6	1042.	0.4	0.4	0.0739	76	138.00	21	7440.	2.8	2.8	0.5280
22	361.00	12	1205.	0.5	0.5	0.0855	77	128.00	10	1057.	0.4	0.4	0.0750
23	351.00	10	148.	0.3	0.3	0.0185	78	127.00	21	1696.	0.6	0.6	0.1204
24	348.00	10	854.	0.7	0.7	0.0606	79	126.00	17	10628.	4.0	4.0	0.7542
25	325.00	17	1836.	0.6	0.6	0.1110	80	125.00	17	3309.	1.3	1.3	0.2348
26	326.00	6	1564.	0.3	0.3	0.0500	81	115.00	21	12064.	4.6	4.6	0.8561
27	339.00	6	704.	0.8	0.8	0.1481	82	114.00	10	1108.	0.4	0.4	0.0786
28	325.00	17	2087.	0.8	0.8	0.1481	83	113.00	12	3452.	1.3	1.3	0.2450
29	322.00	6	10084.	3.8	3.8	0.7156	84	112.00	25	822.	0.3	0.3	0.0583
30	307.00	10	436.	0.2	0.2	0.0309	85	111.00	21	9603.	3.6	3.6	0.6814
31	298.00	6	1428.	0.5	0.5	0.1013	86	110.00	21	1.	0.0	0.0	0.0001
32	297.00	17	4107.	1.6	1.6	0.2914	87	100.00	21	8291.	3.1	3.1	0.5883
33	279.00	10	10719.	4.1	4.1	0.7686	88	99.00	17	741.	0.3	0.3	0.0526*
34	270.00	12	446.	0.2	0.2	0.0316	89	97.00	25	7207.	2.7	2.7	0.5114
35	269.00	17	2987.	1.1	1.1	0.2120	90	86.00	43	65808.	24.9	24.9	4.6698*
36	268.00	12	20342.	7.7	7.7	0.0869	91	85.00	17	5703.	2.2	2.2	0.4047
37	266.00	6	1225.	0.5	0.5	0.0869	92	83.00	25	54565.	20.7	20.7	3.8720
38	264.00	10	1812.	0.7	0.7	0.1286	93	83.00	29	9280.	3.5	3.5	0.6585
39	264.00	6	1606.	0.6	0.6	0.1140	94	72.00	21	14944.	5.7	5.7	1.0604
40	263.00	14	5909.	2.2	2.2	0.4193	95	71.00	29	147404.	55.9	55.9	*10.46
41	262.00	6	1563.	0.6	0.6	0.1109	96	69.00	35	28968.	11.0	11.0	2.0556
42	261.00	8	1423.	0.5	0.5	0.1010	97	64.00	6	1685.	0.6	0.6	0.1196
43	258.00	8	3053.	1.2	1.2	0.2166	98	63.00	6	1240.	0.5	0.5	0.0880
44	257.00	17	16060.	6.1	6.1	0.2166	99	59.00	17	3239.	1.2	1.2	0.2298
45	256.00	25	161832.	61.3	61.3	*1.1396	100	58.00	35	9595.	3.6	3.6	0.6809
46	255.00	21	2357.	0.9	0.9	*1.148	101	57.00	35	263872.	100.0	100.0	*18.72*
47	250.00	6	1482.	0.6	0.6	0.1673	102	56.00	25	49039.	18.6	18.6	3.4799
48	248.00	6	17.	0.0	0.0	0.1052	103	55.00	29	22676.	8.6	8.6	1.6091
49	245.00	10	153.	0.1	0.1	0.0812	104	45.00	21	2308.	0.9	0.9	0.1695
50	241.00	14	2273.	0.9	0.9	0.1613	105	43.00	35	130040.	49.3	49.3	9.2278
51	238.00	6	484.	0.2	0.2	0.0343	106	42.00	35	32596.	12.4	12.4	2.3131*
52	231.00	14	23.	0.0	0.0	0.0816	107	41.00	29	61824.	23.4	23.4	4.3871
53	228.00	6	422.	0.2	0.2	0.0299							
54	227.00	14	11229.	4.3	4.3	0.7968							
55	226.00	6	573.	0.2	0.2	0.0407							

EXAV11.1 [TIC-143385488, 188X-19574784] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	70.00	25	1335168.	6.8	6.8	0.9312
222	69.00	35	6173696.	31.5	31.5	4.3058*
223	68.00	25	928784.	4.7	4.7	0.6478
224	67.00	25	967952.	4.9	4.9	0.6751
225	66.00	14	46463.	0.2	0.2	0.0324*
226	65.00	17	80792.	0.4	0.4	0.0563
227	64.00	17	70612.	0.4	0.4	0.0492*
228	63.00	6	5561.	0.0	0.0	0.0039
229	62.00	8	1453.	0.0	0.0	0.0010
230	61.00	14	44006.	0.2	0.2	0.0307*
231	60.00	10	24017.	0.1	0.1	0.0168
232	59.00	17	106824.	0.5	0.5	0.0745*
233	58.00	29	612736.	3.1	3.1	0.4273
234	57.00	43	12136704.	62.0	62.0	8.4647*
235	56.00	35	2341632.	12.0	12.0	1.6332
236	55.00	35	9408768.	48.1	48.1	6.5621
237	54.00	25	751152.	3.8	3.8	0.5239*
238	53.00	25	370784.	1.9	1.9	0.2586*
239	52.00	12	19877.	0.1	0.1	0.0139
240	51.00	25	561744.	2.9	2.9	0.3918*
241	50.00	10	10222.	0.1	0.1	0.0071
242	49.00	6	916.	0.0	0.0	0.0006
243	47.00	17	50536.	0.3	0.3	0.0352*
244	45.00	25	141316.	0.7	0.7	0.0986*
245	44.00	35	833008.	4.3	4.3	0.5810*
246	43.00	51	19574784.	100.0	100.0	*13.65*
247	42.00	35	2172544.	11.1	11.1	1.5152
248	41.00	35	8360960.	42.7	42.7	5.8313*
249	40.00	25	205512.	1.0	1.0	0.1433
250	39.00	35	933104.	4.8	4.8	0.6508*
251	38.00	12	42100.	0.2	0.2	0.0294*
252	37.00	10	18366.	0.1	0.1	0.0128*
253	36.00	21	127388.	0.7	0.7	0.0888*
254	35.00	10	10835.	0.1	0.1	0.0076

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	220.00	6	1798.	0.0	0.0	0.0013	166	140.00	17	88620.	0.5	0.5	0.0618*
112	219.00	14	5504.	0.0	0.0	0.0038*	167	139.00	21	278784.	1.4	1.4	0.1944*
113	213.00	12	64744.	0.3	0.3	0.0452	168	138.00	17	106908.	0.5	0.5	0.0746*
114	211.00	6	1814.	0.0	0.0	0.0013	169	137.00	17	104620.	0.5	0.5	0.0730
115	210.00	10	38077.	0.2	0.2	0.0266	170	136.00	12	40055.	0.2	0.2	0.0279
116	209.00	17	71912.	0.4	0.4	0.0502*	171	135.00	21	179108.	0.9	0.9	0.1249
117	208.00	17	110644.	0.6	0.6	0.0772	172	134.00	6	2035.	0.0	0.0	0.0014
118	207.00	21	454384.	2.3	2.3	0.3169	173	133.00	17	89084.	0.5	0.5	0.0621*
119	204.00	6	2276.	0.0	0.0	0.0016	174	131.00	12	14930.	0.1	0.1	0.0104
120	203.00	8	1229.	0.0	0.0	0.0009	175	128.00	12	26009.	0.1	0.1	0.0181*
121	202.00	10	2296.	0.0	0.0	0.0016	176	127.00	21	339648.	1.7	1.7	0.2369
122	201.00	6	1429.	0.0	0.0	0.0010	177	126.00	17	153356.	0.8	0.8	0.1070
123	198.00	6	1648.	0.0	0.0	0.0011	178	125.00	25	570752.	2.9	2.9	0.3981
124	197.00	12	33416.	0.2	0.2	0.0233*	179	124.00	17	190420.	1.0	1.0	0.1328
125	196.00	8	22861.	0.1	0.1	0.0159	180	123.00	21	218472.	1.1	1.1	0.1524
126	195.00	14	42220.	0.2	0.2	0.0294	181	122.00	17	57577.	0.3	0.3	0.0402*
127	194.00	17	104176.	0.5	0.5	0.0727	182	121.00	17	171064.	0.9	0.9	0.1193
128	193.00	10	29854.	0.2	0.2	0.0208	183	119.00	6	190252.	0.0	0.0	0.0007
129	192.00	8	3111.	0.0	0.0	0.0022	184	118.00	21	3756.	0.0	0.0	0.0026
130	191.00	14	38718.	0.2	0.2	0.0270*	185	115.00	6	36370.	0.2	0.2	0.0254*
131	189.00	6	956.	0.0	0.0	0.0007	186	114.00	17	807936.	4.1	4.1	0.5635*
132	187.00	8	1730.	0.0	0.0	0.0012	187	113.00	35	318272.	1.6	1.6	0.2220
133	185.00	8	1175.	0.0	0.0	0.0008	188	112.00	25	112280.	5.7	5.7	0.7831
134	184.00	8	4957.	0.0	0.0	0.0035	189	111.00	25	297360.	1.5	1.5	0.2074*
135	183.00	17	109048.	0.6	0.6	0.0761*	190	110.00	21	335200.	1.7	1.7	0.2338
136	182.00	10	26966.	0.1	0.1	0.0188	191	109.00	21	52037.	0.3	0.3	0.0363*
137	181.00	17	74088.	0.4	0.4	0.0517*	192	108.00	17	136560.	0.7	0.7	0.0952
138	180.00	17	72012.	0.4	0.4	0.0502	193	107.00	21	14996.	0.1	0.1	0.0105
139	179.00	10	13396.	0.1	0.1	0.0093	194	105.00	10	2604.	0.0	0.0	0.0018
140	177.00	12	31020.	0.2	0.2	0.0216	195	103.00	8	135408.	0.7	0.7	0.0944*
141	176.00	6	1515.	0.0	0.0	0.0011	196	100.00	25	867776.	4.4	4.4	0.6052
142	174.00	6	1813.	0.0	0.0	0.0013	197	99.00	25	1173760.	6.0	6.0	0.8186
143	170.00	6	1828.	0.0	0.0	0.0013	198	98.00	29	2682112.	13.7	13.7	1.8706
144	169.00	17	137724.	0.7	0.7	0.0961	199	97.00	35	684000.	3.5	3.5	0.4771*
145	168.00	14	47108.	0.2	0.2	0.0329	200	96.00	35	885376.	4.5	4.5	0.6175
146	167.00	17	90100.	0.5	0.5	0.0628	201	95.00	35	91936.	0.5	0.5	0.0641*
147	166.00	14	57905.	0.3	0.3	0.0404*	202	94.00	17	153880.	0.8	0.8	0.1073
148	165.00	8	17518.	0.1	0.1	0.0122*	203	93.00	17	23286.	0.1	0.1	0.0162
149	164.00	10	1971.	0.0	0.0	0.0014	204	91.00	12	7561.	0.0	0.0	0.0053
150	163.00	14	52760.	0.3	0.3	0.0368*	205	87.00	8	206472.	1.1	1.1	0.1440
151	161.00	8	10743.	0.1	0.1	0.0075	206	86.00	21	3208832.	16.4	16.4	2.2380*
152	158.00	6	1891.	0.0	0.0	0.0013	207	85.00	35	1474752.	7.5	7.5	1.0286
153	156.00	10	11120.	0.1	0.1	0.0078	208	84.00	35	3582784.	18.3	18.3	2.4988
154	155.00	21	194596.	1.0	1.0	0.1357*	209	83.00	35	714736.	3.7	3.7	0.4985
155	154.00	17	71332.	0.4	0.4	0.0498	210	82.00	25	812528.	4.2	4.2	0.5667
156	153.00	17	141084.	0.7	0.7	0.0984	211	81.00	25	110112.	0.6	0.6	0.0768*
157	152.00	14	75172.	0.4	0.4	0.0524	212	80.00	17	201356.	1.0	1.0	0.1404*
158	151.00	14	48257.	0.2	0.2	0.0337*	213	79.00	21	18180.	0.1	0.1	0.0127*
159	150.00	8	11843.	0.1	0.1	0.0083	214	78.00	12	63969.	0.3	0.3	0.0446
160	149.00	17	91832.	0.5	0.5	0.0640	215	77.00	14	15976.	0.1	0.1	0.0111
161	148.00	6	2740.	0.0	0.0	0.0019	216	75.00	14	11288.	0.1	0.1	0.0079
162	147.00	17	22193.	0.1	0.1	0.0155*	217	74.00	10	209480.	1.1	1.1	0.1461
163	145.00	6	954.	0.0	0.0	0.0007	218	73.00	21	266800.	1.4	1.4	0.1856
164	142.00	10	17904.	0.1	0.1	0.0125	219	72.00	21	5769472.	29.5	29.5	4.0239
165	141.00	21	263760.	1.3	1.3	0.1840	220	71.00	35

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	495.00	12	2092.	0.4	0.4	0.0759	56	298.00	10	2642.	0.6	0.6	0.0958
2	494.00	14	10115.	2.1	2.1	0.3670	57	297.00	17	4459.	0.9	0.9	0.1621
3	493.00	8	1740.	0.4	0.4	0.0631	58	295.00	17	3922.	0.8	0.8	0.1423
4	492.00	8	1977.	0.4	0.4	0.0717	59	294.00	14	3977.	0.8	0.8	0.1443
5	490.00	6	111.	0.0	0.0	0.0040	60	293.00	17	6192.	1.3	1.3	0.2246
6	479.00	8	2179.	0.5	0.5	0.0791	61	284.00	8	1198.	0.2	0.2	0.0435
7	478.00	8	992.	0.2	0.2	0.0360	62	283.00	17	7644.	1.6	1.6	0.2773
8	477.00	12	3733.	0.8	0.8	0.1354	63	280.00	12	4906.	1.0	1.0	0.1780
9	476.00	14	7734.	1.6	1.6	0.2806	64	279.00	17	1453.	0.3	0.3	0.0527*
10	472.00	12	1547.	0.3	0.3	0.0561	65	277.00	14	6857.	1.4	1.4	0.2480
11	467.00	8	1769.	0.4	0.4	0.0642	66	276.00	14	6920.	1.4	1.4	0.2510
12	466.00	17	7390.	1.5	1.5	0.2681	67	273.00	10	331.	0.1	0.1	0.0120
13	465.00	8	1769.	0.4	0.4	0.0642	68	271.00	8	2272.	0.5	0.5	0.0824
14	464.00	6	699.	0.1	0.1	0.0254	69	270.00	21	9910.	2.1	2.1	0.3595
15	456.00	6	595.	0.1	0.1	0.0216	70	269.00	21	125772.	26.2	26.2	4.5628
16	455.00	6	735.	0.2	0.2	0.0267	71	267.00	10	2918.	0.6	0.6	0.1059
17	453.00	8	865.	0.2	0.2	0.0314	72	266.00	17	3871.	0.8	0.8	0.1404*
18	451.00	8	1361.	0.3	0.3	0.0494	73	264.00	6	733.	0.2	0.2	0.0266
19	439.00	6	167.	0.0	0.0	0.0061	74	261.00	10	2905.	0.6	0.6	0.1054
20	434.00	6	1510.	0.3	0.3	0.0548	75	259.00	10	264.	0.1	0.1	0.0096
21	429.00	8	265.	0.1	0.1	0.0096	76	257.00	17	538.	0.1	0.1	0.0195*
22	427.00	6	269.	0.1	0.1	0.0098	77	255.00	21	4051.	0.8	0.8	0.1470
23	425.00	8	2135.	0.4	0.4	0.0775	78	254.00	6	630.	0.1	0.1	0.0229
24	424.00	8	727.	0.2	0.2	0.0264	79	253.00	17	4221.	0.9	0.9	0.1531
25	423.00	10	3220.	0.7	0.7	0.1168	80	252.00	14	4165.	0.9	0.9	0.1511
26	420.00	6	708.	0.1	0.1	0.0257	81	251.00	17	5659.	1.2	1.2	0.2053
27	415.00	10	1941.	0.4	0.4	0.0704	82	250.00	17	20711.	4.3	4.3	0.7514
28	410.00	10	4368.	0.9	0.9	0.1585	83	243.00	17	9490.	2.0	2.0	0.3443
29	409.00	14	6626.	1.4	1.4	0.2404	84	242.00	25	22684.	4.7	4.7	0.8229*
30	404.00	12	606.	0.1	0.1	0.0220	85	241.00	17	9451.	2.0	2.0	0.3429
31	401.00	6	992.	0.2	0.2	0.0360	86	229.00	8	1767.	0.4	0.4	0.0641
32	395.00	6	1942.	0.4	0.4	0.0705	87	227.00	21	7825.	1.6	1.6	0.2839
33	393.00	6	791.	0.2	0.2	0.0287	88	226.00	14	3274.	0.7	0.7	0.1188*
34	390.00	10	938.	0.2	0.2	0.0340	89	225.00	12	1778.	0.4	0.4	0.0645*
35	389.00	12	62.	0.0	0.0	0.0022	90	223.00	14	2040.	0.4	0.4	0.0740
36	381.00	12	6507.	1.4	1.4	0.2361	91	212.00	6	1676.	0.3	0.3	0.0608
37	375.00	14	1665.	0.3	0.3	0.0604	92	209.00	25	9220.	1.9	1.9	0.3345
38	367.00	8	2641.	0.6	0.6	0.0958	93	199.00	17	5560.	1.2	1.2	0.2017
39	365.00	12	643.	0.1	0.1	0.0233	94	197.00	17	4166.	0.9	0.9	0.1511
40	364.00	12	1165.	0.2	0.2	0.0423	95	196.00	8	2127.	0.4	0.4	0.0772
41	357.00	6	903.	0.2	0.2	0.0328	96	195.00	14	1569.	0.3	0.3	0.0569
42	353.00	12	1961.	0.4	0.4	0.0711	97	194.00	17	3345.	0.7	0.7	0.1214
43	351.00	12	1069.	0.2	0.2	0.0388	98	186.00	8	1416.	0.3	0.3	0.0514
44	341.00	10	1401.	0.3	0.3	0.0508	99	185.00	17	2283.	0.5	0.5	0.0828
45	340.00	12	5719.	1.2	1.2	0.2075	100	184.00	17	3903.	0.8	0.8	0.1416
46	339.00	17	20258.	4.2	4.2	0.7349	101	183.00	21	7504.	1.6	1.6	0.2722
47	338.00	6	333.	0.1	0.1	0.0121	102	182.00	14	3977.	0.8	0.8	0.1443
48	336.00	8	620.	0.1	0.1	0.0225	103	181.00	21	2875.	0.6	0.6	0.1043
49	335.00	12	2535.	0.5	0.5	0.0920	104	180.00	12	716.	0.1	0.1	0.0260
50	326.00	8	1407.	0.3	0.3	0.0510	105	171.00	21	748.	0.2	0.2	0.0821
51	325.00	17	939.	0.2	0.2	0.0341	106	170.00	6	778.	0.2	0.2	0.0282
52	319.00	6	323.	0.1	0.1	0.0117	107	168.00	14	6240.	1.3	1.3	0.2264
53	312.00	12	4435.	0.9	0.9	0.1609	108	167.00	21	11401.	2.4	2.4	0.4136
54	311.00	17	11148.	2.3	2.3	0.4044	109	160.00	8	770.	0.2	0.2	0.0279
55	306.00	8	1231.	0.3	0.3	0.0447	110	159.00	17	278.	0.1	0.1	0.0101

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	156.00	12	1318.	0.3	0.3	0.0478	166	38.00	25	136.	0.0	0.0	0.0049
112	155.00	17	338.	0.1	0.1	0.0123	167	37.00	14	3290.	0.7	0.7	0.1194*
113	154.00	17	802.	0.2	0.2	0.0291							
114	153.00	21	4066.	0.8	0.8	0.1475							
115	152.00	25	270.	0.1	0.1	0.0098							
116	150.00	21	3908.	0.8	0.8	0.1418*							
117	149.00	25	5971.	1.2	1.2	0.2166							
118	148.00	14	2216.	0.5	0.5	0.0804							
119	144.00	14	2865.	0.6	0.6	0.1039							
120	141.00	25	9124.	1.9	1.9	0.3310							
121	140.00	17	11546.	2.4	2.4	0.4189							
122	139.00	25	35700.	7.4	7.4	1.2951							
123	127.00	25	12863.	2.7	2.7	0.4666							
124	126.00	21	16481.	3.4	3.4	0.5979							
125	125.00	21	15278.	3.2	3.2	0.5543							
126	120.00	21	1198.	0.2	0.2	0.0435							
127	116.00	6	1018.	0.2	0.2	0.0369							
128	114.00	10	3352.	0.7	0.7	0.1216							
129	113.00	35	43969.	9.2	9.2	1.5951							
130	112.00	21	22532.	4.7	4.7	0.8174							
131	111.00	25	52563.	10.9	10.9	1.9069							
132	101.00	17	2163.	0.5	0.5	0.0785*							
133	100.00	21	7047.	1.5	1.5	0.2557*							
134	99.00	25	39464.	8.2	8.2	1.4317							
135	98.00	25	21245.	4.4	4.4	0.7707							
136	97.00	29	87940.	18.3	18.3	3.1903							
137	89.00	8	1724.	0.4	0.4	0.0625							
138	87.00	17	2932.	0.6	0.6	0.1064*							
139	86.00	21	10951.	2.3	2.3	0.3973							
140	85.00	35	113116.	23.6	23.6	4.1036*							
141	84.00	21	10331.	2.2	2.2	0.3748							
142	83.00	25	41152.	8.6	8.6	1.4929							
143	72.00	25	23305.	4.9	4.9	0.8455							
144	71.00	35	274784.	57.2	57.2	9.9687							
145	70.00	25	28473.	5.9	5.9	1.0329							
146	69.00	35	119320.	24.9	24.9	4.3287							
147	64.00	17	1780.	0.4	0.4	0.0646*							
148	62.00	10	3030.	0.6	0.6	0.1099							
149	61.00	10	793.	0.2	0.2	0.0288							
150	60.00	12	3524.	0.7	0.7	0.1278							
151	59.00	8	1951.	0.4	0.4	0.0708							
152	58.00	21	21849.	4.6	4.6	0.7926							
153	57.00	35	480112.	100.0	100.0	*17.41							
154	56.00	29	69040.	14.4	14.4	2.5046							
155	55.00	35	113664.	23.7	23.7	4.1235							
156	53.00	21	357.	0.1	0.1	0.0130							
157	51.00	25	10772.	2.2	2.2	0.3908							
158	50.00	8	1496.	0.3	0.3	0.0543							
159	47.00	17	3310.	0.7	0.7	0.1201							
160	44.00	35	7058.	1.5	1.5	0.2561							
161	43.00	43	304752.	63.5	63.5	*11.05							
162	42.00	25	27754.	5.8	5.8	1.0072							
163	41.00	25	90036.	18.8	18.8	3.2663							
164	40.00	25	6878.	1.4	1.4	0.2495							
165	39.00	29	8996.	1.9	1.9	0.3264							

EXAV12.1 [TIC-286278656. 188X-27664384] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	233.00	8	6230.	0.0	0.0	0.0030	166	150.00	8	15972.	0.1	0.1	0.0077
112	232.00	6	1150.	0.0	0.0	0.0005	167	149.00	17	151504.	0.5	0.5	0.0734
113	229.00	6	5263.	0.0	0.0	0.0026	168	147.00	17	49528.	0.2	0.2	0.0240*
114	228.00	8	24933.	0.1	0.1	0.0121	169	145.00	6	2517.	0.0	0.0	0.0012
115	227.00	21	635696.	2.3	2.3	0.3082	170	142.00	10	31752.	0.1	0.1	0.0154*
116	225.00	8	4021.	0.0	0.0	0.0019	171	141.00	21	339248.	1.2	1.2	0.1645
117	224.00	12	43302.	0.2	0.2	0.0210*	172	140.00	17	136652.	0.5	0.5	0.0662
118	223.00	12	31316.	0.1	0.1	0.0152*	173	139.00	21	444400.	1.6	1.6	0.2154*
119	222.00	12	26369.	0.1	0.1	0.0128*	174	138.00	17	157824.	0.6	0.6	0.0765
120	221.00	12	40394.	0.1	0.1	0.0196*	175	137.00	17	154216.	0.6	0.6	0.0748*
121	219.00	6	1039.	0.0	0.0	0.0005	176	136.00	10	29007.	0.1	0.1	0.0141
122	217.00	6	910.	0.0	0.0	0.0004	177	135.00	21	261588.	0.9	0.9	0.1268*
123	216.00	6	2441.	0.0	0.0	0.0012	178	134.00	8	4561.	0.0	0.0	0.0022
124	215.00	6	1098.	0.0	0.0	0.0005	179	133.00	17	132324.	0.5	0.5	0.0641*
125	214.00	6	1973.	0.0	0.0	0.0010	180	131.00	10	32623.	0.1	0.1	0.0158*
126	213.00	14	75268.	0.3	0.3	0.0365	181	128.00	12	42314.	0.2	0.2	0.0205
127	211.00	10	35670.	0.1	0.1	0.0173	182	127.00	21	482768.	1.7	1.7	0.2340
128	210.00	12	24942.	0.1	0.1	0.0121*	183	126.00	17	210516.	0.8	0.8	0.1021
129	209.00	21	168896.	0.6	0.6	0.0819*	184	125.00	25	903296.	3.3	3.3	0.4379*
130	208.00	25	273104.	1.0	1.0	0.1324*	185	124.00	21	239328.	0.9	0.9	0.1160*
131	207.00	21	816768.	3.0	3.0	0.3960	186	123.00	12	334576.	1.2	1.2	0.1622
132	205.00	6	2397.	0.0	0.0	0.0012	187	122.00	12	52879.	0.2	0.2	0.0256
133	204.00	8	1146.	0.0	0.0	0.0006	188	121.00	21	256684.	0.9	0.9	0.1244*
134	198.00	10	5079.	0.0	0.0	0.0005	189	119.00	21	243640.	0.9	0.9	0.1181*
135	197.00	17	111700.	0.4	0.4	0.0542	190	115.00	8	10363.	0.0	0.0	0.0050
136	196.00	10	31224.	0.1	0.1	0.0151	191	114.00	17	66628.	0.2	0.2	0.0323
137	195.00	12	83589.	0.2	0.2	0.0308*	192	113.00	35	1130624.	4.1	4.1	0.5481
138	194.00	17	90816.	0.3	0.3	0.0440	193	112.00	25	483360.	1.7	1.7	0.2343
139	193.00	12	43112.	0.2	0.2	0.0209	194	111.00	29	1777280.	6.4	6.4	0.8616
140	192.00	8	10523.	0.0	0.0	0.0051	195	110.00	21	419152.	1.5	1.5	0.2032
141	191.00	17	98648.	0.4	0.4	0.0478*	196	109.00	21	533488.	0.2	0.2	0.0322*
142	184.00	8	15813.	0.1	0.1	0.0077*	197	108.00	12	66504.	0.6	0.6	0.0829
143	183.00	21	159792.	0.6	0.6	0.0775*	198	107.00	17	171044.	0.1	0.1	0.0122*
144	182.00	10	41745.	0.2	0.2	0.0202*	199	105.00	8	25093.	0.0	0.0	0.0041
145	181.00	17	96868.	0.4	0.4	0.0470*	200	103.00	10	8514.	0.0	0.0	0.0011
146	180.00	14	60578.	0.2	0.2	0.0294	201	102.00	6	2340.	0.0	0.0	0.0009
147	179.00	10	29230.	0.1	0.1	0.0142*	202	101.00	25	172140.	0.6	0.6	0.0835*
148	177.00	14	56831.	0.2	0.2	0.0276*	203	100.00	25	1348224.	4.9	4.9	0.6536
149	170.00	8	13615.	0.0	0.0	0.0055	204	99.00	25	1754560.	6.3	6.3	0.8506
150	169.00	21	212176.	0.8	0.8	0.1029	205	98.00	35	4036544.	14.6	14.6	1.9568
151	168.00	10	54828.	0.2	0.2	0.0266	206	97.00	29	1648400.	3.8	3.8	0.5082*
152	167.00	17	132568.	0.5	0.5	0.0543	207	96.00	35	1315200.	4.8	4.8	0.6376*
153	166.00	12	56209.	0.2	0.2	0.0272	208	95.00	17	128816.	0.5	0.5	0.0624*
154	165.00	12	37700.	0.1	0.1	0.0183*	209	94.00	21	206840.	0.7	0.7	0.1003*
155	164.00	8	7871.	0.0	0.0	0.0038	210	93.00	8	3072.	0.0	0.0	0.0015
156	163.00	17	92408.	0.3	0.3	0.0448*	211	92.00	17	70764.	0.3	0.3	0.0343*
157	162.00	8	6114.	0.0	0.0	0.0030	212	91.00	8	2681.	0.0	0.0	0.0013
158	161.00	10	26087.	0.1	0.1	0.0126*	213	89.00	6	1216.	0.0	0.0	0.0006
159	160.00	6	933.	0.0	0.0	0.0005	214	88.00	10	13974.	0.1	0.1	0.0068
160	156.00	8	5947.	0.0	0.0	0.0029	215	87.00	21	286416.	1.0	1.0	0.1388*
161	155.00	21	266080.	1.0	1.0	0.1290	216	86.00	35	4917760.	17.8	17.8	2.3840*
162	154.00	14	95136.	0.3	0.3	0.0461*	217	85.00	29	2145920.	7.8	7.8	1.0403
163	153.00	21	246368.	0.9	0.9	0.1194	218	84.00	35	5575424.	20.2	20.2	2.7029
164	152.00	14	103844.	0.4	0.4	0.0503	219	83.00	25	1114944.	4.0	4.0	0.5405
165	151.00	12	65944.	0.2	0.2	0.0320	220	82.00					

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	81.00	25	1260480.	4.6	4.6	0.6111
222	80.00	21	145228.	0.5	0.5	0.0704*
223	79.00	21	279392.	1.0	1.0	0.1354
224	78.00	10	43251.	0.2	0.2	0.0210*
225	77.00	14	56411.	0.2	0.2	0.0273*
226	75.00	12	46328.	0.2	0.2	0.0225
227	74.00	10	7866.	0.0	0.0	0.0038*
228	73.00	21	319184.	1.2	1.2	0.1547
229	72.00	25	443232.	1.6	1.6	0.2149
230	71.00	35	8648192.	31.3	31.3	4.1925
231	70.00	29	1990336.	7.2	7.2	0.9649
232	69.00	35	9186048.	33.2	33.2	4.4532*
233	68.00	29	1364224.	4.9	4.9	0.6614*
234	67.00	25	1439232.	5.2	5.2	0.6977*
235	66.00	17	86568.	0.3	0.3	0.0420*
236	65.00	14	87412.	0.3	0.3	0.0424*
237	64.00	17	94716.	0.3	0.3	0.0459
238	63.00	10	11972.	0.0	0.0	0.0058
239	62.00	6	1043.	0.0	0.0	0.0005
240	61.00	14	64189.	0.2	0.2	0.0311*
241	60.00	241	25119.	0.1	0.1	0.0122
242	59.00	21	143708.	0.5	0.5	0.0697*
243	58.00	29	893904.	3.2	3.2	0.4333
244	57.00	43	18105344.	65.4	65.4	8.7771*
245	56.00	35	3385408.	12.2	12.2	1.6412
246	55.00	35	13559808.	49.0	49.0	6.5735
247	54.00	25	1021520.	3.7	3.7	0.4952
248	53.00	25	497360.	1.8	1.8	0.2411
249	52.00	12	30040.	0.1	0.1	0.0146*
250	51.00	25	690208.	2.5	2.5	0.3346*
251	50.00	10	24117.	0.1	0.1	0.0117*
252	49.00	8	5895.	0.0	0.0	0.0029
253	47.00	12	47890.	0.2	0.2	0.0232*
254	45.00	25	208944.	0.8	0.8	0.1013*
255	44.00	35	1152896.	4.2	4.2	0.5589*
256	43.00	51	27664384.	100.0	100.0	*13.41*
257	42.00	35	3048000.	11.0	11.0	1.4776
258	41.00	35	11222272.	40.6	40.6	5.4403
259	40.00	25	274672.	1.0	1.0	0.1332*
260	39.00	29	1216960.	4.4	4.4	0.5900*
261	38.00	14	61119.	0.2	0.2	0.0296*
262	37.00	8	5022.	0.0	0.0	0.0024
263	36.00	21	124916.	0.5	0.5	0.0606*
264	35.00	8	8975.	0.0	0.0	0.0044

AY3AV.1 [TIC-20031488, 100X-39293952] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	299.00	12	65467.	0.2	0.2	0.327	56	169.00	17	145896.	0.4	0.4	0.728
2	297.00	21	618960.	1.6	1.6	0.3090	57	164.00	8	3078.	0.0	0.0	0.0015
3	296.00	35	408032.	10.4	10.4	2.0308*	58	163.00	10	39248.	0.1	0.1	0.00196
4	295.00	21	436336.	0.0	0.0	0.20308*	59	162.00	6	1964.	0.0	0.0	0.0010
5	294.00	8	11911.	0.0	0.0	0.0059*	60	161.00	14	97752.	0.2	0.2	0.0488
6	292.00	8	18299.	0.0	0.0	0.0091	61	151.00	8	2292.	0.0	0.0	0.0011
7	291.00	14	211032.	0.5	0.5	0.1054	62	150.00	14	46649.	0.1	0.1	0.0233*
8	279.00	10	31069.	0.1	0.1	0.0155	63	149.00	6	12867.	0.0	0.0	0.0064
9	278.00	8	17264.	0.0	0.0	0.0086	64	145.00	8	1516.	0.0	0.0	0.0008
10	277.00	14	139556.	0.4	0.4	0.0697	65	135.00	14	95032.	0.2	0.2	0.0474
11	270.00	8	20192.	0.1	0.1	0.0101	66	134.00	6	787.	0.0	0.0	0.0004
12	269.00	17	260052.	0.7	0.7	0.1298	67	133.00	17	211692.	0.0	0.0	0.1057
13	268.00	29	3309248.	8.4	8.4	1.6520*	68	132.00	10	6070.	0.0	0.0	0.0040
14	267.00	17	193588.	0.5	0.5	0.0966*	69	131.00	17	196692.	0.5	0.5	0.0982
15	266.00	8	4803.	0.0	0.0	0.0024	70	129.00	10	12845.	0.0	0.0	0.0064
16	265.00	8	1638.	0.0	0.0	0.0008	71	121.00	6	1202.	0.0	0.0	0.0006
17	258.00	8	4348.	0.0	0.0	0.0022	72	120.00	8	5422.	0.0	0.0	0.0027
18	257.00	21	220056.	0.6	0.6	0.1138*	73	119.00	25	1682496.	4.3	4.3	0.8399
19	256.00	35	2360896.	6.0	6.0	1.1786*	74	115.00	8	6929.	0.0	0.0	0.0035
20	255.00	59	33617920.	85.6	85.6	*16.78*	75	114.00	10	48050.	0.1	0.1	0.0240*
21	254.00	25	107500.	0.3	0.3	0.0537*	76	113.00	25	1409728.	3.6	3.6	0.7038
22	253.00	21	270768.	0.7	0.7	0.1352*	77	112.00	6	4084.	0.0	0.0	0.0020
23	252.00	10	3224.	0.0	0.0	0.0016*	78	111.00	10	33552.	0.1	0.1	0.0167
24	251.00	6	1823.	0.0	0.0	0.0009	79	109.00	17	220920.	0.6	0.6	0.1103
25	243.00	10	7109.	0.0	0.0	0.0035*	80	105.00	10	14403.	0.0	0.0	0.0072
26	242.00	17	175116.	0.4	0.4	0.0874	81	104.00	6	2493.	0.0	0.0	0.0012
27	241.00	10	67084.	0.2	0.2	0.0335*	82	103.00	6	2488.	0.0	0.0	0.0012
28	240.00	10	55207.	0.1	0.1	0.0276	83	101.00	10	51862.	0.1	0.1	0.0259*
29	239.00	12	82320.	0.2	0.2	0.0411	84	100.00	21	741824.	1.9	1.9	0.3703
30	236.00	10	19768.	0.1	0.1	0.0099	85	99.00	17	191384.	0.5	0.5	0.0955
31	235.00	17	371584.	0.9	0.9	0.1855	86	98.00	21	562272.	1.4	1.4	0.2807
32	231.00	8	3925.	0.0	0.0	0.0020	87	97.00	35	9574656.	24.4	24.4	4.7798*
33	229.00	8	10504.	0.0	0.0	0.0052	88	96.00	25	767488.	2.0	2.0	0.3831*
34	227.00	12	65196.	0.2	0.2	0.0325	89	95.00	29	1959424.	5.0	5.0	0.9782
35	226.00	8	18971.	0.0	0.0	0.0095	90	94.00	14	25793.	0.1	0.1	0.0129*
36	223.00	8	10704.	0.0	0.0	0.0053	91	93.00	12	74936.	0.2	0.2	0.0374
37	221.00	6	5371.	0.0	0.0	0.0027	92	91.00	8	16630.	0.0	0.0	0.0083
38	220.00	29	88308.	0.2	0.2	0.0441*	93	86.00	8	8813.	0.0	0.0	0.0044
39	219.00	17	43205.	0.1	0.1	0.0216*	94	86.00	8	3014.	0.0	0.0	0.0015
40	218.00	8	3390.	0.0	0.0	0.0017	95	85.00	21	301856.	0.8	0.8	0.1507*
41	217.00	10	26386.	0.1	0.1	0.0132*	96	84.00	10	22253.	0.1	0.1	0.0111*
42	216.00	12	20319.	0.1	0.1	0.0101*	97	83.00	25	403984.	1.0	1.0	0.2017
43	213.00	14	83864.	0.2	0.2	0.0419	98	82.00	17	99432.	0.3	0.3	0.0496*
44	210.00	10	13150.	0.0	0.0	0.0066	99	81.00	21	443056.	1.1	1.1	0.2212
45	209.00	21	539456.	1.4	1.4	0.2693	100	80.00	21	128148.	0.3	0.3	0.0640
46	207.00	8	3768.	0.0	0.0	0.0019	101	79.00	25	1247424.	3.2	3.2	0.6227
47	206.00	8	5929.	0.0	0.0	0.0030	102	78.00	6	2985.	0.0	0.0	0.0015
48	203.00	6	2526.	0.0	0.0	0.0013	103	77.00	14	77900.	0.2	0.2	0.0389
49	193.00	6	2297.	0.0	0.0	0.0011	104	76.00	6	2356.	0.0	0.0	0.0012
50	191.00	8	12232.	0.0	0.0	0.0061	105	75.00	17	155416.	0.4	0.4	0.0776
51	187.00	6	3597.	0.0	0.0	0.0018	106	74.00	8	4369.	0.0	0.0	0.0022
52	183.00	12	11174.	0.0	0.0	0.0056	107	73.00	21	419040.	1.1	1.1	0.2092
53	181.00	12	55517.	0.1	0.1	0.0277*	108	72.00	6	24751.	0.1	0.1	0.0124
54	178.00	6	1091.	0.0	0.0	0.0005	109	71.00	21	207492.	0.5	0.5	0.1036*
55	177.00	14	95556.	0.2	0.2	0.0477	110	70.00	35	1772224.	4.5	4.5	0.8847

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	69.00	71	39293952.	100.0	100.0	*19.61*
112	68.00	43	6808832.	17.3	17.3	3.3991*
113	67.00	43	9222912.	23.5	23.5	4.6042*
114	66.00	35	751024.	1.9	1.9	0.3749*
115	65.00	29	1096384.	2.8	2.8	0.5473*
116	64.00	25	1030320.	2.6	2.6	0.5144
117	63.00	25	270880.	0.7	0.7	0.1352*
118	62.00	14	81820.	0.2	0.2	0.0408*
119	61.00	17	131024.	0.3	0.3	0.0654*
120	60.00	8	8890.	0.0	0.0	0.0044
121	59.00	12	48669.	0.1	0.1	0.0243*
122	58.00	8	16697.	0.0	0.0	0.0003*
123	57.00	29	627328.	1.6	1.6	0.3132*
124	56.00	25	487456.	1.2	1.2	0.2433
125	55.00	43	12063488.	30.7	30.7	6.0223*
126	54.00	25	525632.	1.3	1.3	0.2624
127	53.00	35	1867712.	4.8	4.8	0.9324
128	52.00	21	203576.	0.5	0.5	0.1016
129	51.00	35	3399104.	8.7	8.7	1.6969
130	50.00	21	284240.	0.7	0.7	0.1419*
131	49.00	21	98496.	0.3	0.3	0.0492*
132	47.00	17	137384.	0.3	0.3	0.0686*
133	45.00	29	629856.	1.6	1.6	0.3144
134	44.00	25	243844.	0.6	0.6	0.1217*
135	43.00	35	1407040.	3.6	3.6	0.7024*
136	42.00	35	5815808.	14.8	14.8	2.9033
137	41.00	51	27784192.	70.7	70.7	*13.87*
138	40.00	35	2679616.	6.8	6.8	1.3377*
139	39.00	35	10747136.	27.4	27.4	5.3651*
140	38.00	29	701424.	1.8	1.8	0.3502*
141	37.00	29	196264.	0.5	0.5	0.0980*
142	36.00	17	131168.	0.3	0.3	0.0655*
143	35.00	12	10870.	0.0	0.0	0.0094*

AC4PK.1 [TIC=119652352, 188X-28866384] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	312.00	10	35906.	0.2	0.2	0.0300	56	113.00	25	664608.	3.3	3.3	0.5554*
2	311.00	21	416560.	2.1	0.2	0.3481*	57	112.00	21	196936.	1.0	1.0	0.1646
3	310.00	29	3040640.	15.2	15.2	2.5412	58	111.00	25	2862208.	14.3	14.3	2.3921
4	309.00	17	129860.	0.6	0.6	0.1085*	59	110.00	25	2203136.	11.0	11.0	1.8413
5	295.00	10	12696.	0.1	0.1	0.0106	60	109.00	25	449643.	2.2	2.2	0.3758
6	295.00	17	348896.	1.7	1.7	0.2916	61	101.00	8	632.	0.0	0.0	0.0054
7	293.00	8	1302.	0.0	0.0	0.0011	62	100.00	21	308064.	1.5	1.5	0.2575
8	292.00	10	22019.	0.1	0.1	0.0184	63	99.00	14	78120.	0.4	0.4	0.0653*
9	291.00	10	66664.	0.3	0.3	0.0557	64	98.00	10	2007.	0.0	0.0	0.0017
10	283.00	12	2895.	0.0	0.0	0.0024	65	97.00	10	13026.	0.1	0.1	0.0189*
11	282.00	14	164992.	0.8	0.8	0.1379	66	96.00	8	5196.	0.0	0.0	0.0043
12	281.00	25	1052352.	5.2	5.2	0.8795*	67	95.00	25	573376.	2.9	2.9	0.4792*
13	270.00	10	50323.	0.3	0.3	0.0421	68	94.00	12	60278.	0.3	0.3	0.0504*
14	269.00	17	588464.	2.9	2.9	0.4918	69	93.00	25	725232.	3.6	3.6	0.6061
15	268.00	17	503136.	2.5	2.5	0.4205*	70	92.00	12	62873.	0.3	0.3	0.0525*
16	267.00	12	66788.	0.3	0.3	0.0558*	71	91.00	14	80596.	0.4	0.4	0.0674
17	257.00	12	53018.	0.3	0.3	0.0443*	72	87.00	8	2652.	0.0	0.0	0.0022
18	256.00	25	578128.	2.9	2.9	0.4832*	73	86.00	6	1930.	0.0	0.0	0.0016
19	255.00	43	6911488.	34.4	34.4	5.7763*	74	85.00	17	134008.	0.7	0.7	0.1120*
20	254.00	14	51377.	0.3	0.3	0.0429*	75	84.00	25	882496.	4.4	4.4	0.7376
21	253.00	17	128968.	0.6	0.6	0.1078	76	83.00	35	14470912.	72.1	72.1	*12.09*
22	244.00	8	4202.	0.0	0.0	0.0035	77	82.00	35	3128320.	15.6	15.6	2.6145*
23	243.00	17	315904.	4.3	4.3	0.2640*	78	81.00	35	4024384.	20.1	20.1	3.3634*
24	242.00	21	869855.	1.6	1.6	0.7270*	79	80.00	21	236996.	1.2	1.2	0.1981
25	241.00	10	15912.	0.1	0.1	0.0133	80	79.00	25	918224.	4.6	4.6	0.7674
26	240.00	10	47627.	0.2	0.2	0.0398	81	78.00	17	109900.	0.5	0.5	0.0918*
27	239.00	12	100000.	0.5	0.5	0.0836	82	77.00	25	300960.	1.9	1.9	0.3184*
28	237.00	6	2543.	0.0	0.0	0.0021	83	76.00	8	3743.	0.0	0.0	0.0031
29	236.00	8	2498.	0.0	0.0	0.0021	84	75.00	12	62055.	0.3	0.3	0.0519*
30	235.00	14	120968.	0.6	0.6	0.1011	85	73.00	17	122024.	0.6	0.6	0.1020*
31	229.00	12	34245.	0.2	0.2	0.0286	86	71.00	17	94668.	0.5	0.5	0.0791*
32	228.00	8	10149.	0.1	0.1	0.0085	87	70.00	21	131040.	0.7	0.7	0.1095*
33	227.00	17	326864.	1.6	1.6	0.2732	88	69.00	35	4826624.	24.1	24.1	4.0339*
34	217.00	10	3505.	0.0	0.0	0.0030	89	68.00	35	7384576.	36.8	36.8	6.1717*
35	216.00	6	709.	0.0	0.0	0.0006	90	67.00	25	3231616.	16.1	16.1	2.7008*
36	213.00	10	21923.	0.1	0.1	0.0183	91	66.00	25	305728.	1.5	1.5	0.2555
37	210.00	14	12606.	0.1	0.1	0.0186*	92	65.00	21	292160.	1.5	1.5	0.2442
38	209.00	17	308320.	1.5	1.5	0.2577	93	64.00	35	394320.	2.0	2.0	0.3296
39	191.00	10	18153.	0.1	0.1	0.0152	94	63.00	12	58374.	0.3	0.3	0.0488*
40	183.00	10	5172.	0.0	0.0	0.0043	95	62.00	8	14382.	0.1	0.1	0.0120*
41	181.00	10	25600.	0.1	0.1	0.0214	96	61.00	17	78052.	0.4	0.4	0.0652*
42	169.00	12	62648.	0.3	0.3	0.0524	97	60.00	6	530.	0.0	0.0	0.0004
43	163.00	10	2309.	0.0	0.0	0.0019	98	59.00	10	20275.	0.1	0.1	0.0169*
44	162.00	6	2945.	0.0	0.0	0.0025	99	58.00	8	4284.	0.0	0.0	0.0036
45	161.00	12	44070.	0.2	0.2	0.0368*	100	57.00	25	502016.	2.5	2.5	0.4696*
46	150.00	8	16038.	0.1	0.1	0.0134	101	56.00	35	5622016.	28.0	28.0	*16.77*
47	136.00	8	4994.	0.0	0.0	0.0042	102	55.00	51	20066304.	100.0	100.0	1.6969
48	135.00	8	12130.	0.1	0.1	0.0101	103	54.00	29	2030400.	10.1	10.1	1.6114
49	133.00	14	97632.	0.5	0.5	0.0816	104	53.00	29	1928064.	9.6	9.6	1.6114
50	131.00	17	105876.	0.5	0.5	0.0885	105	52.00	21	280592.	1.4	1.4	0.2345*
51	127.00	10	15094.	0.1	0.1	0.0126	106	51.00	35	2050240.	10.2	10.2	1.7135
52	123.00	6	1165.	0.0	0.0	0.0010	107	50.00	21	178736.	0.9	0.9	0.1494*
53	120.00	6	1259.	0.0	0.0	0.0011	108	49.00	8	21431.	0.1	0.1	0.0179*
54	119.00	21	794608.	4.0	4.0	0.6641	109	47.00	17	79284.	0.4	0.4	0.0663*
55	114.00	8	6158.	0.0	0.0	0.0051	110	45.00	25	295568.	1.5	1.5	0.2470*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	44.00	25	231200.	1.2	1.2	0.1932
112	43.00	35	2210240.	11.0	11.0	1.8472
113	42.00	35	1325568.	6.6	6.6	1.1078
114	41.00	43	10360320.	51.6	51.6	8.6587*
115	40.00	35	733984.	3.7	3.7	0.6134*
116	39.00	35	4235520.	21.1	21.1	3.5399*
117	38.00	21	143316.	0.7	0.7	0.1198*
118	37.00	10	18964.	0.1	0.1	0.0158*
119	36.00	25	87436.	0.4	0.4	0.0731*
120	35.00	6	3489.	0.0	0.0	0.0029

AV4AV.1 [TIC-219365376, 180X-51459872] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	326.00	10	36631.	0.1	0.1	0.0167	56	207.00	8	18860.	0.0	0.0	0.0086
2	325.00	21	505616.	6.6	1.0	0.2305*	57	205.00	14	42913.	0.1	0.1	0.0196
3	324.00	35	3404672.	1.0	6.6	1.5521*	58	192.00	6	709.	0.0	0.0	0.0003
4	323.00	12	12238.	0.0	0.0	0.0056*	59	191.00	8	2478.	0.0	0.0	0.0011
5	311.00	10	6168.	0.0	0.0	0.0028	60	183.00	12	55464.	0.1	0.1	0.0253
6	310.00	14	147884.	0.3	0.3	0.0074	61	181.00	8	13647.	0.0	0.0	0.0062
7	309.00	21	1437568.	2.8	2.8	0.5553	62	169.00	12	85308.	0.2	0.2	0.0389
8	308.00	8	3558.	0.0	0.0	0.0016	63	163.00	8	10149.	0.0	0.0	0.0046
9	307.00	8	4184.	0.0	0.0	0.0019	64	161.00	14	66324.	0.1	0.1	0.0302
10	306.00	6	1797.	0.0	0.0	0.0008	65	159.00	6	2087.	0.0	0.0	0.0010
11	305.00	10	15859.	0.0	0.0	0.0072	66	150.00	12	33910.	0.1	0.1	0.0155
12	296.00	10	46069.	0.1	0.1	0.0210	67	149.00	12	39837.	0.1	0.1	0.0182
13	295.00	17	332256.	0.6	0.6	0.1515	68	145.00	8	2466.	0.0	0.0	0.0011
14	293.00	6	7152.	0.0	0.0	0.0033	69	141.00	8	2322.	0.0	0.0	0.0011
15	287.00	8	2062.	0.0	0.0	0.0009	70	135.00	8	5816.	0.0	0.0	0.0027
16	283.00	12	86680.	0.2	0.2	0.0395	71	133.00	17	182312.	0.4	0.4	0.0831*
17	282.00	17	219692.	0.4	0.4	0.1001	72	132.00	8	1445.	0.0	0.0	0.0007
18	281.00	14	98476.	0.2	0.2	0.0449	73	131.00	17	171680.	0.3	0.3	0.0783
19	279.00	6	1380.	0.0	0.0	0.0006	74	127.00	8	23009.	0.0	0.0	0.0105
20	271.00	12	70744.	0.1	0.1	0.0322	75	126.00	17	109604.	0.2	0.2	0.0500
21	270.00	25	839184.	1.6	1.6	0.3826*	76	125.00	21	826096.	1.6	1.6	0.3766
22	269.00	43	10940672.	21.3	21.3	4.9874*	77	124.00	21	634848.	1.2	1.2	0.2894
23	268.00	17	121736.	0.2	0.2	0.0555*	78	123.00	21	294128.	0.6	0.6	0.1341*
24	267.00	14	127604.	0.2	0.2	0.0582	79	122.00	6	1613.	0.0	0.0	0.0007
25	258.00	10	5043.	0.0	0.0	0.0023	80	121.00	6	1168.	0.0	0.0	0.0005
26	257.00	14	103036.	0.2	0.2	0.0470	81	120.00	8	6739.	0.0	0.0	0.0031
27	256.00	25	1497920.	2.9	2.9	0.6828	82	119.00	25	1349248.	2.6	2.6	0.6151
28	255.00	17	423920.	0.8	0.8	0.1932*	83	114.00	10	42620.	0.1	0.1	0.0194
29	254.00	10	41563.	0.1	0.1	0.0189	84	113.00	25	1328384.	2.6	2.6	0.6056
30	253.00	12	88588.	0.2	0.2	0.0404	85	112.00	6	1677.	0.0	0.0	0.0008
31	251.00	8	2241.	0.0	0.0	0.0010	86	111.00	12	48368.	0.1	0.1	0.0220
32	250.00	6	981.	0.0	0.0	0.0004	87	110.00	10	10519.	0.0	0.0	0.0048
33	249.00	10	67948.	0.1	0.1	0.0310	88	109.00	21	297248.	0.6	0.6	0.1355*
34	243.00	12	50339.	0.1	0.1	0.0229	89	108.00	12	37932.	0.1	0.1	0.0173
35	242.00	17	109440.	0.2	0.2	0.0499*	90	107.00	21	277440.	0.5	0.5	0.1265
36	241.00	21	982368.	1.9	1.9	0.4478	91	106.00	6	4660.	0.0	0.0	0.0021
37	240.00	10	23081.	0.0	0.0	0.0105	92	105.00	12	13967.	0.0	0.0	0.0064
38	239.00	14	150860.	0.3	0.3	0.0688	93	101.00	12	27198.	0.1	0.1	0.0124
39	235.00	8	26390.	0.1	0.1	0.0120	94	100.00	21	511520.	1.0	1.0	0.2332
40	230.00	6	1483.	0.0	0.0	0.0007	95	99.00	17	168964.	0.3	0.3	0.0770
41	229.00	8	8449.	0.0	0.0	0.0039	96	98.00	35	3543936.	6.9	6.9	1.6155*
42	228.00	10	41254.	0.1	0.1	0.0188*	97	97.00	87	51459072.	100.0	100.0	*23.45*
43	227.00	21	696384.	1.4	1.4	0.3175	98	96.00	35	2230400.	4.3	4.3	1.0168*
44	226.00	6	1150.	0.0	0.0	0.0005	99	95.00	35	3867776.	7.5	7.5	1.7632*
45	225.00	10	48289.	0.1	0.1	0.0220*	100	94.00	14	105012.	0.2	0.2	0.0479
46	224.00	12	44881.	0.1	0.1	0.0205*	101	93.00	21	288928.	0.6	0.6	0.1317
47	223.00	29	706784.	1.4	1.4	0.3222*	102	92.00	8	26534.	0.1	0.1	0.0121
48	222.00	17	3529.	0.0	0.0	0.0016*	103	91.00	21	264512.	0.5	0.5	0.1206
49	221.00	10	6625.	0.0	0.0	0.0030	104	87.00	8	26162.	0.1	0.1	0.0119
50	219.00	10	16902.	0.0	0.0	0.0077	105	85.00	14	59710.	0.1	0.1	0.0272*
51	216.00	8	4131.	0.0	0.0	0.0019	106	84.00	10	26734.	0.1	0.1	0.0122
52	215.00	10	5372.	0.0	0.0	0.0024	107	83.00	29	874960.	1.7	1.7	0.3989
53	213.00	12	69216.	0.1	0.1	0.0316	108	82.00	29	1479040.	2.9	2.9	0.6742
54	211.00	6	2479.	0.0	0.0	0.0011	109	81.00	35	5285888.	10.3	10.3	2.4096*
55	209.00	10	39031.	0.1	0.1	0.0178	110	80.00	21	302544.	0.6	0.6	0.1379*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	79.00	25	1258304.	2.4	2.4	0.5736
112	78.00	17	155496.	0.3	0.3	0.0709*
113	77.00	25	756688.	1.5	1.5	0.3449*
114	76.00	6	3036.	0.0	0.0	0.0014
115	75.00	14	82852.	0.2	0.2	0.0378*
116	74.00	8	4703.	0.0	0.0	0.0021
117	73.00	14	41276.	0.1	0.1	0.0188
118	71.00	21	184592.	0.4	0.4	0.0841*
119	70.00	29	1206528.	2.3	2.3	0.5500
120	69.00	43	11623424.	22.6	22.6	5.2987*
121	68.00	29	1738432.	3.4	3.4	0.7925*
122	67.00	35	4195072.	8.2	8.2	1.9124*
123	66.00	25	319408.	0.6	0.6	0.1456*
124	65.00	25	680944.	1.3	1.3	0.3104
125	64.00	25	729200.	1.4	1.4	0.3324
126	63.00	17	149964.	0.3	0.3	0.0684*
127	62.00	12	27739.	0.1	0.1	0.0126
128	61.00	17	100872.	0.2	0.2	0.0460*
129	59.00	17	173216.	0.3	0.3	0.0790
130	58.00	10	52453.	0.1	0.1	0.0239*
131	57.00	35	1334208.	2.6	2.6	0.6082
132	56.00	35	6781952.	13.2	13.2	3.0916*
133	55.00	71	47989760.	93.3	93.3	*21.87*
134	54.00	29	1877696.	3.6	3.6	0.8560*
135	53.00	35	3598864.	6.8	6.8	1.5996*
136	52.00	25	371536.	0.7	0.7	0.1694
137	51.00	35	3699776.	7.2	7.2	1.6866*
138	50.00	21	235724.	0.5	0.5	0.1075*
139	49.00	21	62826.	0.1	0.1	0.0286*
140	48.00	8	17842.	0.0	0.0	0.0081*
141	47.00	21	170708.	0.3	0.3	0.0778*
142	46.00	10	36887.	0.1	0.1	0.0168*
143	45.00	29	636304.	1.2	1.2	0.2901
144	44.00	29	278432.	0.5	0.5	0.1269*
145	43.00	35	4991744.	9.7	9.7	2.2755
146	42.00	29	1373888.	2.7	2.7	0.6263
147	41.00	43	14003200.	27.2	27.2	6.3835*
148	40.00	35	1340544.	2.6	2.6	0.6111*
149	39.00	35	6404096.	12.4	12.4	2.9194*
150	38.00	21	231704.	0.5	0.5	0.1056*
151	37.00	17	42629.	0.1	0.1	0.0194*
152	36.00	17	133080.	0.3	0.3	0.0607*
153	35.00	12	22291.	0.0	0.0	0.0102*

AG8AV.1 [TIC=175665152, 188X=27262976] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	PEAK NO.	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	339.00	10	25637.	0.1	0.1	0.0146	120.00	56	25	909744.	3.3	3.2	0.5175*
2	338.00	10	96520.	0.4	0.4	0.0549	119.00	57	25	1149376.	4.2	4.2	0.6543
3	321.00	8	1826.	0.0	0.0	0.0010	118.00	58	8	2160.	0.0	0.0	0.0012
4	320.00	12	121800.	0.4	0.4	0.0693	114.00	59	12	19877.	0.1	0.1	0.0113*
5	319.00	10	28502.	0.1	0.1	0.0162	113.00	60	21	1117248.	4.1	4.1	0.6360
6	310.00	12	139172.	0.5	0.5	0.0792	111.00	61	17	237128.	0.9	0.9	0.1350
7	309.00	17	699040.	2.6	2.6	0.3979	110.00	62	21	581632.	2.1	2.1	0.3311*
8	291.00	8	9871.	0.0	0.0	0.0056	109.00	63	25	622512.	2.3	2.3	0.3544
9	282.00	12	3329.	0.0	0.0	0.0019	108.00	64	12	20124.	0.1	0.1	0.0115
10	281.00	8	34601.	0.1	0.1	0.0197	107.00	65	10	45440.	0.2	0.2	0.0259
11	279.00	6	1100.	0.0	0.0	0.0006	106.00	66	21	42075.	0.2	0.2	0.0240*
12	278.00	8	21958.	0.1	0.1	0.0125	105.00	67	17	96052.	0.4	0.4	0.0547*
13	269.00	8	10024.	0.0	0.0	0.0057	104.00	68	14	4960.	0.0	0.0	0.0028*
14	267.00	8	6514.	0.0	0.0	0.0037	103.00	69	10	12989.	0.0	0.0	0.0074*
15	265.00	8	4076.	0.0	0.0	0.0023	101.00	70	10	6300.	0.0	0.0	0.0036
16	257.00	12	91032.	0.3	0.3	0.0518	100.00	71	21	41880.	1.5	1.5	0.2385
17	256.00	21	917488.	3.4	3.4	0.5223	99.00	72	12	64924.	0.2	0.2	0.0370
18	255.00	35	4990464.	18.3	18.3	2.8409*	98.00	73	29	2009664.	7.4	7.4	1.1440*
19	254.00	10	19377.	0.1	0.1	0.0110*	97.00	74	29	27231232.	99.9	99.9	*15.50*
20	253.00	17	244900.	0.9	0.9	0.1394	96.00	75	59	3131136.	11.5	11.5	1.7824
21	252.00	8	9533.	0.0	0.0	0.0054	95.00	76	35	4411392.	16.2	16.2	2.5113*
22	244.00	10	30951.	0.1	0.1	0.0176	94.00	77	25	1735296.	6.4	6.4	0.9878
23	243.00	21	712736.	2.6	2.6	0.4057*	93.00	78	25	1160512.	4.3	4.3	0.6606
24	242.00	29	3405120.	12.5	12.5	1.9384*	92.00	79	25	175508.	0.6	0.6	0.0999*
25	241.00	10	43864.	0.2	0.2	0.0250	91.00	80	21	489392.	1.8	1.8	0.2786
26	240.00	8	55042.	0.2	0.2	0.0694	89.00	81	8	7789.	0.0	0.0	0.0044
27	239.00	14	121928.	0.4	0.4	0.0694	85.00	82	10	40715.	0.1	0.1	0.0232*
28	237.00	8	3753.	0.0	0.0	0.0021	84.00	83	25	613072.	2.2	2.2	0.3490
29	235.00	12	86992.	0.3	0.3	0.0495	83.00	84	35	8170496.	30.0	30.0	4.6512*
30	227.00	17	191740.	0.7	0.7	0.1092	82.00	85	25	1072512.	3.9	3.9	0.6105
31	222.00	10	4642.	0.0	0.0	0.0026	81.00	86	35	4918016.	18.0	18.0	2.7997*
32	219.00	6	2331.	0.0	0.0	0.0013	80.00	87	21	406944.	1.5	1.5	0.2317*
33	213.00	10	44068.	0.2	0.2	0.0251	79.00	88	29	1883456.	6.9	6.9	1.0722
34	209.00	8	25899.	0.1	0.1	0.0147	78.00	89	17	184764.	0.7	0.7	0.1052
35	207.00	8	3721.	0.0	0.0	0.0021	77.00	90	25	601952.	2.2	2.2	0.3427*
36	183.00	10	24218.	0.1	0.1	0.0138*	76.00	91	8	1338.	0.0	0.0	0.0000
37	181.00	8	9662.	0.0	0.0	0.0055	75.00	92	14	96300.	0.4	0.4	0.0548*
38	169.00	8	82240.	0.3	0.3	0.0468	74.00	93	8	6187.	0.0	0.0	0.0035
39	163.00	8	11638.	0.0	0.0	0.0066	73.00	94	17	125988.	0.5	0.5	0.0717*
40	161.00	8	9481.	0.0	0.0	0.0054	72.00	95	10	4727.	0.0	0.0	0.0027*
41	150.00	8	27347.	0.1	0.1	0.0156	71.00	96	17	137588.	0.5	0.5	0.0783*
42	145.00	8	6030.	0.0	0.0	0.0034	70.00	97	21	255312.	0.9	0.9	0.1453*
43	142.00	6	1309.	0.0	0.0	0.0007	69.00	98	35	6544128.	24.0	24.0	3.7253*
44	141.00	8	5182.	0.0	0.0	0.0029	68.00	99	35	2702976.	9.9	9.9	1.5387*
45	140.00	17	263376.	11.3	11.3	0.1499*	67.00	100	35	6021888.	22.1	22.1	3.4280*
46	139.00	29	3689152.	11.3	11.3	1.7585*	66.00	101	25	450256.	1.7	1.7	0.2563*
47	138.00	21	894160.	3.3	3.3	0.5090	65.00	102	25	541584.	2.0	2.0	0.3083
48	137.00	17	200544.	0.7	0.7	0.1142	64.00	103	25	465600.	1.7	1.7	0.2650*
49	136.00	10	23042.	0.1	0.1	0.0131	63.00	104	14	97228.	0.4	0.4	0.0553*
50	135.00	8	2268.	0.0	0.0	0.0013	62.00	105	10	30758.	0.1	0.1	0.0175
51	133.00	14	127004.	0.5	0.5	0.0723	61.00	106	14	118804.	0.4	0.4	0.0676*
52	131.00	17	116928.	0.4	0.4	0.0656	60.00	107	10	41603.	0.2	0.2	0.0237*
53	123.00	14	92796.	0.3	0.3	0.0528*	59.00	108	12	45590.	0.2	0.2	0.0260*
54	122.00	21	443344.	1.6	1.6	0.2524	58.00	109	14	855528.	0.3	0.3	0.0487*
55	121.00	35	4789504.	17.6	17.6	2.7265*	57.00	110	35	1965440.	7.2	7.2	1.1189*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	56.00	35	2131904.	7.8	7.8	1.2136
112	55.00	51	27262976.	100.0	100.0	*15.51*
113	54.00	29	3159232.	11.6	11.6	1.7984
114	53.00	29	2428544.	8.9	8.9	1.3825*
115	52.00	25	336608.	1.2	1.2	0.1916*
116	51.00	35	2586496.	9.5	9.5	1.4724*
117	50.00	17	204404.	0.7	0.7	0.1164*
118	49.00	10	36030.	0.1	0.1	0.0205*
119	48.00	8	12272.	0.0	0.0	0.0070
120	47.00	12	44777.	0.2	0.2	0.0255
121	46.00	10	10454.	0.0	0.0	0.0060
122	45.00	21	396496.	1.5	1.5	0.2257*
123	44.00	35	619488.	2.3	2.3	0.3527*
124	43.00	43	6781184.	24.9	24.9	3.8603
125	42.00	35	2931136.	10.8	10.8	1.6686*
126	41.00	35	14893568.	54.6	54.6	8.4784*
127	40.00	29	895856.	3.3	3.3	0.5100*
128	39.00	35	4970496.	18.2	18.2	2.8295*
129	38.00	17	109896.	0.4	0.4	0.0626*
130	37.00	10	19438.	0.1	0.1	0.0111*
131	36.00	17	70188.	0.3	0.3	0.0400*

EXAV9.1 [TIC=151089162.100X-16320000] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	466.00	8	1762.	0.5	0.5	0.0012	281.00	17	137644.	0.9	0.9	0.0911
2	465.00	12	74028.	0.5	0.5	0.0490	280.00	8	6794.	0.0	0.0	0.0045
3	464.60	17	298720.	1.9	1.9	0.1977	270.00	10	7683.	0.1	0.1	0.0051
4	462.00	10	6574.	0.0	0.0	0.0044	269.00	17	174104.	1.1	1.1	0.1152
5	447.00	6	4184.	0.0	0.0	0.0028	268.00	10	7916.	0.1	0.1	0.0052
6	446.00	12	50913.	0.3	0.3	0.0337	267.00	17	118276.	0.8	0.8	0.0783
7	445.00	10	21773.	0.1	0.1	0.0144	266.00	21	272896.	1.8	1.8	0.1806
8	436.00	8	3306.	0.0	0.0	0.0022	265.00	25	1387520.	9.1	9.1	0.9183
9	432.00	6	987.	0.0	0.0	0.0007	264.00	17	541760.	3.5	3.5	0.3586
10	429.00	6	1586.	0.0	0.0	0.0010	263.00	6	4762.	0.0	0.0	0.0032
11	421.00	6	4243.	0.0	0.0	0.0028	256.00	10	58214.	0.4	0.4	0.0385
12	408.00	8	2658.	0.0	0.0	0.0018	255.00	21	655776.	4.3	4.3	0.4340
13	407.00	6	11392.	0.1	0.1	0.0075	254.00	8	18975.	0.1	0.1	0.0126
14	395.00	8	8229.	0.1	0.1	0.0054	253.00	17	223144.	1.5	1.5	0.1477
15	394.00	6	2529.	0.0	0.0	0.0017	252.00	8	2247.	0.0	0.0	0.0015
16	393.00	10	19496.	0.1	0.1	0.0129	248.00	8	10894.	0.1	0.1	0.0072
17	381.00	8	19828.	0.1	0.1	0.0131	247.00	17	120720.	0.8	0.8	0.0799
18	380.00	8	9846.	0.1	0.1	0.0065	246.00	14	82988.	0.5	0.5	0.0549
19	379.00	10	23517.	0.2	0.2	0.0156	244.00	8	2154.	0.0	0.0	0.0014
20	378.00	8	2629.	0.0	0.0	0.0017	243.00	17	106216.	0.7	0.7	0.0703
21	368.00	10	28499.	0.2	0.2	0.0189	242.00	17	451152.	2.9	2.9	0.2986
22	367.00	8	9928.	0.1	0.1	0.0066	241.00	17	167044.	1.1	1.1	0.1106
23	366.00	6	1302.	0.0	0.0	0.0009	239.00	12	66940.	0.4	0.4	0.0443
24	365.00	12	37835.	0.2	0.2	0.0250	236.00	14	114964.	0.8	0.8	0.0761
25	364.00	8	5423.	0.0	0.0	0.0036	235.00	10	48397.	0.3	0.3	0.0320
26	356.00	6	1008.	0.0	0.0	0.0007	231.00	17	88748.	0.6	0.6	0.0587
27	355.00	10	11227.	0.1	0.1	0.0074	228.00	6	1904.	0.0	0.0	0.0013
28	354.00	8	14817.	0.1	0.1	0.0098	227.00	8	5111.	0.0	0.0	0.0040
29	353.00	8	21965.	0.1	0.1	0.0145	224.00	17	395344.	2.6	2.6	0.2617
30	352.00	8	12515.	0.1	0.1	0.0083	223.00	8	1232.	0.0	0.0	0.0008
31	351.00	12	53681.	0.4	0.4	0.0355	222.00	17	118828.	0.8	0.8	0.0786
32	345.00	10	21015.	0.1	0.1	0.0139	221.00	21	649968.	4.2	4.2	0.4302
33	341.00	6	1464.	0.0	0.0	0.0010	220.00	17	141520.	0.9	0.9	0.0937
34	340.00	10	2123.	0.0	0.0	0.0014	219.00	17	325228.	2.1	2.1	0.2156
35	339.00	8	49390.	0.3	0.3	0.0327	218.00	6	1233.	0.0	0.0	0.0008
36	338.00	8	4629.	0.0	0.0	0.0031	213.00	12	59255.	0.4	0.4	0.0392
37	337.00	10	43583.	0.3	0.3	0.0288	210.00	8	2630.	0.0	0.0	0.0017
38	327.00	8	1695.	0.0	0.0	0.0011	209.00	12	45904.	0.3	0.3	0.0304
39	326.00	10	6495.	0.0	0.0	0.0043	208.00	17	90364.	0.6	0.6	0.0596
40	325.00	12	67468.	0.4	0.4	0.0447	207.00	21	315840.	2.1	2.1	0.2090
41	324.00	8	2393.	0.0	0.0	0.0016	205.00	8	2303.	0.0	0.0	0.0015
42	323.00	10	36793.	0.2	0.2	0.0244	203.00	8	4228.	0.0	0.0	0.0028
43	311.00	8	10184.	0.1	0.1	0.0067	196.00	8	4701.	0.0	0.0	0.0031
44	310.00	14	107588.	0.7	0.7	0.0712	195.00	10	36513.	0.2	0.2	0.0242
45	310.00	10	32702.	0.2	0.2	0.0216	194.00	17	128388.	0.8	0.8	0.0850
46	309.00	17	225144.	1.5	1.5	0.1490	193.00	17	131336.	0.9	0.9	0.0869
47	308.00	6	2282.	0.0	0.0	0.0015	192.00	8	12124.	0.1	0.1	0.0080
48	298.00	10	34989.	0.2	0.2	0.0232	191.00	10	42722.	0.3	0.3	0.0283
49	297.00	17	149636.	1.0	1.0	0.0990	189.00	8	2825.	0.0	0.0	0.0019
50	296.00	14	152776.	1.0	1.0	0.1011	188.00	10	25838.	0.2	0.2	0.0171
51	295.00	14	107648.	0.7	0.7	0.0712	183.00	12	29143.	0.2	0.2	0.0193
52	292.00	8	1877.	0.0	0.0	0.0012	182.00	10	27987.	0.2	0.2	0.0185
53	284.00	12	37698.	0.2	0.2	0.0012	181.00	17	113108.	0.7	0.7	0.0749
54	283.00	17	256360.	1.7	1.7	0.1697	180.00	21	325600.	2.1	2.1	0.2155
55	282.00	17	136716.	0.9	0.9	0.0905	179.00	17	186500.	1.2	1.2	0.1234

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	178.00	8	10963.	0.1	0.1	0.0073	166	100.00	14	85520.	0.6	0.6	0.0566*
112	177.00	12	37078.	0.2	0.2	0.0245*	167	99.00	25	291856.	1.9	1.9	0.1932
113	176.00	8	11573.	0.1	0.1	0.0077	168	98.00	29	2169472.	14.2	14.2	1.4359
114	175.00	14	57064.	0.4	0.4	0.0378*	169	96.00	35	5847808.	38.2	38.2	3.8704
115	169.00	10	56184.	0.4	0.4	0.0372	170	96.00	35	3841728.	25.1	25.1	2.5427*
116	168.00	14	74252.	0.5	0.5	0.0491	171	95.00	35	2458800.	16.0	16.0	1.6274
117	167.00	21	172408.	1.1	1.1	0.1141	172	94.00	21	339312.	2.2	2.2	0.2246
118	166.00	21	289456.	1.9	1.9	0.1916	173	93.00	21	410048.	2.7	2.7	0.2714
119	165.00	21	320944.	2.1	2.1	0.2124	174	92.00	10	37519.	0.2	0.2	0.0248*
120	164.00	14	46181.	0.3	0.3	0.0306*	175	91.00	21	226096.	1.5	1.5	0.1496
121	163.00	14	77888.	0.5	0.5	0.0516	176	87.00	10	2719.	0.0	0.0	0.0018
122	162.00	10	32930.	0.2	0.2	0.0218	177	86.00	14	58642.	0.4	0.4	0.0388*
123	161.00	17	134160.	0.9	0.9	0.0888	178	85.00	29	1117056.	7.3	7.3	0.7393
124	155.00	10	22593.	0.1	0.1	0.0150*	179	84.00	35	3884352.	25.3	25.3	2.5709*
125	154.00	17	164572.	1.1	1.1	0.1089*	180	83.00	35	8355328.	54.5	54.5	5.5301*
126	153.00	21	301808.	2.0	2.0	0.1998	181	82.00	29	3066048.	20.0	20.0	2.0293
127	152.00	21	407264.	2.7	2.7	0.2696	182	81.00	35	3617152.	23.6	23.6	2.3941
128	151.00	25	442768.	2.9	2.9	0.2931	183	80.00	21	424688.	2.8	2.8	0.2811
129	150.00	14	74780.	0.5	0.5	0.0495*	184	79.00	21	777936.	5.1	5.1	0.5149
130	149.00	21	184052.	1.2	1.2	0.1218	185	78.00	10	64573.	0.4	0.4	0.0427*
131	148.00	17	112128.	0.7	0.7	0.0742	186	77.00	21	226416.	1.5	1.5	0.1499
132	147.00	21	237004.	1.5	1.5	0.1569	187	76.00	10	4525.	0.0	0.0	0.0030
133	141.00	10	45245.	0.3	0.3	0.0299	188	75.00	8	16087.	0.1	0.1	0.0106
134	140.00	21	274352.	1.8	1.8	0.1816	189	73.00	17	124044.	0.8	0.8	0.0821*
135	139.00	21	539152.	3.5	3.5	0.3568	190	72.00	17	97448.	0.6	0.6	0.0645*
136	138.00	25	617680.	4.0	4.0	0.4088	191	71.00	29	2195680.	14.3	14.3	1.4538
137	137.00	21	557408.	3.6	3.6	0.3689	192	70.00	35	4786432.	31.2	31.2	3.1680
138	136.00	17	137516.	0.9	0.9	0.0910*	193	69.00	43	11674624.	76.2	76.2	7.7270
139	135.00	25	388688.	2.5	2.5	0.2573	194	68.00	35	3938176.	25.7	25.7	2.6065
140	134.00	17	193540.	1.3	1.3	0.1281	195	67.00	35	4289024.	28.0	28.0	2.8387
141	133.00	25	312592.	2.0	2.0	0.2069*	196	66.00	21	246352.	1.6	1.6	0.1631*
142	131.00	8	19552.	0.1	0.1	0.0129	197	65.00	21	253436.	1.7	1.7	0.1677*
143	127.00	14	66948.	0.4	0.4	0.0443*	198	64.00	12	66064.	0.4	0.4	0.0437*
144	126.00	21	458112.	3.0	3.0	0.3032	199	63.00	6	6046.	0.0	0.0	0.0040
145	125.00	25	1159936.	7.6	7.6	0.7677	200	62.00	8	7176.	0.0	0.0	0.0047
146	124.00	25	915456.	6.0	6.0	0.6059	201	61.00	12	37749.	0.2	0.2	0.0250*
147	123.00	25	1006672.	6.6	6.6	0.6663	202	59.00	12	37358.	0.2	0.2	0.0247*
148	122.00	21	193056.	1.3	1.3	0.1278*	203	58.00	25	255728.	1.7	1.7	0.1693*
149	121.00	21	367040.	2.4	2.4	0.2429	204	57.00	35	6200320.	40.5	40.5	4.1037
150	120.00	17	85476.	0.6	0.6	0.0566	205	56.00	35	5503488.	35.9	35.9	3.6425
151	119.00	25	429376.	2.8	2.8	0.2842	206	55.00	43	15328000.	100.0	100.0	*10.14*
152	118.00	8	4715.	0.0	0.0	0.0031	207	54.00	29	3592576.	23.4	23.4	2.3778
153	117.00	6	1548.	0.0	0.0	0.0010	208	53.00	25	900912.	5.9	5.9	0.5963
154	115.00	6	1501.	0.0	0.0	0.0010	209	52.00	14	37693.	0.2	0.2	0.0249*
155	114.00	6	1771.	0.0	0.0	0.0012	210	51.00	25	740640.	4.9	4.9	0.4955
156	113.00	29	481088.	3.1	3.1	0.3184*	211	50.00	10	32460.	0.2	0.2	0.0188*
157	112.00	25	883008.	5.8	5.8	0.5844	212	47.00	12	32460.	0.2	0.2	0.0215*
158	111.00	29	2587904.	16.9	16.9	1.7128	213	45.00	21	145396.	0.9	0.9	0.0962*
159	110.00	25	1540032.	10.0	10.0	1.0193	214	44.00	35	456640.	3.0	3.0	0.3022*
160	109.00	25	1283456.	8.4	8.4	0.8495	215	43.00	43	9488896.	61.9	61.9	6.2803*
161	108.00	21	242348.	1.6	1.6	0.1604	216	42.00	35	2242624.	14.6	14.6	1.4843
162	107.00	21	298928.	2.0	2.0	0.1978	217	41.00	35	10033408.	65.5	65.5	6.6407
163	106.00	8	12509.	0.1	0.1	0.0083	218	40.00	21	300624.	2.0	2.0	0.1990*
164	105.00	17	105604.	0.7	0.7	0.0725*	219	39.00	29	1515968.	9.9	9.9	1.0034*
165	103.00	6	6023.	0.0	0.0	0.0040	220	38.00	14	73800.	0.5	0.5	0.048*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	37.00	10	5552.	0.0	0.0	0.0037*
222	36.00	29	247644.	1.6	1.6	0.1639*
223	35.00	8	11425.	0.1	0.1	0.0075*

EXAV4.1 [TIC-113816832, 188X-47469568] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	306.00	12	55169.	0.1	0.1	0.0488	56	76.00	29	1442112.	3.0	3.0	1.2760*
2	305.00	25	780704.	1.6	1.6	0.6908*	57	75.00	25	949696.	2.0	2.0	0.8403
3	304.00	35	6942720.	14.6	14.6	6.1431*	58	74.00	25	972256.	2.0	2.0	0.8603*
4	303.00	21	208852.	0.4	0.4	0.1848*	59	73.00	21	142704.	0.3	0.3	0.1263*
5	286.00	10	32328.	0.1	0.1	0.0286	60	71.00	8	1419.	0.0	0.0	0.0013
6	285.00	17	358864.	0.8	0.8	0.0286	61	70.00	8	19290.	0.0	0.0	0.0171
7	284.00	6	837.	0.0	0.0	0.0007	62	69.00	29	3324544.	7.0	7.0	2.9416*
8	259.00	8	10318.	0.0	0.0	0.0091	63	65.00	17	119204.	0.3	0.3	0.1055*
9	240.00	8	5155.	0.0	0.0	0.0046	64	64.00	25	534560.	1.1	1.1	0.4730*
10	239.00	6	1735.	0.0	0.0	0.0015	65	63.00	21	180264.	0.4	0.4	0.1595*
11	219.00	8	4888.	0.0	0.0	0.0043	66	62.00	17	122268.	0.3	0.3	0.1082*
12	207.00	6	1787.	0.0	0.0	0.0016	67	61.00	12	39408.	0.1	0.1	0.0349*
13	185.00	17	166232.	0.4	0.4	0.01471	68	57.00	8	19333.	0.0	0.0	0.0171*
14	181.00	8	3212.	0.0	0.0	0.0028	69	56.00	25	86084.	0.2	0.2	0.0762*
15	169.00	14	149384.	0.3	0.3	0.0122	70	53.00	17	133644.	0.3	0.3	0.1183
16	165.00	10	13848.	0.0	0.0	0.0123	71	52.00	35	543728.	1.1	1.1	0.4811*
17	163.00	10	8254.	0.0	0.0	0.0073	72	51.00	43	18899200.	23.0	23.0	9.6439*
18	150.00	12	22630.	0.0	0.0	0.0200	73	50.00	35	3830976.	8.1	8.1	3.3897*
19	141.00	14	31852.	0.2	0.2	0.0724*	74	49.00	21	164112.	0.3	0.3	0.1452*
20	140.00	8	24861.	0.1	0.1	0.0220	75	47.00	8	4039.	0.0	0.0	0.0036
21	135.00	17	122360.	0.3	0.3	0.1583	76	45.00	17	193736.	0.4	0.4	0.1714*
22	134.00	10	2522.	0.0	0.0	0.0022	77	44.00	17	82284.	0.2	0.2	0.0728*
23	133.00	8	10423.	0.0	0.0	0.0092	78	40.00	6	1290.	0.0	0.0	0.0011
24	131.00	14	76920.	0.2	0.2	0.0681*	79	39.00	25	698496.	1.5	1.5	0.6180
25	123.00	6	2019.	0.0	0.0	0.0018	80	38.00	35	447488.	0.9	0.9	0.3959*
26	121.00	10	7061.	0.0	0.0	0.0062	81	37.00	21	121416.	0.3	0.3	0.1074*
27	120.00	17	155420.	0.3	0.3	0.1375	82	36.00	21	145436.	0.3	0.3	0.1287*
28	119.00	25	783552.	1.7	1.7	0.6933	83	35.00	8	6590.	0.0	0.0	0.0058
29	114.00	6	1426.	0.0	0.0	0.0013							
30	113.00	17	219444.	3.5	0.5	0.1942							
31	111.00	6	2563.	0.0	0.0	0.0023							
32	109.00	8	3970.	0.0	0.0	0.0035							
33	108.00	10	2348.	0.0	0.0	0.0021							
34	107.00	21	197624.	0.4	0.4	0.1749							
35	106.00	35	3446784.	7.3	7.3	3.0498*							
36	105.00	87	47469568.	100.0	100.0	*42.00*							
37	104.00	35	343352.	0.7	0.7	0.3082*							
38	103.00	12	37103.	0.1	0.1	0.0328*							
39	102.00	6	2482.	0.0	0.0	0.0022							
40	101.00	12	8615.	0.0	0.0	0.0076*							
41	100.00	21	450080.	0.9	0.9	0.3982							
42	96.00	8	13634.	0.0	0.0	0.0121							
43	95.00	21	254932.	0.5	0.5	0.2256							
44	94.00	8	4214.	0.0	0.0	0.0037							
45	93.00	14	40533.	0.1	0.1	0.0359							
46	92.00	35	350000.	0.7	0.7	0.3097*							
47	91.00	21	365664.	0.8	0.8	0.3235							
48	85.00	10	4587.	0.0	0.0	0.0041							
49	83.00	17	112200.	0.2	0.2	0.0993*							
50	82.00	12	48952.	0.1	0.1	0.0433							
51	81.00	12	8392.	0.0	0.0	0.0074							
52	80.00	10	4307.	0.0	0.0	0.0038							
53	79.00	10	53834.	0.1	0.1	0.0476*							
54	78.00	25	1538800.	3.2	3.2	1.3616							
55	77.00	59	22766592.	48.0	48.0	*20.14*							

AC6PK.1 [TIC-183186432, 183X-22321152] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	* INT. BASE	* INT. NREF	* TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	* INT. BASE	* INT. NREF	* TOT. ION
1	320.00	14	72136.	0.3	0.3	0.0699	56	93.00	12	46258.	0.2	0.2	0.0448*
2	319.00	21	713328.	3.2	3.2	0.6913*	57	92.00	25	1162112.	5.2	5.2	1.1262
3	318.00	43	5958912.	26.7	26.7	5.7749*	58	91.00	51	15353088.	68.8	68.8	*14.87*
4	317.00	21	311776.	1.4	1.4	0.3021*	59	90.00	35	4137344.	18.5	18.5	4.0096*
5	316.00	6	732.	0.0	0.0	0.0007	60	89.00	35	2488960.	11.2	11.2	2.4121*
6	304.00	10	9172.	0.0	0.0	0.0089	61	88.00	17	86224.	0.4	0.4	0.0036*
7	303.00	17	204616.	0.9	0.9	0.1983	62	87.00	14	98508.	0.4	0.4	0.0055
8	301.00	8	1763.	0.0	0.0	0.0017	63	86.00	17	96596.	0.4	0.4	0.0036*
9	300.00	10	57852.	0.3	0.3	0.0561	64	85.00	10	39968.	0.2	0.2	0.0087*
10	299.00	17	441728.	2.0	2.0	0.4281	65	83.00	17	122148.	0.5	0.5	0.1184*
11	289.00	6	1401.	0.0	0.0	0.0014	66	82.00	10	44192.	0.2	0.2	0.0428*
12	273.00	10	29873.	0.1	0.1	0.0290	67	81.00	8	12991.	0.1	0.1	0.0126
13	269.00	8	3366.	0.0	0.0	0.0033	68	80.00	14	90240.	0.4	0.4	0.0075*
14	255.00	12	2282.	0.0	0.0	0.0022	69	79.00	25	1300096.	5.8	5.8	1.2599
15	254.00	9	5789.	0.0	0.0	0.0056	70	78.00	21	286144.	1.3	1.3	0.2773
16	253.00	8	1333.	0.0	0.0	0.0013	71	77.00	25	1650176.	7.4	7.4	1.5992
17	219.00	8	2454.	0.0	0.0	0.0024	72	76.00	17	158204.	0.7	0.7	0.1533*
18	200.00	6	1277.	0.0	0.0	0.0012	73	75.00	21	279520.	1.3	1.3	0.2709
19	199.00	17	101460.	0.0	0.0	0.0083	74	74.00	21	191644.	0.9	0.9	0.1057
20	181.00	10	4555.	0.0	0.0	0.0044	75	73.00	8	16043.	0.1	0.1	0.0155
21	169.00	14	81320.	0.4	0.4	0.0788	76	70.00	17	67008.	0.3	0.3	0.0649*
22	164.00	6	1888.	0.0	0.0	0.0018	77	69.00	35	2692928.	12.1	12.1	2.6098*
23	163.00	10	5575.	0.0	0.0	0.0054	78	68.00	10	1911.	0.0	0.0	0.0019
24	156.00	6	1335.	0.0	0.0	0.0013	79	67.00	8	6963.	0.0	0.0	0.0067
25	155.00	14	69592.	0.3	0.3	0.0674	80	66.00	21	344608.	1.5	1.5	0.3340
26	151.00	6	1636.	0.0	0.0	0.0016	81	65.00	35	6736384.	30.2	30.2	6.5204*
27	150.00	10	25009.	0.1	0.1	0.0242	82	64.00	25	1092032.	4.9	4.9	1.0583
28	149.00	12	59343.	0.3	0.3	0.0575	83	63.00	29	2401088.	10.8	10.8	2.3269
29	140.00	6	1642.	0.0	0.0	0.0016	84	62.00	25	684544.	3.1	3.1	0.6634
30	137.00	12	42467.	0.2	0.2	0.0412*	85	61.00	21	173004.	0.8	0.8	0.1677*
31	136.00	17	224300.	1.0	1.0	0.2174	86	60.00	10	4140.	0.0	0.0	0.0040
32	135.00	29	2800576.	12.5	12.5	2.7141*	87	59.00	29	369008.	1.7	1.7	0.3576*
33	134.00	17	121784.	0.5	0.5	0.1180	88	57.00	10	3871.	0.0	0.0	0.0038
34	133.00	21	285936.	1.3	1.3	0.2771	89	55.00	10	25564.	0.1	0.1	0.0248*
35	132.00	10	6226.	0.0	0.0	0.0060	90	53.00	25	210108.	0.9	0.9	0.2836
36	131.00	12	76580.	0.3	0.3	0.0742	91	52.00	21	364912.	1.6	1.6	0.3536
37	124.00	6	1237.	0.0	0.0	0.0012	92	51.00	29	2079488.	9.3	9.3	2.0153
38	121.00	17	113864.	0.5	0.5	0.1103*	93	50.00	25	805408.	3.6	3.6	0.7805
39	120.00	35	1767936.	7.9	7.9	1.7133*	94	49.00	10	32709.	0.1	0.1	0.0317*
40	119.00	71	22321152.	100.0	100.0	*21.63*	95	47.00	6	4840.	0.0	0.0	0.0047
41	118.00	59	14084608.	63.1	63.1	*13.64*	96	46.00	10	23265.	0.1	0.1	0.0225*
42	117.00	8	2759.	0.0	0.0	0.0027	97	45.00	43	567168.	2.5	2.5	0.5497*
43	116.00	6	2102.	0.0	0.0	0.0020	98	44.00	29	179600.	0.8	0.8	0.1741*
44	115.00	8	1751.	0.0	0.0	0.0017	99	43.00	14	57957.	0.3	0.3	0.0562*
45	113.00	17	207836.	0.9	0.9	0.0014	100	42.00	8	5920.	0.0	0.0	0.0057
46	109.00	17	102204.	0.5	0.5	0.0990	101	41.00	25	693456.	3.1	3.1	0.6720*
47	107.00	17	195648.	0.9	0.9	0.1935	102	40.00	25	269392.	1.2	1.2	0.2611*
48	106.00	17	114248.	0.5	0.5	0.1107*	103	39.00	35	3169600.	14.2	14.2	3.0717
49	105.00	25	539008.	2.4	2.4	0.5224	104	38.00	25	429696.	1.9	1.9	0.4164*
50	104.00	6	4339.	0.0	0.0	0.0042	105	37.00	14	86308.	0.4	0.4	0.0361*
51	101.00	8	3380.	0.0	0.0	0.0033	106	36.00	8	23667.	0.1	0.1	0.0229
52	100.00	25	404208.	1.8	1.8	0.3917*							
53	99.00	14	75116.	0.3	0.3	0.0728							
54	97.00	8	2719.	0.0	0.0	0.0026							
55	95.00	17	239868.	1.1	1.1	0.2325							

EXAV6.1 [TIC-151927712, 199X-55695240] EI

3-methylbenzoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	320.00	17	126844.	0.2	0.2	0.5840	56	101.00	8	12459.	0.8	0.8	0.0082
2	319.00	25	1253184.	2.3	2.3	0.8298*	57	100.00	21	470112.	0.8	0.8	0.3113
3	318.00	43	11512064.	20.7	20.7	7.6225*	58	99.00	21	272912.	0.5	0.5	0.1807*
4	317.00	25	661408.	1.2	1.2	0.4379*	59	96.00	8	2678.	0.0	0.0	0.0018
5	316.00	17	49053.	0.1	0.1	0.0325*	60	95.00	17	263792.	0.5	0.5	0.1747
6	315.00	8	1148.	0.0	0.0	0.0008	61	94.00	6	1650.	0.0	0.0	0.0011
7	304.00	8	11662.	0.0	0.0	0.0077	62	93.00	17	84740.	0.2	0.2	0.0561*
8	303.00	17	200184.	0.4	0.4	0.1325	63	92.00	29	1971456.	3.5	3.5	1.3054
9	301.00	8	1719.	0.0	0.0	0.0011	64	91.00	59	26208256.	47.1	47.1	*17.35*
10	300.00	14	73432.	0.1	0.1	0.0486	65	90.00	35	2716608.	4.9	4.9	1.7987*
11	299.00	17	634048.	1.1	1.1	0.4198	66	89.00	35	3223040.	5.8	5.8	2.1341*
12	289.00	6	2301.	0.0	0.0	0.0015	67	88.00	29	169360.	0.3	0.3	0.1121*
13	273.00	10	60837.	0.1	0.1	0.0403	68	87.00	21	205164.	0.4	0.4	0.1358
14	269.00	6	1035.	0.0	0.0	0.0007	69	86.00	17	173772.	0.3	0.3	0.1151
15	254.00	6	2244.	0.0	0.0	0.0015	70	85.00	12	52632.	0.1	0.1	0.0348*
16	253.00	8	2074.	0.0	0.0	0.0014	71	84.00	6	1375.	0.0	0.0	0.0009
17	207.00	6	1793.	0.0	0.0	0.0012	72	83.00	17	128124.	0.2	0.2	0.0848
18	200.00	6	2908.	0.0	0.0	0.0019	73	82.00	14	71368.	0.1	0.1	0.0473*
19	199.00	17	169656.	0.3	0.3	0.1123	74	81.00	12	43076.	0.1	0.1	0.0285*
20	181.00	8	2024.	0.0	0.0	0.0013	75	80.00	10	13463.	0.0	0.0	0.0089
21	179.00	8	11859.	0.0	0.0	0.0079	76	79.00	17	112164.	0.2	0.2	0.0743*
22	169.00	17	158996.	0.3	0.3	0.1053*	77	78.00	21	255136.	0.5	0.5	0.1689
23	163.00	8	5719.	0.0	0.0	0.0038	78	77.00	25	487600.	0.9	0.9	0.3229
24	155.00	10	27304.	0.0	0.0	0.0181	79	76.00	21	261360.	0.5	0.5	0.1731
25	154.00	10	19963.	0.0	0.0	0.0132	80	75.00	21	435664.	0.8	0.8	0.2885
26	151.00	8	8918.	0.1	0.1	0.0059	81	74.00	21	274720.	0.5	0.5	0.1819
27	150.00	12	65450.	0.0	0.0	0.0433	82	73.00	10	15344.	0.0	0.0	0.0102
28	149.00	17	270912.	0.5	0.5	0.1794	83	71.00	6	1692.	0.0	0.0	0.0011
29	148.00	8	4121.	0.0	0.0	0.0027	84	70.00	35	145108.	0.3	0.3	0.0961*
30	141.00	8	1990.	0.0	0.0	0.0013	85	69.00	71	3873216.	7.0	7.0	2.5646*
31	137.00	8	4634.	0.0	0.0	0.0031	86	68.00	8	2952.	0.0	0.0	0.0020
32	136.00	8	8899.	0.0	0.0	0.0059	87	67.00	8	11893.	0.0	0.0	0.0079
33	135.00	17	268736.	0.5	0.5	0.1779	88	66.00	21	543664.	1.0	1.0	0.3600
34	134.00	17	127328.	0.2	0.2	0.0843	89	65.00	43	9952512.	17.9	17.9	6.5899*
35	133.00	17	268640.	0.5	0.5	0.1779	90	64.00	29	1511680.	2.7	2.7	1.0009*
36	132.00	8	11102.	0.0	0.0	0.0074	91	63.00	35	3450304.	6.2	6.2	2.2846
37	131.00	14	78504.	0.1	0.1	0.0520	92	62.00	25	1097344.	2.0	2.0	0.7266
38	127.00	6	1679.	0.0	0.0	0.0011	93	61.00	21	245428.	0.4	0.4	0.1625*
39	125.00	6	2555.	0.0	0.0	0.0017	94	60.00	17	10050.	0.0	0.0	0.0067
40	123.00	8	1685.	0.0	0.0	0.0011	95	59.00	35	531408.	1.0	1.0	0.3519*
41	122.00	12	13495.	0.0	0.0	0.0089	96	57.00	8	7062.	0.0	0.0	0.0047
42	121.00	21	276832.	0.5	0.5	0.1833	97	55.00	6	2820.	0.0	0.0	0.0019
43	120.00	35	4682240.	8.4	8.4	3.1003*	98	53.00	25	283456.	0.5	0.5	0.1877
44	119.00	87	55605248.	100.0	100.0	*36.81*	99	52.00	25	529088.	1.0	1.0	0.3508
45	118.00	51	821168.	1.5	1.5	0.5437*	100	51.00	35	2644992.	4.8	4.8	1.7513
46	117.00	17	71388.	0.1	0.1	0.0473*	101	50.00	25	1341632.	2.4	2.4	0.8883*
47	116.00	6	1994.	0.0	0.0	0.0013	102	49.00	17	53384.	0.1	0.1	0.0353*
48	114.00	10	4662.	0.0	0.0	0.0031	103	47.00	8	14139.	0.0	0.0	0.0094*
49	113.00	17	251020.	0.5	0.5	0.0031	104	46.00	17	55237.	0.1	0.1	0.0366*
50	109.00	10	2468.	0.0	0.0	0.1662	105	45.00	51	890400.	1.6	1.6	0.5896*
51	107.00	10	51773.	0.1	0.1	0.0016	106	44.00	43	293584.	0.5	0.5	0.1944*
52	107.00	12	70756.	0.1	0.1	0.0343	107	43.00	17	119320.	0.2	0.2	0.0790*
53	106.00	17	158112.	0.3	0.3	0.0468*	108	42.00	12	28157.	0.1	0.1	0.0186*
54	105.00	25	524832.	0.9	0.9	0.1047	109	41.00	25	1164032.	2.1	2.1	0.7707
55	104.00	8	1212.	0.0	0.0	0.0008	110	40.00	25	340512.	0.6	0.6	0.2255*

PAGE 3

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	39.00	29	4349696.	7.8	7.8	2.8801
112	38.00	35	623152.	1.1	1.1	0.4126*
113	37.00	21	139896.	0.3	0.3	0.0926*
114	36.00	21	173524.	0.3	0.3	0.1149*
115	35.00	8	13881.	0.0	0.0	0.0392

EV3PK.1 [TIC-78958912, 188X-27618384] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	321.00	8	2773.	0.0	0.0	0.0039	56	112.00	8	1123.	0.0	0.0	0.0016
2	320.00	17	52019.	0.2	0.2	0.0733*	57	111.00	8	2309.	0.0	0.0	0.0033
3	319.00	29	519008.	0.2	0.2	0.07315*	58	110.00	8	3040.	0.0	0.0	0.0043
4	318.00	35	4920576.	17.8	17.8	6.9352*	59	109.00	12	26466.	0.1	0.1	0.00373*
5	317.00	25	244612.	0.9	0.9	0.3448*	60	108.00	10	4801.	0.0	0.0	0.0068
6	316.00	14	21355.	0.1	0.1	0.0301*	61	107.00	21	141340.	0.5	0.5	0.1992
7	315.00	6	914.	0.0	0.0	0.0013	62	106.00	17	82116.	0.3	0.3	0.1157*
8	303.00	12	41922.	0.2	0.2	0.0591*	63	105.00	21	284976.	1.0	1.0	0.4017
9	300.00	14	43108.	0.2	0.2	0.0608*	64	104.00	17	10742.	0.0	0.0	0.0151
10	299.00	25	347968.	1.3	1.3	0.4904	65	101.00	8	2568.	0.0	0.0	0.0036
11	298.00	8	3262.	0.0	0.0	0.0046	66	100.00	25	281360.	1.0	1.0	0.3966
12	289.00	17	86984.	0.3	0.3	0.1226*	67	99.00	17	124660.	0.5	0.5	0.1757*
13	281.00	6	889.	0.0	0.0	0.0013	68	96.00	8	1438.	0.0	0.0	0.0020
14	273.00	8	6769.	0.0	0.0	0.0095	69	95.00	25	227812.	0.8	0.8	0.0097
15	269.00	8	761.	0.0	0.0	0.0011	70	94.00	10	6885.	0.2	0.2	0.0853*
16	254.00	8	9047.	0.0	0.0	0.0128	71	93.00	17	60552.	2.9	2.9	*15.00*
17	249.00	10	3141.	0.0	0.0	0.0044	72	92.00	35	797392.	38.5	38.5	1.7469*
18	237.00	8	795.	0.0	0.0	0.0011	73	91.00	51	10643968.	4.5	4.5	2.1154*
19	224.00	10	7022.	0.0	0.0	0.0034	74	90.00	35	1239424.	5.4	5.4	0.1101*
20	219.00	8	2384.	0.0	0.0	0.0023	75	89.00	43	1500864.	0.3	0.3	0.1511*
21	200.00	10	1615.	0.0	0.0	0.0034	76	88.00	29	78100.	0.2	0.2	0.0802*
22	199.00	17	85084.	0.3	0.3	0.1199	77	87.00	17	107176.	0.4	0.4	0.0382*
23	185.00	10	3536.	0.0	0.0	0.0050	78	86.00	17	87896.	0.3	0.3	0.0686*
24	181.00	8	11889.	0.0	0.0	0.0168	79	85.00	17	41857.	0.2	0.2	0.0590
25	179.00	10	3906.	0.0	0.0	0.0055	80	83.00	17	56879.	0.1	0.1	0.0802*
26	171.00	6	786.	0.0	0.0	0.0011	81	82.00	17	30719.	0.1	0.1	0.0382*
27	169.00	21	115392.	0.4	0.4	0.1626	82	81.00	10	27094.	0.1	0.1	0.0270*
28	164.00	10	7286.	0.0	0.0	0.0103	83	80.00	10	19133.	0.2	0.2	0.0686*
29	163.00	8	701.	0.0	0.0	0.0010	84	79.00	17	48643.	0.6	0.6	0.2264*
30	155.00	12	42297.	0.2	0.2	0.0596*	85	78.00	21	160612.	0.7	0.7	0.2913
31	154.00	6	1385.	0.0	0.0	0.0020	86	77.00	21	206672.	0.5	0.5	0.1774*
32	153.00	8	1247.	0.0	0.0	0.0018	87	76.00	21	125868.	0.8	0.8	0.3079*
33	150.00	14	34300.	0.1	0.1	0.0483*	88	75.00	25	219428.	0.6	0.6	0.2243*
34	149.00	17	81436.	0.3	0.3	0.1148	89	74.00	21	159176.	0.4	0.4	0.1447*
35	148.00	8	2049.	0.0	0.0	0.0029	90	73.00	12	13272.	0.0	0.0	0.0187
36	145.00	10	3918.	0.0	0.0	0.0055	91	70.00	43	102680.	7.4	7.4	2.8981*
37	141.00	8	2997.	0.0	0.0	0.0042	92	69.00	59	2056256.	0.0	0.0	0.0050
38	137.00	10	3247.	0.0	0.0	0.0046*	93	67.00	8	3580.	0.9	0.9	0.3528*
39	136.00	6	896.	0.0	0.0	0.0013	94	66.00	25	250292.	17.2	17.2	6.6779*
40	135.00	17	50684.	0.2	0.2	0.0714*	95	65.00	43	4738048.	2.5	2.5	0.9758*
41	134.00	14	41675.	0.2	0.2	0.0587*	96	64.00	35	692336.	5.8	5.8	2.2434
42	133.00	17	118612.	0.4	0.4	0.1672*	97	63.00	35	1591680.	1.9	1.9	0.7440
43	132.00	12	17221.	0.1	0.1	0.0243*	98	62.00	29	527904.	0.5	0.5	0.1911*
44	131.00	17	60889.	0.2	0.2	0.0858	99	61.00	21	135608.	0.4	0.4	0.0125
45	127.00	6	1167.	0.0	0.0	0.0016	100	60.00	8	8874.	0.4	0.4	0.1596*
46	126.00	8	2673.	0.0	0.0	0.0038	101	59.00	25	113256.	0.1	0.1	0.0420*
47	122.00	6	1035.	0.0	0.0	0.0015	102	57.00	17	29815.	0.0	0.0	0.0184*
48	121.00	21	130016.	0.5	0.5	0.1832*	103	56.00	12	13057.	0.1	0.1	0.0302
49	120.00	43	2231360.	8.1	8.1	3.1449*	104	55.00	10	21407.	0.0	0.0	0.0052
50	119.00	87	27618304.	100.0	100.0	*38.92*	105	54.00	10	3665.	0.0	0.0	0.2238*
51	118.00	51	350560.	1.3	1.3	0.4941*	106	53.00	29	158763.	0.6	0.6	0.3443
52	117.00	17	33876.	0.1	0.1	0.0477*	107	52.00	25	244256.	0.9	0.9	1.8504
53	115.00	6	3446.	0.0	0.0	0.0049	108	51.00	35	1312896.	4.8	4.8	0.9281*
54	114.00	8	1994.	0.0	0.0	0.0028	109	50.00	35	658464.	2.4	2.4	0.0490*
55	113.00	21	130276.	0.5	0.5	0.1836*	110	49.00	17	34763.	0.1	0.1	

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	47.00	6	2302.	0.0	0.0	0.0032
112	46.00	21	27216.	0.1	0.1	0.0384*
113	45.00	51	412016.	1.5	1.5	0.5807*
114	44.00	35	174332.	0.6	0.6	0.2457*
115	43.00	14	37350.	0.1	0.1	0.0526*
116	42.00	8	5471.	0.0	0.0	0.0077
117	41.00	35	520128.	1.9	1.9	0.7331
118	40.00	25	206284.	0.7	0.7	0.2907*
119	39.00	35	2065280.	7.5	7.5	2.9109
120	38.00	35	288848.	1.0	1.0	0.4071*
121	37.00	17	73912.	0.3	0.3	0.1042*
122	36.00	21	91660.	0.3	0.3	0.1292*
123	35.00	10	10887.	0.0	0.0	0.0153*

AG6AV.1 [TIC-148382288, 188X-74358592] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	415.00	6	1487.	0.0	0.0	0.0011	88.00	17	97140.	0.1	0.1	0.0692*
2	321.00	8	1809.	0.0	0.0	0.0013	87.00	14	108428.	0.1	0.1	0.0772*
3	320.00	12	82052.	0.1	0.1	0.0584*	86.00	12	100532.	0.1	0.1	0.0716*
4	319.00	25	966400.	1.3	1.3	0.6884*	85.00	10	34075.	0.0	0.0	0.0243
5	318.00	43	8571648.	11.5	11.5	6.1059*	83.00	17	206356.	0.3	0.3	0.1470
6	317.00	12	55517.	0.1	0.1	0.0395*	82.00	12	75784.	0.1	0.1	0.0540
7	316.00	6	1378.	0.0	0.0	0.0010	81.00	10	28058.	0.0	0.0	0.0200*
8	301.00	8	2125.	0.0	0.0	0.0015	80.00	12	33812.	0.0	0.0	0.0241*
9	300.00	8	14670.	0.0	0.0	0.0105	79.00	21	527552.	0.7	0.7	0.3758*
10	299.00	17	255772.	0.3	0.3	0.1822	78.00	21	417712.	0.6	0.6	0.2976
11	290.00	10	10226.	0.0	0.0	0.0073	77.00	21	568368.	0.8	0.8	0.4849
12	289.00	12	80548.	0.1	0.1	0.0574	76.00	17	148732.	0.2	0.2	0.1059
13	276.00	10	87828.	0.1	0.1	0.0626	75.00	21	303904.	0.4	0.4	0.2165*
14	259.00	12	6305.	0.0	0.0	0.0045	74.00	17	201940.	0.3	0.3	0.1439*
15	253.00	6	2080.	0.0	0.0	0.0015	73.00	10	33981.	0.0	0.0	0.0242*
16	251.00	6	7180.	0.0	0.0	0.0051	70.00	10	19145.	0.0	0.0	0.0136*
17	219.00	8	2156.	0.0	0.0	0.0015	69.00	29	4242688.	5.7	5.7	3.0222*
18	199.00	12	90128.	0.1	0.1	0.0642	67.00	6	1517.	0.0	0.0	0.0011
19	183.00	8	15741.	0.0	0.0	0.0112	66.00	21	462400.	0.6	0.6	0.3294*
20	181.00	10	2196.	0.0	0.0	0.0016	65.00	35	9344768.	12.6	12.6	6.6567*
21	169.00	14	124608.	0.2	0.2	0.0888	64.00	25	1572736.	2.1	2.1	1.1203
22	158.00	10	60337.	0.1	0.1	0.0430	63.00	35	3089088.	4.2	4.2	2.2805
23	150.00	6	1164.	0.0	0.0	0.0008	62.00	25	816016.	1.1	1.1	0.5813
24	136.00	8	2538.	0.0	0.0	0.0018	61.00	21	279312.	0.4	0.4	0.1990*
25	135.00	17	162704.	0.2	0.2	0.1159	60.00	8	7475.	0.0	0.0	0.0053
26	133.00	14	16671.	0.0	0.0	0.0119	59.00	14	119092.	0.2	0.2	0.0848*
27	133.00	8	112888.	0.2	0.2	0.0804*	57.00	8	22301.	0.0	0.0	0.0159*
28	132.00	8	10253.	0.0	0.0	0.0073	55.00	8	10262.	0.0	0.0	0.0073*
29	131.00	14	128320.	0.2	0.2	0.0914	53.00	17	119596.	0.2	0.2	0.0852*
30	121.00	8	2363.	0.0	0.0	0.0017	52.00	25	681664.	0.9	0.9	0.485E
31	120.00	14	114156.	0.2	0.2	0.0813	51.00	35	3968576.	5.3	5.3	2.8270
32	119.00	29	2395200.	3.2	3.2	1.7062	50.00	29	1169024.	1.6	1.6	0.8327
33	118.00	21	866496.	1.2	1.2	0.6172	49.00	12	66688.	0.1	0.1	0.0475*
34	117.00	8	3426.	0.0	0.0	0.0024	47.00	12	12922.	0.0	0.0	0.0092*
35	114.00	10	11674.	0.0	0.0	0.0083	46.00	21	115272.	0.2	0.2	0.0821*
36	113.00	21	674240.	0.9	0.9	0.4803	45.00	43	1569344.	2.1	2.1	1.1179*
37	111.00	8	9911.	0.0	0.0	0.0071*	44.00	25	312192.	0.4	0.4	0.2224*
38	110.00	12	5485.	0.0	0.0	0.0039	43.00	14	65190.	0.1	0.1	0.0464*
39	109.00	14	111828.	0.2	0.2	0.0797	42.00	21	162848.	0.2	0.2	0.1160*
40	108.00	8	1737.	0.0	0.0	0.0012	41.00	25	1074176.	1.4	1.4	0.7652
41	107.00	17	246400.	0.3	0.3	0.1755	40.00	25	332496.	0.4	0.4	0.2369*
42	106.00	14	151372.	0.2	0.2	0.1078*	39.00	35	4732160.	6.4	6.4	3.3709
43	105.00	17	236448.	0.3	0.3	0.1684*	38.00	25	695440.	0.9	0.9	0.4954
44	104.00	6	1720.	0.0	0.0	0.0012	37.00	17	128824.	0.2	0.2	0.0918*
45	101.00	10	16313.	0.0	0.0	0.0116	36.00	10	49293.	0.1	0.1	0.0351
46	100.00	25	602752.	0.8	0.8	0.4294*						
47	99.00	6	11193.	0.0	0.0	0.0080						
48	96.00	8	3916.	0.0	0.0	0.0028						
49	95.00	21	545824.	0.7	0.7	0.3888						
50	94.00	8	6300.	0.0	0.0	0.0045						
51	93.00	17	199788.	0.3	0.3	0.1423						
52	92.00	35	5435392.	7.3	7.3	3.8719*						
53	91.00	87	74350592.	100.0	100.0	*52.96*						
54	90.00	35	2437184.	3.3	3.3	1.7361*						
55	89.00	35	2932800.	3.9	3.9	2.0892*						

EXAV7.1 [TIC-144682784, 188X-24534816] EI

2,3-dimethylbenzoic acid.
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	335.00	8	4589.	0.5	0.5	0.0032	56	104.00	43	6481920.	26.4	26.4	4.4857*
2	334.00	17	112960.	0.5	0.5	0.0782*	57	103.00	35	4998656.	20.4	20.4	3.4592*
3	333.00	29	839808.	3.4	0.5	0.5812*	58	102.00	29	772752.	3.1	3.1	0.5348*
4	332.00	43	8495872.	34.6	34.6	5.8794*	59	101.00	35	223596.	0.9	0.9	0.1547*
5	331.00	21	502048.	2.0	2.0	0.3474*	60	100.00	21	389488.	1.6	1.6	0.2695
6	330.00	12	34996.	0.1	0.1	0.0242*	61	99.00	14	11532.	0.5	0.5	0.0802*
7	329.00	8	1170.	0.0	0.0	0.0008	62	98.00	10	2551.	0.1	0.1	0.0177*
8	318.00	10	50363.	0.2	0.2	0.0008	63	97.00	6	2528.	0.0	0.0	0.0017*
9	317.00	17	371440.	1.5	0.2	0.0349	64	96.00	12	4984.	0.0	0.0	0.0034
10	314.00	14	97488.	0.4	1.5	0.2570	65	95.00	21	307152.	1.3	1.3	0.2126
11	313.00	21	792120.	3.2	0.4	0.0675	66	94.00	14	38358.	0.2	0.2	0.0265*
12	289.00	6	1272.	0.0	3.2	0.5482*	67	93.00	25	64448.	2.6	2.6	0.4460*
13	288.00	8	5310.	0.0	0.0	0.0009	68	92.00	17	216216.	0.9	0.9	0.1396
14	287.00	12	67588.	0.3	0.0	0.0037	69	91.00	29	2020992.	8.2	8.2	1.3986
15	273.00	6	1313.	0.0	0.3	0.0468	70	90.00	21	41742.	1.7	1.7	0.7889
16	268.00	6	2573.	0.0	0.0	0.0009	71	89.00	25	736656.	3.0	3.0	0.5098
17	214.00	12	2685.	0.0	0.0	0.0018	72	88.00	12	30412.	0.1	0.1	0.0210*
18	207.00	17	159448.	0.6	0.0	0.0019	73	87.00	17	128196.	0.5	0.5	0.0887*
19	169.00	17	141516.	0.6	0.6	0.1103	74	86.00	12	64157.	0.3	0.3	0.0444*
20	168.00	10	14010.	0.1	0.0	0.0008	75	85.00	10	18606.	0.1	0.1	0.0129*
21	163.00	14	73888.	0.3	0.1	0.0097	76	84.00	8	4269.	0.0	0.0	0.0030
22	162.00	6	3057.	0.0	0.3	0.0021	77	83.00	59	352608.	1.4	1.4	0.2440*
23	154.00	8	1802.	0.0	0.0	0.0012	78	82.00	43	178284.	0.7	0.7	0.1234*
24	151.00	12	61208.	0.2	0.0	0.00424	79	81.00	25	61327.	0.2	0.2	0.0424*
25	150.00	21	395760.	1.6	1.6	0.2739	80	80.00	35	333568.	1.4	1.4	0.2308
26	149.00	29	4030912.	16.4	0.2	0.1076*	81	79.00	35	5243648.	21.4	21.4	3.6288*
27	148.00	21	155496.	0.6	16.4	2.7895	82	78.00	35	3603456.	14.7	14.7	2.4937
28	147.00	17	283152.	1.2	0.6	0.1959	83	76.00	43	9001728.	36.7	36.7	6.2294*
29	139.00	6	3929.	0.0	0.0	0.0016	84	75.00	21	476560.	1.9	1.9	0.3298*
30	137.00	6	2115.	0.0	0.0	0.0027	85	74.00	29	531280.	2.2	2.2	0.3677*
31	136.00	6	202924.	0.0	0.0	0.0015	86	73.00	21	291872.	1.2	1.2	0.2020
32	135.00	17	2254016.	9.2	0.0	0.0015	87	70.00	10	13787.	0.1	0.1	0.0095
33	134.00	29	24534016.	100.0	0.8	0.1404*	88	69.00	8	13624.	0.1	0.1	0.0094
34	133.00	59	20958208.	85.4	9.2	0.15598*	89	67.00	29	3331520.	13.6	13.6	2.3055*
35	132.00	71	359072.	1.5	100.0	*16.97*	90	66.00	17	91148.	0.4	0.4	0.0631
36	131.00	35	2060.	0.0	0.0	*14.50*	91	65.00	43	951072.	4.0	4.0	0.6858*
37	130.00	10	42701.	0.0	1.5	0.2485*	92	64.00	43	1654144.	6.7	6.7	1.1447*
38	129.00	12	6649.	0.0	0.0	0.0014	93	63.00	29	850288.	3.5	3.5	0.5884*
39	128.00	10	11537.	0.2	0.0	0.0046*	94	62.00	21	1851136.	7.5	7.5	1.2810
40	127.00	8	301648.	0.0	0.2	0.0296	95	61.00	21	480016.	2.0	2.0	0.3322*
41	126.00	21	145636.	1.2	0.0	0.0080	96	60.00	21	129516.	0.5	0.5	0.0896*
42	125.00	21	1506560.	0.6	1.2	0.0087	97	59.00	6	12615.	0.1	0.1	0.0087*
43	124.00	29	160140.	0.7	0.6	0.2007	98	58.00	43	419008.	1.7	1.7	0.2905*
44	119.00	10	7353.	0.0	0.0	0.1108	99	57.00	8	3063.	0.0	0.0	0.0021
45	118.00	17	10990.	0.0	6.1	1.0426	100	56.00	3	8462.	0.0	0.0	0.0059
46	117.00	6	10990.	0.0	0.7	0.0051*	101	55.00	6	2246.	0.0	0.0	0.0016
47	116.00	10	8690.	0.0	0.0	0.0008	102	54.00	7	76376.	0.3	0.3	0.0529*
48	115.00	10	295088.	1.2	0.0	0.0060	103	53.00	12	46248.	0.2	0.2	0.0320*
49	113.00	17	3847.	0.0	1.2	0.2042	104	52.00	29	1270784.	5.2	5.2	0.8794*
50	111.00	8	1392.	0.0	0.0	0.0027	105	51.00	35	1044304.	4.3	4.3	0.7227*
51	109.00	12	37824.	0.2	0.0	0.0010	106	50.00	51	4467200.	18.2	18.2	3.0914*
52	107.00	17	79556.	0.3	0.2	0.0262*	107	49.00	25	1056704.	4.3	4.3	0.7313
53	106.00	35	1437440.	5.9	0.3	0.0551*	108	48.00	12	42403.	0.2	0.2	0.0293*
54	105.00	51	15559424.	63.4	5.9	0.9947*	109	45.00	21	260376.	1.1	1.1	0.1002
55	105.00	51	15559424.	63.4	53.4	*10.76*	110	44.00	17	101752.	0.4	0.4	0.0704*

PAGE	3	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
		111	43.00	21	223804.	0.9	0.9	0.1549*
		112	42.00	8	8669.	0.0	0.0	0.0060
		113	41.00	21	370032.	1.5	1.5	0.2561
		114	40.00	21	205660.	0.8	0.8	0.1423
		115	39.00	29	2568256.	10.5	10.5	1.7773
		116	38.00	29	354928.	1.4	1.4	0.2456*
		117	37.00	10	34130.	0.1	0.1	0.0236*
		118	36.00	21	167960.	0.7	0.7	0.1162*
		119	35.00	8	3360.	0.0	0.0	0.0023

AC7PK.1 [TIC=96272384, 189X=17732688] EI

2,6-dimethylbenzoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	335.00	8	1415.	0.0	0.4	0.0015	56	80.00	21	217108.	1.2	1.2	0.2255
2	334.00	14	77680.	0.4	0.4	0.0007*	57	79.00	29	3581184.	20.2	20.2	3.7198
3	333.00	25	792160.	4.5	4.5	0.0228*	58	78.00	29	2646080.	14.9	14.9	2.7485*
4	332.00	35	5847296.	33.0	33.0	0.0737*	59	77.00	35	5906688.	33.3	33.3	6.1354*
5	331.00	21	224432.	1.3	1.3	0.2331*	60	76.00	25	295608.	1.7	1.7	0.3070*
6	318.00	8	16899.	0.1	0.1	0.0176*	61	75.00	25	283696.	1.6	1.6	0.2947*
7	317.00	17	192168.	1.1	0.1	0.1996	62	74.00	21	174816.	1.0	1.0	0.1816
8	314.00	12	76456.	0.4	0.4	0.0794	63	70.00	10	6718.	0.0	0.0	0.0070
9	313.00	17	546224.	3.1	3.1	0.5674	64	69.00	29	2176176.	12.3	12.3	2.2625
10	213.00	14	85932.	0.5	0.5	0.0893	65	67.00	17	81920.	0.5	0.5	0.0851*
11	169.00	10	60884.	0.3	0.3	0.0632	66	66.00	43	681936.	3.8	3.8	0.7083*
12	163.00	8	1855.	0.0	0.0	0.0019	67	65.00	35	1031776.	5.8	5.8	1.0717*
13	151.00	8	16265.	0.1	0.1	0.0169	68	64.00	25	505552.	2.9	2.9	0.5255
14	150.00	17	163552.	0.9	0.9	0.1699	69	63.00	25	1123136.	6.3	6.3	1.1666
15	149.00	25	1438208.	8.1	8.1	1.4939	70	62.00	21	324272.	1.8	1.8	0.3368*
16	148.00	14	84844.	0.5	0.5	0.0881	71	61.00	17	99208.	0.6	0.6	0.1030
17	147.00	17	201536.	1.1	1.1	0.2093	72	60.00	8	5233.	0.0	0.0	0.0054
18	135.00	17	114636.	0.6	0.6	0.1191*	73	59.00	17	116684.	0.7	0.7	0.1211*
19	134.00	29	1599808.	9.0	9.0	1.6618*	74	58.00	12	5754.	0.0	0.0	0.0060*
20	133.00	71	17732608.	100.0	100.0	*18.41*	75	57.00	8	3540.	0.0	0.0	0.0037
21	132.00	59	15804160.	89.1	89.1	*16.41*	76	56.00	6	2728.	0.0	0.0	0.0028
22	131.00	21	200784.	1.1	1.1	0.2086*	77	55.00	14	29419.	0.2	0.2	0.0306*
23	123.00	10	27289.	0.2	0.2	0.0283	78	54.00	10	23408.	0.1	0.1	0.0243
24	121.00	17	144392.	0.8	0.8	0.1500	79	53.00	29	801040.	4.5	4.5	0.8321
25	120.00	14	90124.	0.5	0.5	0.0936*	80	52.00	29	719040.	4.1	4.1	0.7469*
26	119.00	25	720032.	4.1	4.1	0.7479	81	51.00	43	2926208.	16.5	16.5	3.0395*
27	118.00	14	75228.	0.4	0.4	0.0781*	82	50.00	29	599104.	3.4	3.4	0.6223*
28	114.00	6	1320.	0.0	0.0	0.0014	83	49.00	8	10740.	0.1	0.1	0.0112
29	113.00	17	179108.	1.0	1.0	0.1860	84	45.00	17	120060.	0.7	0.7	0.1247
30	109.00	8	2093.	0.0	0.0	0.0022	85	44.00	17	93920.	0.5	0.5	0.0976*
31	107.00	12	34952.	0.2	0.2	0.0363*	86	43.00	21	210880.	1.2	1.2	0.2190*
32	106.00	25	827824.	4.7	4.7	0.8599*	87	42.00	8	3674.	0.0	0.0	0.0038
33	105.00	43	9876736.	55.7	55.7	*10.25*	88	41.00	21	279712.	1.6	1.6	0.2085*
34	104.00	35	4257536.	24.0	24.0	4.4224*	89	40.00	25	194632.	1.1	1.1	0.2022*
35	103.00	35	3342464.	18.8	18.8	3.4719*	90	39.00	29	1909312.	10.8	10.8	1.9832
36	102.00	25	501552.	2.8	2.8	0.5210*	91	38.00	21	217672.	1.2	1.2	0.2261*
37	101.00	21	118072.	0.7	0.7	0.1226*	92	37.00	10	17137.	0.1	0.1	0.0178*
38	100.00	17	263776.	1.5	1.5	0.2740	93	36.00	12	22664.	0.1	0.1	0.0235*
39	99.00	8	7495.	0.0	0.0	0.0078	94	35.00	6	1094.	0.0	0.0	0.0011
40	98.00	6	6701.	0.0	0.0	0.0070							
41	97.00	6	4617.	0.0	0.0	0.0048							
42	95.00	17	211064.	1.2	1.2	0.2192							
43	94.00	8	6628.	0.0	0.0	0.0069							
44	93.00	21	339056.	1.9	1.9	0.3522							
45	92.00	17	134308.	0.8	0.8	0.1395							
46	91.00	25	1297856.	7.3	7.3	1.3481							
47	90.00	21	223640.	1.3	1.3	0.2323*							
48	89.00	21	423280.	2.4	2.4	0.4397							
49	88.00	12	577.	0.0	0.0	0.0089							
50	87.00	14	68908.	0.4	0.4	0.0716*							
51	86.00	10	35820.	0.2	0.2	0.0372							
52	85.00	8	6215.	0.0	0.0	0.0065							
53	83.00	35	223604.	1.3	1.3	0.2323*							
54	82.00	17	55681.	0.3	0.3	0.0578*							
55	81.00	8	24825.	0.1	0.1	0.0258*							

AV6AV.1 [TIC-162163296, 166X-23454726] EI

100 90 80 70 60 50 40 30 20 10 0

132

RELATIVE INTENSITY (%)

77 165

51

69

39

81

149

166

150

200

250

300

332 M⁺

317

m/z

2-ethylbenzoic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	334.00	12	78076.	0.3	0.3	0.0482*	56	129.00	14	58285.	0.2	0.2	0.0360*
2	333.00	25	821312.	3.5	3.5	3.5067*	57	128.00	8	2625.	0.0	0.0	0.0016
3	332.00	43	7374848.	31.4	31.4	4.5495*	58	127.00	8	2778.	0.0	0.0	0.0017
4	331.00	17	162428.	0.7	0.7	0.1002*	59	123.00	6	1399.	0.0	0.0	0.0009
5	330.00	8	8885.	0.0	0.0	0.0055	60	122.00	10	6974.	0.0	0.0	0.0043
6	329.00	8	2465.	0.0	0.0	0.0015	61	121.00	12	54917.	0.0	0.0	0.0339
7	319.00	8	13257.	0.1	0.1	0.0082	62	120.00	17	117084.	0.2	0.5	0.0722*
8	318.00	17	243544.	1.0	1.0	0.1502*	63	119.00	29	1433984.	0.5	0.5	0.0846
9	317.00	25	2097664.	8.9	8.9	1.2940*	64	118.00	21	374112.	6.1	6.1	0.2308
10	316.00	12	24554.	0.1	0.1	0.0152*	65	117.00	12	36650.	0.2	1.6	0.0226*
11	315.00	12	101744.	0.4	0.4	0.0628	66	116.00	21	85896.	0.4	0.4	0.0226*
12	314.00	12	84080.	0.4	0.4	0.0519	67	115.00	35	709344.	3.0	3.0	0.0530*
13	313.00	21	675328.	2.9	2.9	0.4166	68	114.00	10	15447.	0.1	0.1	0.4376*
14	312.00	10	1790.	0.0	0.0	0.0011	69	113.00	21	401240.	0.1	1.7	0.0095
15	305.00	8	3449.	0.0	0.0	0.0021	70	111.00	12	10530.	0.0	1.7	0.2475
16	304.00	8	2917.	0.0	0.0	0.0018	71	110.00	12	19295.	0.1	0.1	0.0068
17	303.00	10	75580.	0.3	0.3	0.0466	72	109.00	21	447864.	1.9	1.9	0.0119
18	297.00	6	1759.	0.0	0.0	0.0011	73	108.00	8	5978.	0.0	0.0	0.2764
19	293.00	6	2385.	0.0	0.0	0.0015	74	107.00	17	130288.	0.6	0.6	0.0037
20	289.00	10	15682.	0.1	0.1	0.0097	75	106.00	35	821504.	3.5	3.5	0.0804
21	287.00	8	15490.	0.1	0.1	0.0096	76	105.00	43	9830912.	41.9	41.9	0.5068*
22	285.00	12	54563.	0.2	0.2	0.0337	77	104.00	43	7698432.	32.8	32.8	6.0646*
23	281.00	8	1057.	0.0	0.0	0.0007	78	103.00	51	9225216.	39.3	39.3	4.7491*
24	219.00	8	4441.	0.0	0.0	0.0027	79	102.00	35	1038640.	4.4	4.4	5.6909*
25	214.00	8	2558.	0.0	0.0	0.0016	80	101.00	29	397216.	1.7	1.7	0.6407*
26	213.00	17	161716.	0.7	0.7	0.0098	81	99.00	21	439360.	0.9	1.9	0.2450*
27	190.00	6	861.	0.0	0.0	0.0005	82	98.00	21	202780.	0.1	0.9	0.1251*
28	185.00	8	2510.	0.0	0.0	0.0015	83	97.00	10	32919.	0.0	0.1	0.0203
29	183.00	8	3045.	0.0	0.0	0.0019	84	96.00	12	4236.	0.0	0.0	0.0026*
30	181.00	8	7405.	0.0	0.0	0.0046	85	95.00	8	9710.	0.0	0.0	0.0060
31	169.00	8	119036.	0.5	0.5	0.0734	86	94.00	21	488576.	2.1	2.1	0.3014
32	164.00	12	2652.	0.0	0.0	0.0016	87	94.00	10	10838.	0.0	0.0	0.0067*
33	163.00	10	9290.	0.0	0.0	0.0057	88	93.00	17	127492.	0.0	0.0	0.0078
34	162.00	12	3715.	0.0	0.0	0.0023*	89	92.00	21	260876.	0.5	0.5	0.0076
35	161.00	6	2384.	0.0	0.0	0.0015	90	91.00	29	2736448.	1.1	1.1	0.1609
36	153.00	8	1823.	0.0	0.0	0.0011	91	90.00	25	1591424.	11.7	11.7	1.6881*
37	151.00	10	29565.	0.1	0.1	0.0182	92	89.00	29	1836288.	6.8	6.8	0.9817
38	150.00	21	273776.	1.2	1.2	0.1689*	93	88.00	17	80964.	0.3	0.3	0.499*
39	149.00	29	2776192.	11.8	11.8	1.7126*	94	87.00	17	121976.	0.5	0.5	0.0752
40	148.00	17	102104.	0.4	0.4	0.0630*	95	86.00	12	44423.	0.2	0.2	0.0274
41	147.00	17	241936.	1.0	1.0	0.1492	96	85.00	10	16218.	0.1	0.1	0.0100*
42	146.00	8	3555.	0.0	0.0	0.0022	97	84.00	8	5622.	0.0	0.0	0.0035
43	145.00	8	8016.	0.0	0.0	0.0049	98	83.00	25	300000.	1.3	1.3	0.1851*
44	141.00	8	5605.	0.0	0.0	0.0041	99	82.00	35	144832.	0.6	0.6	0.0893*
45	140.00	8	5724.	0.0	0.0	0.0035	100	81.00	43	215760.	0.9	0.9	0.1331*
46	139.00	8	2538.	0.0	0.0	0.0016	101	80.00	21	310016.	1.3	1.3	0.1912*
47	138.00	10	6639.	0.0	0.0	0.0041	102	79.00	35	5108736.	21.8	21.8	3.1515*
48	137.00	17	217956.	0.9	0.9	0.1345	103	78.00	29	3048512.	13.0	13.0	1.8806
49	136.00	14	144340.	0.6	0.6	0.0890*	104	77.00	35	9830144.	41.9	41.9	6.0641*
50	135.00	25	1895040.	8.1	8.1	1.1690*	105	76.00	29	830896.	4.5	4.5	0.6468*
51	134.00	35	1595264.	6.8	6.8	0.9841*	106	75.00	25	563552.	3.5	3.5	0.5126*
52	133.00	59	18051072.	77.0	77.0	*11.13*	107	74.00	21	36771.	2.4	2.4	0.3476
53	132.00	71	23454720.	100.0	100.0	*14.46*	108	73.00	17	36771.	0.2	0.2	0.0227*
54	131.00	71	15114752.	64.4	64.4	9.3241*	109	71.00	8	1653.	0.0	0.0	0.0010
55	130.00	35	330816.	1.4	1.4	0.2041*	110	70.00	12	17035.	0.1	0.1	0.0105*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	69.00	29	4049408.	17.3	17.3	2.4980*
112	67.00	10	28809.	0.1	0.1	0.0178*
113	66.00	25	263312.	1.1	1.1	0.1624*
114	65.00	35	1235456.	5.3	5.3	3.7621*
115	64.00	29	1036912.	4.4	4.4	0.6397
116	63.00	25	1900672.	8.1	8.1	1.1725
117	62.00	25	510160.	2.2	2.2	0.3147*
118	61.00	17	164884.	0.7	0.7	0.1017*
119	60.00	10	7848.	0.0	0.0	0.0048
120	59.00	35	881984.	3.8	3.8	0.5441*
121	58.00	8	5248.	0.0	0.0	0.0032
122	57.00	17	65495.	0.3	0.3	0.0404*
123	56.00	8	8618.	0.0	0.0	0.0053
124	55.00	25	549168.	2.3	2.3	0.3388*
125	54.00	10	27763.	0.1	0.1	0.0171
126	53.00	35	725312.	3.1	3.1	0.4474*
127	52.00	35	811008.	3.5	3.5	0.5003*
128	51.00	43	5157120.	22.0	22.0	5.1814*
129	50.00	25	1582592.	6.7	6.7	0.9763*
130	49.00	17	98408.	0.4	0.4	0.0607*
131	47.00	8	5149.	0.0	0.0	0.0032
132	46.00	6	2947.	0.0	0.0	0.0018
133	45.00	25	528128.	2.3	2.3	0.3258*
134	44.00	17	135432.	0.6	0.6	0.0835*
135	43.00	25	435712.	1.9	1.9	0.2688*
136	42.00	8	12560.	0.1	0.1	0.0077
137	41.00	21	178416.	0.8	0.8	0.1101
138	40.00	21	209504.	0.9	0.9	0.1292*
139	39.00	29	2116480.	9.0	9.0	1.3056
140	38.00	25	357664.	1.5	1.5	0.2206*
141	37.00	17	63936.	0.3	0.3	0.0394*
142	36.00	14	100016.	0.4	0.4	0.0617*
143	35.00	12	9551.	0.0	0.0	0.0059*

EW4PK.1 [TIC=86288512, 188X=42347520] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	335.00	8	3872.	0.0	0.0	0.0045	56	116.00	6	2772.	0.0	0.0	0.0032
2	334.00	21	68576.	0.2	0.2	0.0795*	57	115.00	8	6886.	0.0	0.0	0.0078
3	333.00	25	678592.	1.6	1.6	0.7872*	58	114.00	10	13453.	0.0	0.0	0.0155
4	332.00	43	5397760.	12.7	12.7	6.2613*	59	113.00	25	341104.	0.8	0.8	0.3957
5	331.00	21	115292.	0.1	0.1	0.1337*	60	112.00	6	1252.	0.0	0.0	0.0015
6	330.00	17	26902.	0.1	0.1	0.0312*	61	111.00	8	8673.	0.0	0.0	0.0101
7	314.00	8	25913.	0.1	0.1	0.0301*	62	109.00	14	28528.	0.1	0.1	0.0331*
8	313.00	21	249076.	0.6	0.6	0.2889	63	108.00	8	6564.	0.0	0.0	0.0076
9	304.00	8	3867.	0.0	0.0	0.0045	64	107.00	21	187684.	0.4	0.4	0.2177
10	303.00	17	65061.	0.2	0.2	0.0755	65	106.00	51	3140064.	0.6	0.6	4.2224*
11	290.00	12	31234.	0.1	0.1	0.0362*	66	105.00	87	42347520.	100.0	100.0	*49.12*
12	289.00	17	120088.	0.3	0.3	0.1393*	67	104.00	71	2399232.	5.7	5.7	2.7831*
13	285.00	8	6542.	0.0	0.0	0.0076	68	103.00	43	2408768.	5.7	5.7	2.7941*
14	273.00	6	4920.	0.0	0.0	0.0057	69	102.00	43	359488.	0.8	0.8	0.4170*
15	267.00	10	8845.	0.0	0.0	0.0103	70	101.00	43	160888.	0.4	0.4	0.1865*
16	266.00	8	1455.	0.0	0.0	0.0017	71	100.00	29	234892.	0.6	0.6	0.2725*
17	265.00	10	23311.	0.1	0.1	0.0270	72	98.00	12	5779.	0.0	0.0	0.0067
18	232.00	6	1356.	0.0	0.0	0.0016	73	97.00	6	2068.	0.0	0.0	0.0024
19	231.00	8	1050.	0.0	0.0	0.0012	74	96.00	12	12048.	0.0	0.0	0.0140*
20	219.00	6	2036.	0.0	0.0	0.0024	75	95.00	25	361616.	0.9	0.9	0.4195
21	217.00	10	2454.	0.0	0.0	0.0028	76	94.00	14	18296.	0.0	0.0	0.0212*
22	213.00	17	57736.	0.1	0.1	0.0670	77	93.00	25	151532.	0.4	0.4	0.1758*
23	197.00	6	1148.	0.0	0.0	0.0013	78	92.00	25	106476.	0.3	0.3	0.1235*
24	183.00	10	3997.	0.0	0.0	0.0046	79	91.00	29	683088.	1.6	1.6	0.7924
25	181.00	14	14400.	0.0	0.0	0.0167	80	90.00	25	157728.	0.4	0.4	0.1830
26	169.00	17	71780.	0.2	0.2	0.0833	81	89.00	25	341888.	0.8	0.8	0.3966
27	164.00	12	17214.	0.0	0.0	0.0030	82	88.00	12	5394.	0.0	0.0	0.0063
28	163.00	8	2574.	0.0	0.0	0.0030	83	87.00	14	42842.	0.1	0.1	0.0497*
29	155.00	6	1951.	0.0	0.0	0.0023	84	86.00	10	19290.	0.0	0.0	0.0224
30	154.00	6	1139.	0.0	0.0	0.0013	85	85.00	8	21447.	0.1	0.1	0.0249
31	151.00	6	1849.	0.0	0.0	0.0021	86	83.00	21	115440.	0.3	0.3	0.1339
32	150.00	14	34245.	0.1	0.1	0.0397*	87	82.00	12	32181.	0.1	0.1	0.0373*
33	149.00	21	124672.	0.3	0.3	0.1146*	88	81.00	12	22116.	0.1	0.1	0.0257*
34	148.00	8	4659.	0.0	0.0	0.0054	89	80.00	25	187804.	0.4	0.4	0.2178
35	147.00	8	9516.	0.0	0.0	0.0110	90	79.00	35	2744960.	6.5	6.5	3.1841*
36	146.00	6	9017.	0.0	0.0	0.0010	91	78.00	35	2015808.	4.8	4.8	2.3383*
37	145.00	10	5017.	0.0	0.0	0.0058	92	77.00	35	4067904.	9.6	9.6	4.7187*
38	141.00	10	2202.	0.0	0.0	0.0026	93	76.00	29	267896.	0.6	0.6	0.3050*
39	137.00	14	2853.	0.0	0.0	0.0033*	94	75.00	35	271536.	0.6	0.6	0.3150*
40	135.00	6	620.	0.0	0.0	0.0007	95	74.00	25	135444.	0.3	0.3	0.1571*
41	134.00	12	39941.	0.1	0.1	0.0463	96	73.00	14	16950.	0.0	0.0	0.0197*
42	133.00	25	366704.	0.9	0.9	0.4254	97	71.00	8	2870.	0.0	0.0	0.0033
43	132.00	25	435072.	1.0	1.0	0.5747	98	70.00	10	12310.	0.0	0.0	0.0143
44	131.00	25	167680.	0.4	0.4	0.1910*	99	69.00	35	2087680.	4.9	4.9	2.4217*
45	129.00	6	2415.	0.0	0.0	0.0028	100	68.00	10	3177.	0.0	0.0	0.0037
46	126.00	8	1163.	0.0	0.0	0.0014	101	67.00	12	16512.	0.0	0.0	0.0192*
47	125.00	6	1902.	0.0	0.0	0.0022	102	66.00	35	242204.	0.6	0.6	0.2810*
48	124.00	6	2114.	0.0	0.0	0.0025	103	65.00	29	689824.	1.6	1.6	0.8002
49	123.00	12	19835.	0.0	0.0	0.0230*	104	64.00	35	464144.	1.1	1.1	0.5384*
50	122.00	8	6305.	0.0	0.0	0.0073	105	63.00	35	822816.	1.9	1.9	0.9544*
51	121.00	17	96104.	0.2	0.2	0.1115	106	62.00	29	249580.	0.6	0.6	0.2895*
52	120.00	17	69728.	0.2	0.2	0.0809*	107	61.00	25	102308.	0.2	0.2	0.1187*
53	119.00	35	653456.	1.5	1.5	0.7580	108	60.00	12	15570.	0.0	0.0	0.0181*
54	118.00	8	5241.	0.0	0.0	0.0061	109	59.00	29	58345.	0.1	0.1	0.0677*
55	117.00	10	12310.	0.0	0.0	0.0143*	110	58.00	10	14346.	0.0	0.0	0.0166*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	57.00	17	33174.	0.1	0.1	0.0385*
112	56.00	14	16224.	0.0	0.0	0.0188*
113	55.00	10	26513.	0.1	0.1	0.0308*
114	54.00	12	28114.	0.1	0.1	0.0326
115	53.00	35	646384.	1.5	1.5	0.7498
116	52.00	59	1513536.	3.6	3.6	1.7557*
117	51.00	51	2946944.	7.0	7.0	3.4184*
118	50.00	35	657040.	1.6	1.6	0.7622*
119	49.00	12	37477.	0.1	0.1	0.0435
120	45.00	21	135620.	0.3	0.3	0.1573*
121	44.00	25	142484.	0.3	0.3	0.1653*
122	43.00	12	14909.	0.0	0.0	0.0173*
123	42.00	21	81916.	0.2	0.2	0.0950*
124	41.00	25	177540.	0.4	0.4	0.2059*
125	40.00	29	135624.	0.3	0.3	0.1573*
126	39.00	35	1435392.	3.4	3.4	1.6650*
127	38.00	35	221408.	0.5	0.5	0.2568*
128	37.00	14	39209.	0.1	0.1	0.0455*
129	36.00	21	104496.	0.2	0.2	0.1212*
130	35.00	14	11275.	0.0	0.0	0.0131*

AG7AV.1 [TIC-15171584N, 155X-46541588] EI

2-phenylbutyric acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	348.00	10	47942.	0.1	0.1	0.0316*	119.00	71	32870400.	71.4	71.4	*21.66*
2	347.00	17	578944.	1.3	0.3	0.3816	118.00	35	2683776.	5.8	5.8	1.7689*
3	346.00	29	3987008.	8.7	8.7	2.6279*	117.00	35	2637568.	5	5.7	1.7385*
4	345.00	8	1002.	0.0	0.0	0.0007	116.00	25	543696.	1.2	1.2	0.3584*
5	331.00	8	31189.	0.1	0.1	0.0206	115.00	29	2107136.	4.6	4.6	1.3889*
6	327.00	8	6520.	0.0	0.0	0.0043	114.00	14	70864.	0.2	0.2	0.0467*
7	319.00	10	59873.	0.1	0.1	0.00395	113.00	25	973904.	2.1	2.1	0.6419*
8	318.00	17	483840.	1.1	0.3	0.3189	111.00	6	318.	0.0	0.0	0.0002
9	317.00	17	327120.	0.7	0.7	0.2156	110.00	6	1665.	0.0	0.0	0.0011
10	303.00	8	1599.	0.0	0.0	0.0011	109.00	17	211260.	0.5	0.5	0.1392
11	298.00	8	9853.	0.0	0.0	0.0065	108.00	8	16212.	0.0	0.0	0.0107
12	291.00	8	3668.	0.0	0.0	0.0024	107.00	21	474688.	1.0	1.0	0.3129
13	290.00	14	210080.	0.5	0.5	0.1385*	106.00	17	213316.	0.5	0.5	0.1406*
14	289.00	21	2004160.	4.4	4.4	1.3210	105.00	25	958240.	2.1	2.1	0.6316
15	286.00	8	12378.	0.0	0.0	0.0082	104.00	29	2381824.	5.2	5.2	1.5699*
16	285.00	14	173232.	0.4	0.4	0.1142	103.00	25	2158848.	4.7	4.7	1.4230*
17	276.00	10	2413.	0.0	0.0	0.0016	102.00	21	483648.	1.1	1.1	0.3188
18	259.00	6	2317.	0.0	0.0	0.0015	101.00	14	68572.	0.1	0.1	0.0452*
19	257.00	6	954.	0.0	0.0	0.0006	100.00	21	388816.	0.0	0.0	0.2563
20	227.00	14	92652.	0.2	0.2	0.0611	98.00	6	1448.	0.0	0.0	0.0014
21	219.00	8	4857.	0.0	0.0	0.0032	97.00	6	2209.	0.0	0.0	0.0015
22	210.00	8	4439.	0.0	0.0	0.0029	96.00	10	5775.	0.0	0.0	0.0038
23	209.00	17	270736.	0.6	0.6	0.1784	95.00	21	741264.	1.6	1.6	0.4886
24	207.00	6	1693.	0.0	0.0	0.0011	93.00	14	140596.	0.3	0.3	0.0927*
25	201.00	8	2321.	0.0	0.0	0.0015	92.00	29	3382080.	7.3	7.3	2.292*
26	198.00	10	37446.	0.1	0.1	0.0247	91.00	71	46041088.	100.0	100.0	*30.34*
27	185.00	10	13622.	0.0	0.0	0.0090	90.00	29	2338176.	5.1	5.1	1.5412*
28	183.00	8	18595.	0.0	0.0	0.0123	89.00	29	1808320.	3.9	3.9	1.1919*
29	181.00	8	5276.	0.0	0.0	0.0035	88.00	17	83684.	0.2	0.2	0.0552*
30	169.00	12	106892.	0.2	0.2	0.0705	87.00	14	114060.	0.2	0.2	0.0752*
31	164.00	8	4517.	0.0	0.0	0.0030	86.00	10	32011.	0.1	0.1	0.0211*
32	163.00	10	12156.	0.0	0.0	0.0080	85.00	14	4451.	0.0	0.0	0.0029*
33	162.00	6	2054.	0.0	0.0	0.0014	83.00	17	229168.	0.5	0.5	0.0162*
34	161.00	8	15303.	0.0	0.0	0.0101	82.00	10	24635.	0.1	0.1	0.0151
35	159.00	8	3040.	0.0	0.0	0.0020	81.00	10	15330.	0.0	0.0	0.0101
36	153.00	8	12523.	0.0	0.0	0.0083	80.00	14	145272.	0.3	0.3	0.0950*
37	151.00	10	6072.	0.0	0.0	0.0040	79.00	29	2376960.	5.2	5.2	1.5667
38	150.00	8	35494.	0.1	0.1	0.0234	78.00	25	2366016.	5.1	5.1	1.5595
39	148.00	8	8747.	0.0	0.0	0.0058	77.00	29	3263808.	7.1	7.1	2.1513*
40	147.00	14	136728.	0.3	0.3	0.0901*	76.00	21	347312.	0.8	0.8	0.2289*
41	146.00	14	163528.	0.4	0.4	0.1078	75.00	21	360336.	0.8	0.8	0.2375*
42	145.00	10	24202.	0.1	0.1	0.0160*	74.00	17	2030088.	0.4	0.4	0.1339*
43	144.00	8	14586.	0.0	0.0	0.0096	73.00	10	13393.	0.0	0.0	0.0088
44	136.00	8	11594.	0.0	0.0	0.0076	71.00	10	10499.	0.0	0.0	0.0069*
45	135.00	17	266256.	0.0	0.0	0.1755	70.00	71	502656.	1.1	1.1	0.3313*
46	134.00	14	89120.	0.2	0.2	0.0587*	69.00	59	40335968.	8.8	8.8	2.6602*
47	133.00	17	256220.	0.6	0.6	0.1689*	68.00	8	6955.	0.0	0.0	0.0046
48	132.00	10	31231.	0.1	0.1	0.0206	67.00	14	15540.	0.0	0.0	0.0102
49	131.00	21	355376.	0.8	0.8	0.2342	66.00	17	149824.	0.3	0.3	0.0908*
50	129.00	14	70236.	0.2	0.2	0.0463	65.00	25	1973696.	4.3	4.3	1.3009*
51	128.00	8	10510.	0.0	0.0	0.0069	64.00	25	877760.	1.9	1.9	0.5786
52	127.00	10	29283.	0.1	0.1	0.0193	63.00	25	1496960.	3.3	3.3	0.9867
53	122.00	10	50494.	0.1	0.1	0.0333	62.00	17	380160.	0.8	0.8	0.2506
54	121.00	14	115724.	0.3	0.3	0.0763*	61.00	12	62378.	0.1	0.1	0.0411
55	120.00	35	2988224.	6.5	6.5	1.9696*	60.00	6	1592.	0.0	0.0	0.0010

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	59.00	8	29816.	0.1	0.1	0.0197
112	58.00	17	134052.	0.3	0.3	0.0884*
113	57.00	25	285088.	0.6	0.6	0.1879*
114	56.00	6	3505.	0.0	0.0	0.0023
115	55.00	17	143500.	0.3	0.3	0.0946*
116	54.00	8	3666.	0.0	0.0	0.0024
117	53.00	21	256928.	0.6	0.6	0.1693*
118	52.00	25	589024.	1.3	1.3	0.3882*
119	51.00	35	4724992.	10.3	10.3	3.1144*
120	50.00	25	838320.	1.8	1.8	0.5526
121	49.00	10	29164.	0.1	0.1	0.0192
122	47.00	8	6804.	0.0	0.0	0.0045
123	46.00	8	2224.	0.0	0.0	0.0015
124	45.00	25	353424.	0.8	0.8	0.2330*
125	44.00	21	199032.	0.4	0.4	0.1312*
126	43.00	17	101696.	0.2	0.2	0.0670*
127	42.00	17	144644.	0.3	0.3	0.0953*
128	41.00	35	4486912.	9.7	9.7	2.9574*
129	40.00	25	250960.	0.5	0.5	0.1654*
130	39.00	35	2800192.	6.1	6.1	1.8457
131	38.00	21	241636.	0.5	0.5	0.1593*
132	37.00	8	31526.	0.1	0.1	0.0208
133	36.00	10	45308.	0.1	0.1	0.0299*

AY7AV.1 [TIC-21863688, 1882-77837568] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	348.00	14	66380.	0.1	0.1	0.0315	56	127.00	12	46900.	0.1	0.1	0.0223*
2	347.00	25	587312.	0.8	0.8	0.2788*	57	124.00	6	951.	0.0	0.0	0.0005
3	346.00	35	4771328.	6.2	6.2	2.2652*	58	123.00	14	88344.	0.1	0.1	0.0419*
4	345.00	12	27411.	0.0	0.0	0.0130*	59	122.00	17	159008.	0.2	0.2	0.0755*
5	344.00	8	1636.	0.0	0.0	0.0008	60	121.00	21	1190208.	1.5	1.5	0.0561
6	343.00	8	7204.	0.0	0.0	0.0034	61	120.00	17	214176.	0.3	0.3	0.1017
7	331.00	12	90784.	0.1	0.1	0.0431	62	119.00	35	4107776.	5.3	5.3	1.9502*
8	330.00	8	2215.	0.0	0.0	0.0011	63	118.00	59	21498880.	27.9	27.9	*10.20*
9	329.00	8	5111.	0.0	0.0	0.0024	64	117.00	43	3297024.	4.3	4.3	1.5653
10	304.00	8	15822.	0.0	0.0	0.0024	65	116.00	43	590384.	0.8	0.8	0.2803*
11	303.00	17	204772.	0.3	0.3	0.0972	66	115.00	25	1532288.	2.0	2.0	0.7275*
12	302.00	8	2043.	0.0	0.0	0.0010	67	114.00	17	75292.	0.1	0.1	0.0357*
13	291.00	12	39946.	0.1	0.1	0.0190	68	113.00	29	1050176.	1.4	1.4	0.4986*
14	290.00	21	632488.	0.8	0.8	0.3003*	69	112.00	6	1379.	0.0	0.0	0.0007
15	289.00	35	13621.	0.0	0.0	0.0065*	70	111.00	8	2651.	0.0	0.0	0.0126
16	288.00	10	3410.	0.0	0.0	0.0016	71	109.00	8	82188.	0.1	0.1	0.0390
17	287.00	10	2285.	0.0	0.0	0.0011	72	108.00	8	8007.	0.0	0.0	0.0038
18	286.00	10	39507.	0.1	0.1	0.0188	73	107.00	21	353504.	0.5	0.5	0.1678
19	285.00	10	1047.	0.0	0.0	0.0005	74	106.00	43	6324224.	8.2	8.2	3.0024*
20	271.00	6	2334.	0.0	0.0	0.0011	75	105.00	57	77037568.	8.0	8.0	*36.57*
21	269.00	6	6679.	0.0	0.0	0.0032	76	104.00	89	6174976.	2.9316*	2.9316*	0.0026
22	255.00	8	58812.	0.1	0.1	0.0279	77	103.00	51	6099200.	7.9	7.9	2.8956*
23	242.00	10	56976.	0.1	0.1	0.0270	78	102.00	43	999904.	1.3	1.3	0.4747*
24	227.00	10	3201.	0.0	0.0	0.0015	79	101.00	35	286272.	0.4	0.4	0.1359*
25	221.00	8	4915.	0.0	0.0	0.0023	80	100.00	21	394968.	0.5	0.5	0.1875
26	219.00	6	1671.	0.0	0.0	0.0008	81	98.00	10	5482.	0.0	0.0	0.0026
27	213.00	6	75712.	0.1	0.1	0.0359	82	97.00	10	3542.	0.0	0.0	0.0017
28	207.00	12	4737.	0.0	0.0	0.0022	83	96.00	12	25742.	0.0	0.0	0.0122
29	201.00	10	1663.	0.0	0.0	0.0008	84	95.00	21	655920.	0.9	0.9	0.3114
30	195.00	6	13049.	0.0	0.0	0.0008	85	94.00	8	6643.	0.0	0.0	0.0032
31	183.00	10	6796.	0.0	0.0	0.0062	86	93.00	17	59846.	0.1	0.1	0.0284
32	181.00	8	2536.	0.0	0.0	0.0032	87	92.00	21	490112.	0.6	0.6	0.2327
33	169.00	17	122684.	0.2	0.2	0.0012	88	91.00	35	6292992.	8.2	8.2	2.9876*
34	165.00	8	7796.	0.0	0.0	0.0037	89	90.00	17	175312.	0.2	0.2	0.0832*
35	164.00	8	1870.	0.0	0.0	0.0009	90	89.00	21	533632.	0.7	0.7	0.2533
36	163.00	14	45604.	0.1	0.1	0.0217*	91	88.00	8	21114.	0.0	0.0	0.0100*
37	162.00	6	1115.	0.0	0.0	0.0005	92	87.00	17	63121.	0.1	0.1	0.0300*
38	161.00	12	54339.	0.0	0.0	0.0031	93	86.00	17	22336.	0.0	0.0	0.0106*
39	150.00	8	12121.	0.1	0.1	0.0258	94	85.00	8	11693.	0.0	0.0	0.0056
40	149.00	8	261080.	0.3	0.3	0.0058	95	83.00	21	272096.	0.4	0.4	0.1292
41	148.00	17	2405056.	3.1	3.1	0.1239	96	82.00	12	30673.	0.0	0.0	0.0146
42	147.00	25	111504.	0.1	0.1	1.1418	97	81.00	14	34221.	0.0	0.0	0.0162*
43	146.00	17	133336.	0.2	0.2	0.0529	98	80.00	25	401024.	0.5	0.5	0.1904
44	145.00	14	9872.	0.0	0.0	0.0633	99	79.00	35	5816320.	7.5	7.5	2.7613*
45	144.00	8	2809.	0.0	0.0	0.0047	100	78.00	29	4692480.	6.1	6.1	2.2278
46	141.00	8	1497.	0.0	0.0	0.0013	101	77.00	35	8053760.	10.5	10.5	3.8235*
47	136.00	6	9780.	0.0	0.0	0.0007	102	76.00	25	587056.	0.8	0.8	0.2787
48	134.00	10	200276.	0.3	0.3	0.0046*	103	75.00	29	557392.	0.7	0.7	0.2646*
49	133.00	21	91688.	0.1	0.1	0.0091	104	74.00	21	411216.	0.5	0.5	0.1952*
50	132.00	14	1013312.	0.1	0.1	0.0435*	105	73.00	35	809568.	1.1	1.1	0.3843*
51	130.00	25	1582.	1.3	1.3	0.4811	106	71.00	8	4117.	0.0	0.0	0.0020
52	129.00	8	35772.	0.0	0.0	0.0008	107	70.00	14	44734.	0.1	0.1	0.0212*
53	129.00	12	16577.	0.0	0.0	0.0170*	108	69.00	35	4365824.	5.7	5.7	2.0727
54	129.00	10	16577.	0.0	0.0	0.0079	109	68.00	6	3323.	0.0	0.0	0.0016
55	128.00	10	16577.	0.0	0.0	0.0079	110	67.00	10	10819.	0.0	0.0	0.0051

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	66.00	21	198788.	0.3	0.3	0.0944
112	65.00	35	1527808.	2.0	2.0	0.7253*
113	64.00	25	703856.	0.9	0.9	0.3342
114	63.00	25	1186496.	1.5	1.5	0.5633
115	62.00	21	286624.	0.4	0.4	0.1361
116	61.00	21	242992.	0.3	0.3	0.1154
117	60.00	21	54450.	0.1	0.1	0.0259*
118	59.00	35	273072.	0.4	0.4	0.1296*
119	58.00	43	646288.	0.8	0.8	0.3068*
120	57.00	43	600032.	0.8	0.8	0.2849*
121	56.00	10	14095.	0.0	0.0	0.6067*
122	55.00	14	8239.	0.1	0.1	0.0391*
123	54.00	8	16034.	0.0	0.0	0.0076
124	53.00	25	532464.	0.7	0.7	0.2528
125	52.00	29	1272768.	1.7	1.7	0.6342*
126	51.00	51	7283968.	9.5	9.5	3.4581*
127	50.00	29	1316288.	1.7	1.7	0.6249
128	49.00	12	39298.	0.1	0.1	0.0187
129	47.00	10	19247.	0.0	0.0	0.0091
130	45.00	25	318784.	0.4	0.4	0.1513*
131	44.00	25	221276.	0.3	0.3	0.1051*
132	43.00	29	1468508.	1.9	1.9	0.6972
133	42.00	35	2391104.	3.1	3.1	1.1352*
134	41.00	35	2980608.	3.9	3.9	1.4150*
135	40.00	35	352800.	0.5	0.5	0.1675*
136	39.00	35	3171648.	4.1	4.1	1.5057*
137	38.00	25	267148.	0.3	0.3	0.1221*
138	37.00	12	31148.	0.0	0.0	0.0148*
139	36.00	17	109304.	0.1	0.1	0.0519*
140	35.00	6	7189.	0.0	0.0	0.0034

EXAV8.1 [TIC-194285568. 100X-59474944] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	348.00	10	27814.	0.0	0.0	0.0143	56	109.00	17	160336.	0.3	0.3	0.0825
2	347.00	17	415664.	0.7	0.7	0.2139	57	108.00	6	1450.	0.0	0.0	0.0007
3	346.00	29	2966592.	5.0	5.0	1.5269*	58	107.00	17	63489.	0.1	0.1	0.0327*
4	345.00	8	1015.	0.0	0.0	0.0005	59	106.00	21	748240.	1.3	1.3	0.3851
5	327.00	8	9854.	0.0	0.0	0.0051	60	105.00	51	12201984.	20.5	20.5	6.2804*
6	307.00	8	1369.	0.0	0.0	0.0007	61	104.00	87	59474944.	100.0	100.0	*30.61*
7	303.00	8	18466.	0.0	0.0	0.0095	62	103.00	59	2239680.	3.8	3.8	1.1528*
8	289.00	8	19855.	0.0	0.0	0.0102	63	102.00	35	444848.	0.7	0.7	0.2290*
9	271.00	8	13015.	0.0	0.0	0.0067	64	101.00	21	88760.	0.1	0.1	0.0457*
10	256.00	6	3493.	0.0	0.0	0.0018	65	100.00	21	321680.	0.5	0.5	0.1656
11	255.00	17	204496.	0.3	0.3	0.1053	66	96.00	10	13279.	0.0	0.0	0.0068
12	249.00	12	52426.	0.1	0.1	0.0270	67	95.00	21	514560.	0.9	0.9	0.2648*
13	243.00	10	48483.	0.1	0.1	0.0250	68	93.00	17	152908.	0.3	0.3	0.0787*
14	242.00	21	939920.	1.6	1.6	0.4838	69	92.00	29	3058112.	5.1	5.1	1.5740
15	241.00	8	1052.	0.0	0.0	0.0005	70	91.00	71	33154048.	55.7	55.7	*17.06*
16	236.00	10	3513.	0.0	0.0	0.0018	71	90.00	29	728880.	1.2	1.2	0.3752*
17	235.00	14	103076.	0.2	0.2	0.0531*	72	89.00	29	1318464.	2.2	2.2	0.6786*
18	227.00	10	32395.	0.1	0.1	0.0167	73	88.00	12	51816.	0.1	0.1	0.0267*
19	213.00	8	7487.	0.0	0.0	0.0039	74	87.00	17	78556.	0.1	0.1	0.0404*
20	209.00	12	84584.	0.1	0.1	0.0435	75	86.00	10	36498.	0.1	0.1	0.0188
21	207.00	12	49671.	0.1	0.1	0.0256	76	85.00	8	16105.	0.0	0.0	0.0083
22	183.00	8	16497.	0.0	0.0	0.0085*	77	84.00	6	1970.	0.0	0.0	0.0010
23	181.00	6	1241.	0.0	0.0	0.0006	78	83.00	17	202552.	0.3	0.3	0.1043
24	169.00	14	90148.	0.2	0.2	0.0464	79	82.00	8	11861.	0.0	0.0	0.0061
25	165.00	8	13152.	0.0	0.0	0.0068	80	81.00	8	15776.	0.0	0.0	0.0081
26	163.00	6	5859.	0.0	0.0	0.0030	81	80.00	14	74704.	0.1	0.1	0.0385*
27	161.00	10	29663.	0.0	0.0	0.0153	82	79.00	25	1107264.	1.9	1.9	0.5699
28	159.00	6	838.	0.0	0.0	0.0004	83	78.00	29	2893824.	4.9	4.9	1.4895*
29	150.00	10	24358.	0.0	0.0	0.0125*	84	77.00	29	2579072.	4.3	4.3	1.3275
30	149.00	14	85300.	0.1	0.1	0.0439	85	76.00	21	284448.	0.5	0.5	0.1454
31	148.00	25	996224.	1.7	1.7	0.5128*	86	75.00	21	299136.	0.5	0.5	0.1540*
32	147.00	43	9997568.	16.8	16.8	5.1458*	87	74.00	25	354080.	0.6	0.6	0.1822*
33	146.00	35	5816064.	9.8	9.8	2.9936*	88	73.00	43	1560320.	2.6	2.6	0.8031*
34	145.00	12	49743.	0.1	0.1	0.0256*	89	70.00	10	24585.	0.0	0.0	0.0127
35	144.00	8	3395.	0.0	0.0	0.0017	90	69.00	29	3120256.	5.2	5.2	1.6060*
36	143.00	6	2149.	0.0	0.0	0.0011	91	67.00	8	18151.	0.0	0.0	0.0093
37	136.00	6	2318.	0.0	0.0	0.0015	92	66.00	21	338784.	0.6	0.6	0.1744*
38	135.00	10	34005.	0.1	0.1	0.0175	93	65.00	35	7014400.	11.8	11.8	3.6104
39	133.00	17	119848.	0.2	0.2	0.0617	94	64.00	25	896864.	1.5	1.5	0.4616*
40	131.00	17	127760.	0.2	0.2	0.0658*	95	63.00	29	1566976.	2.6	2.6	0.8065*
41	130.00	17	154600.	0.3	0.3	0.0796	96	62.00	35	350864.	0.6	0.6	0.1806*
42	129.00	25	1532224.	2.6	2.6	0.7886	97	61.00	25	126836.	0.2	0.2	0.0653*
43	128.00	12	56361.	0.1	0.1	0.0290	98	60.00	21	184336.	0.3	0.3	0.0949
44	127.00	17	102688.	0.2	0.2	0.0529*	99	59.00	43	1340416.	2.3	2.3	0.6899*
45	123.00	12	46817.	0.1	0.1	0.0241	100	58.00	51	1208640.	2.0	2.0	0.6221*
46	121.00	8	8465.	0.0	0.0	0.0044	101	57.00	43	940832.	1.6	1.6	0.4843*
47	120.00	14	48024.	0.1	0.1	0.0247*	102	56.00	21	241492.	0.4	0.4	0.1243*
48	119.00	29	1090304.	1.8	1.8	0.5612	103	55.00	25	1226432.	2.1	2.1	0.6313
49	118.00	21	877184.	1.5	1.5	0.4515	104	54.00	10	13196.	0.0	0.0	0.0068
50	117.00	29	2668160.	4.5	4.5	1.3733*	105	53.00	21	276240.	0.5	0.5	0.1422
51	116.00	21	437792.	0.7	0.7	0.2253*	106	52.00	25	804384.	1.4	1.4	0.4142*
52	115.00	25	1619520.	2.7	2.7	0.8336	107	51.00	35	4435712.	7.5	7.5	2.2831*
53	114.00	17	65568.	0.1	0.1	0.0337*	108	50.00	25	930704.	1.6	1.6	0.4790
54	113.00	35	847872.	1.4	1.4	0.4364*	109	49.00	10	26244.	0.0	0.0	0.0135
55	111.00	8	13395.	0.0	0.0	0.0069	110	48.00	8	2619.	0.0	0.0	0.0013

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	47.00	8	6674.	0.0	0.0	0.0034
112	46.00	17	22621.	0.0	0.0	0.0116*
113	45.00	21	263328.	0.4	0.4	0.1355*
114	44.00	29	579840.	1.0	1.0	0.2984
115	43.00	35	4287480.	7.2	7.2	2.2068
116	42.00	25	832224.	1.4	1.4	0.4284*
117	41.00	29	2442240.	4.1	4.1	1.2570*
118	40.00	25	283616.	0.5	0.5	0.1460
119	39.00	35	3694976.	6.2	6.2	1.9018*
120	38.00	29	310624.	0.5	0.5	0.1599*
121	37.00	10	34404.	0.1	0.1	0.0177
122	36.00	21	185188.	0.3	0.3	0.0953*
123	35.00	8	9968.	0.0	0.0	0.0051

AC8PK.1 [TIC-94187528, 188X-21456896] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	349.00	8	1519.	0.0	0.0	0.0016	56	102.00	21	307136.	1.4	1.4	0.3261*
2	348.00	14	84620.	0.4	0.4	0.0098	57	101.00	12	61345.	0.3	0.3	0.0651*
3	347.00	21	856528.	4.0	4.0	0.0094*	58	100.00	17	200872.	0.9	0.9	0.2133
4	346.00	35	6565120.	30.6	30.6	6.9703*	59	99.00	8	2335.	0.0	0.0	0.0025
5	345.00	21	368464.	1.7	1.7	0.3912*	60	98.00	8	4449.	0.0	0.0	0.0047
6	344.00	8	6845.	0.0	0.0	0.0073	61	97.00	29	88808.	0.4	0.4	0.0943*
7	343.00	6	1744.	0.0	0.0	0.0019	62	96.00	29	90320.	0.4	0.4	0.0959*
8	332.00	10	24070.	0.1	0.1	0.0256	63	95.00	25	212008.	1.0	1.0	0.2251*
9	331.00	17	220376.	1.0	1.0	0.2340	64	94.00	10	19460.	0.1	0.1	0.0207*
10	328.00	12	85852.	0.4	0.4	0.0912	65	93.00	25	364816.	1.7	1.7	0.3873
11	327.00	17	661856.	3.1	3.1	0.7027*	66	92.00	21	490528.	2.3	2.3	0.5208
12	318.00	6	1286.	0.0	0.0	0.0014	67	91.00	35	4961280.	23.1	23.1	5.2674*
13	317.00	10	31054.	0.1	0.1	0.0330	68	90.00	17	112468.	0.5	0.5	0.1194*
14	283.00	6	1260.	0.0	0.0	0.0013	69	89.00	21	269632.	1.3	1.3	0.2863
15	227.00	12	77352.	0.4	0.4	0.0821	70	88.00	8	10944.	0.1	0.1	0.0116*
16	207.00	8	2523.	0.0	0.0	0.0027	71	87.00	12	39945.	0.2	0.2	0.0424
17	178.00	14	3923.	0.0	0.0	0.0042*	72	86.00	8	15034.	0.1	0.1	0.0160
18	175.00	6	1075.	0.0	0.0	0.0011	73	83.00	17	93732.	0.4	0.4	0.0995*
19	169.00	14	69836.	0.3	0.3	0.0741	74	82.00	10	12749.	0.1	0.1	0.0135
20	165.00	10	8901.	0.0	0.0	0.0095*	75	81.00	10	22058.	0.1	0.1	0.0234
21	164.00	17	108088.	0.5	0.5	0.1148*	76	80.00	12	56164.	0.3	0.3	0.0596*
22	163.00	21	890032.	4.1	4.1	0.9450	77	79.00	25	1074800.	5.0	5.0	1.1412
23	162.00	14	98036.	0.9	0.9	0.1049*	78	78.00	25	1063744.	5.0	5.0	1.1294
24	161.00	17	186940.	0.9	0.9	0.1063*	79	77.00	29	2446272.	11.4	11.4	2.5972
25	150.00	10	15344.	0.1	0.1	0.0163*	80	76.00	17	168688.	0.8	0.8	0.1791
26	149.00	21	148636.	0.7	0.7	0.1578*	81	75.00	21	240924.	1.1	1.1	0.2558*
27	148.00	43	2170112.	10.1	10.1	2.3040*	82	74.00	29	327056.	1.5	1.5	0.3472*
28	147.00	59	21456896.	100.0	100.0	*22.78*	83	73.00	35	532400.	2.5	2.5	0.5653*
29	146.00	59	13070336.	60.9	60.9	*13.87*	84	72.00	12	48798.	0.2	0.2	0.0518*
30	145.00	17	108296.	0.5	0.5	0.1150*	85	71.00	10	5158.	0.0	0.0	0.0055*
31	143.00	6	1403.	0.0	0.0	0.0015	86	70.00	10	16514.	0.1	0.1	0.0175*
32	137.00	10	14593.	0.1	0.1	0.0155	87	69.00	29	1867904.	8.7	8.7	1.9832
33	136.00	10	4356.	0.0	0.0	0.0046	88	67.00	21	166176.	0.8	0.8	0.1764*
34	135.00	14	79984.	0.4	0.4	0.0849	89	66.00	25	490016.	2.3	2.3	0.5203*
35	134.00	12	81232.	0.4	0.4	0.0862*	90	65.00	25	1192570.	5.6	5.6	1.2662*
36	133.00	21	273680.	1.3	1.3	0.2906	91	64.00	21	327504.	1.5	1.5	0.3477*
37	132.00	17	103568.	0.5	0.5	0.1100*	92	63.00	25	630576.	3.0	3.0	0.6759
38	131.00	17	101648.	0.5	0.5	0.1079	93	62.00	25	184896.	0.9	0.9	0.1963*
39	129.00	6	3204.	0.0	0.0	0.0034	94	61.00	17	45646.	0.2	0.2	0.0485*
40	121.00	8	18673.	0.1	0.1	0.0198	95	60.00	8	1708.	0.0	0.0	0.0018
41	120.00	21	744336.	3.5	3.5	0.7903	96	59.00	10	25424.	0.1	0.1	0.0270
42	119.00	43	7962880.	37.1	37.1	8.4543*	97	58.00	35	513296.	2.4	2.4	0.5450*
43	118.00	29	2201344.	10.3	10.3	2.3372*	98	57.00	35	281840.	1.3	1.3	0.2992*
44	117.00	35	2534400.	11.8	11.8	2.6908*	99	56.00	8	6145.	0.0	0.0	0.0065
45	116.00	35	421312.	2.0	2.0	0.4473*	100	55.00	17	77876.	0.4	0.4	0.0827*
46	115.00	29	1429760.	6.7	6.7	1.5180*	101	54.00	12	17801.	0.1	0.1	0.0189
47	114.00	17	32803.	0.2	0.2	0.0348*	102	53.00	25	685696.	3.2	3.2	0.7280
48	109.00	21	189684.	0.9	0.9	0.2027	103	52.00	25	499968.	2.3	2.3	0.5308*
49	108.00	6	2516.	0.0	0.0	0.0027	104	51.00	29	1942272.	9.1	9.1	2.0621
50	107.00	10	10614.	0.0	0.0	0.0113	105	50.00	25	388912.	1.8	1.8	0.4129
51	106.00	21	247208.	1.2	1.2	0.2625	106	49.00	14	12362.	0.1	0.1	0.0131*
52	105.00	17	99680.	0.5	0.5	0.1058*	107	46.00	8	1777.	0.0	0.0	0.0019
53	104.00	25	591424.	2.8	2.8	0.6279	108	45.00	17	73552.	0.3	0.3	0.0781*
54	103.00	25	1092224.	5.1	5.1	1.1596*	109	44.00	14	90888.	0.4	0.4	0.0965*
55	103.00	29	1752896.	8.2	8.2	1.8611*	110	43.00	17	189612.	0.9	0.9	0.2013

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	42.00	18	27605.	8.1	8.1	8.8293*
112	41.00	29	1877128.	8.7	8.7	1.5938
113	40.00	25	222916.	1.8	1.8	8.2367*
114	39.00	29	1532736.	7.1	7.1	1.6273
115	38.00	17	183932.	8.5	8.5	8.1183*
116	37.00	18	6658.	8.8	8.8	8.8871
117	36.00	8	12195.	8.1	8.1	8.8129

AG9AV.1 [TIC-130215936, 100X-40704000] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	362.00	8	12223.	0.0	0.0	0.0094	56	128.00	17	263632.	0.6	0.6	0.2025*
2	361.00	17	270752.	0.7	0.7	0.2079*	57	127.00	12	78576.	0.2	0.2	0.0603
3	360.00	21	1823616.	4.5	4.5	1.4005*	58	126.00	6	3747.	0.0	0.0	0.0029
4	331.00	6	1420.	0.0	0.0	0.0011	59	123.00	8	1505.	0.0	0.0	0.0012
5	318.00	6	1148.	0.0	0.0	0.0009	60	122.00	12	31638.	0.1	0.1	0.0243*
6	303.00	8	10272.	0.0	0.0	0.0079	61	120.00	12	42649.	0.1	0.1	0.0328
7	269.00	8	2479.	0.0	0.0	0.0019	62	119.00	29	1214080.	3.0	3.0	0.9324
8	282.00	8	2555.	0.0	0.0	0.0020	63	118.00	29	2347584.	5.8	5.8	1.8028*
9	271.00	10	23065.	0.1	0.1	0.0177	64	117.00	35	5698304.	14.0	14.0	4.3760*
10	270.00	10	50035.	0.1	0.1	0.0384	65	116.00	25	471120.	1.2	1.2	0.3618*
11	269.00	17	646672.	1.6	1.6	0.4966	66	115.00	25	1008272.	2.5	2.5	0.7743
12	268.00	6	2407.	0.0	0.0	0.0018	67	114.00	8	39354.	0.1	0.1	0.0302*
13	263.00	6	1764.	0.0	0.0	0.0014	68	113.00	25	823296.	2.0	2.0	0.6323*
14	256.00	10	33190.	0.1	0.1	0.0255	69	112.00	6	2328.	0.0	0.0	0.0018
15	255.00	17	385072.	0.9	0.9	0.2957	70	111.00	10	14765.	0.0	0.0	0.0113
16	251.00	10	8271.	0.0	0.0	0.0064	71	110.00	12	11358.	0.0	0.0	0.0087*
17	243.00	10	42731.	0.1	0.1	0.0328*	72	109.00	21	141148.	0.3	0.3	0.1084*
18	242.00	17	443904.	1.1	1.1	0.3409	73	108.00	6	3681.	0.0	0.0	0.0028
19	240.00	10	9888.	0.0	0.0	0.0076	74	107.00	8	11426.	0.0	0.0	0.0080
20	239.00	10	59473.	0.1	0.1	0.0457	75	106.00	17	256716.	0.6	0.6	0.1971*
21	235.00	10	14947.	0.0	0.0	0.0115	76	105.00	29	3318208.	8.2	8.2	2.5482*
22	228.00	10	68044.	0.2	0.2	0.0523	77	104.00	35	7755008.	19.1	19.1	5.9555*
23	227.00	21	1129472.	2.8	2.8	0.8674	78	103.00	25	1338800.	3.3	3.3	1.0282*
24	222.00	8	11956.	0.0	0.0	0.0092	79	102.00	17	2422000.	0.1	0.1	0.1860
25	221.00	8	18533.	0.0	0.0	0.0142	80	101.00	12	42965.	0.7	0.7	0.0330*
26	215.00	10	2530.	0.0	0.0	0.0019	81	100.00	17	281424.	0.0	0.0	0.2161
27	213.00	8	2605.	0.0	0.0	0.0020	82	99.00	6	1647.	0.0	0.0	0.0013
28	209.00	8	27721.	0.1	0.1	0.0213	83	97.00	6	1022.	0.0	0.0	0.0008
29	208.00	6	1096.	0.0	0.0	0.0008	84	96.00	6	4694.	0.0	0.0	0.0036
30	193.00	14	3214.	0.0	0.0	0.0029	85	95.00	21	565376.	1.4	1.4	0.4342
31	183.00	8	10564.	0.0	0.0	0.0081	86	94.00	8	5855.	0.0	0.0	0.0045
32	181.00	10	2448.	0.0	0.0	0.0019	87	93.00	21*	392736.	1.0	1.0	0.3016*
33	169.00	12	71544.	0.2	0.2	0.0549	88	92.00	29	6242304.	15.3	15.3	4.7938*
34	163.00	8	22646.	0.1	0.1	0.0174	89	91.00	71	40704000.	100.0	100.0	*31.25*
35	162.00	21	453696.	1.1	1.1	0.3484*	90	90.00	29	442064.	1.1	1.1	0.3395*
36	161.00	29	4416000.	10.8	10.8	3.3913*	91	89.00	25	738160.	1.8	1.8	0.5669
37	160.00	35	7057152.	17.3	17.3	5.4196*	92	87.00	10	20852.	0.1	0.1	0.0160
38	159.00	12	88300.	0.2	0.2	0.0678*	93	86.00	10	6935.	0.0	0.0	0.0054
39	158.00	6	2761.	0.0	0.0	0.0021	94	85.00	10	7254.	0.0	0.0	0.0056
40	156.00	8	2125.	0.0	0.0	0.0016	95	83.00	21	228916.	0.6	0.6	0.1758*
41	151.00	6	1867.	0.0	0.0	0.0014	96	82.00	17	62038.	0.2	0.2	0.0476*
42	150.00	8	41429.	0.1	0.1	0.0318	97	81.00	25	428192.	1.1	1.1	0.3200*
43	146.00	6	2041.	0.0	0.0	0.0016	98	80.00	21	202908.	0.5	0.5	0.1550*
44	145.00	14	97900.	0.2	0.2	0.0752*	99	79.00	25	1315264.	3.2	3.2	1.0101
45	144.00	8	13879.	0.0	0.0	0.0107	100	78.00	29	2741184.	6.7	6.7	2.1051
46	143.00	17	214976.	0.5	0.5	0.1651*	101	77.00	25	2446976.	6.0	6.0	1.6792*
47	142.00	21	596288.	1.5	1.5	0.4579	102	76.00	17	189584.	0.5	0.5	0.1450*
48	141.00	8	12136.	0.0	0.0	0.0093	103	75.00	17	260228.	0.6	0.6	0.1990
49	135.00	12	15379.	0.0	0.0	0.0118	104	74.00	17	122532.	0.3	0.3	0.0941*
50	134.00	10	44382.	0.1	0.1	0.0341	105	73.00	8	26167.	0.1	0.1	0.0201*
51	133.00	25	748112.	1.8	1.8	0.5745	106	71.00	12	23616.	0.1	0.1	0.0181*
52	132.00	29	2856896.	7.0	7.0	2.1940*	107	70.00	14	94884.	0.2	0.2	0.0729*
53	131.00	25	469072.	1.2	1.2	0.3602	108	69.00	29	2516928.	6.2	6.2	1.9329
54	130.00	14	154096.	0.4	0.4	0.1182	109	68.00	17	10312.	0.0	0.0	0.0079
55	129.00	21	569984.	1.4	1.4	0.4377*	110	67.00	17	86644.	0.2	0.2	0.0665*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	66.00	25	343264.	0.8	0.8	0.2636*
112	65.00	35	4519424.	11.1	11.1	3.4707*
113	64.00	25	611600.	1.5	1.5	0.4697*
114	63.00	25	916656.	2.3	2.3	0.77040
115	62.00	17	165138.	0.4	0.4	0.1268*
116	61.00	12	82720.	0.2	0.2	0.0635*
117	60.00	8	3769.	0.0	0.0	0.0029
118	59.00	8	2100.	0.0	0.0	0.0016
119	58.00	12	20723.	0.1	0.1	0.0159*
120	57.00	25	341216.	0.8	0.8	0.2620*
121	56.00	17	114508.	0.3	0.3	0.0879*
122	55.00	35	1341312.	3.3	3.3	1.0301
123	54.00	14	89720.	0.2	0.2	0.0689*
124	53.00	21	351664.	0.9	0.9	0.2701*
125	52.00	25	508688.	1.2	1.2	0.3906*
126	51.00	35	3392512.	8.3	8.3	2.6053
127	50.00	25	544416.	1.3	1.3	0.4181*
128	49.00	8	26412.	0.1	0.1	0.0203*
129	47.00	14	71596.	0.2	0.2	0.0550*
130	46.00	8	3281.	0.0	0.0	0.0025
131	45.00	25	317984.	0.8	0.8	0.2442*
132	44.00	21	226944.	0.6	0.6	0.1743*
133	43.00	35	1234944.	3.0	3.0	0.9484
134	42.00	35	2032192.	5.0	5.0	1.5606
135	41.00	25	1636160.	4.0	4.0	1.2565
136	40.00	25	292480.	0.7	0.7	0.2246*
137	39.00	29	2435520.	6.0	6.0	1.8704
138	38.00	17	136264.	0.3	0.3	0.1046*
139	37.00	10	9174.	0.0	0.0	0.0070
140	36.00	10	30385.	0.1	0.1	0.0233
141	35.00	6	1400.	0.0	0.0	0.0011

AG12AV.1 [TIC-109572096, 109X-15101696] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	404.00	12	67832.	0.4	0.4	0.0615	56	205.00	8	28046.	0.2	0.2	0.0256
2	403.00	17	636112.	0.2	4.2	0.5805	57	204.00	21	545904.	3.6	3.6	0.4982*
3	402.00	25	3241152.	21.5	21.5	2.9580*	58	203.00	29	3926720.	26.0	26.0	3.5837*
4	401.00	12	64913.	0.4	0.4	0.0592*	59	202.00	12	46188.	0.3	0.3	0.0422*
5	385.00	8	1757.	0.0	0.0	0.0016	60	201.00	10	35944.	0.2	0.2	0.0328*
6	384.00	12	120700.	0.8	0.8	0.1102	61	198.00	8	5524.	0.0	0.0	0.0050
7	383.00	17	565552.	3.7	0.5161	0.0066	62	191.00	8	2182.	0.0	0.0	0.0020
8	374.00	12	7265.	0.0	0.0	0.0058	63	187.00	8	1974.	0.0	0.0	0.0018
9	373.00	10	76448.	0.5	0.5	0.0069	64	183.00	8	11737.	0.1	0.1	0.0107
10	361.00	6	8348.	0.1	0.1	0.0076	65	177.00	8	7269.	0.0	0.0	0.0056
11	360.00	14	175976.	1.2	1.2	0.1606	66	176.00	14	95832.	0.6	0.6	0.0075
12	359.00	17	728160.	4.8	4.8	0.6645	67	175.00	21	743184.	4.9	4.9	0.6783
13	358.00	10	11260.	0.1	0.1	0.0103	68	174.00	10	46164.	0.3	0.3	0.0421
14	357.00	8	1896.	0.0	0.0	0.0017	69	173.00	10	51692.	0.3	0.3	0.0472
15	347.00	6	1677.	0.0	0.0	0.0015	70	169.00	10	21828.	0.1	0.1	0.0199
16	346.00	10	77108.	0.5	0.5	0.0084	71	164.00	6	9674.	0.1	0.1	0.0088
17	345.00	17	285904.	1.9	1.9	0.2609	72	163.00	8	1767.	0.0	0.0	0.0016
18	344.00	8	24800.	0.2	0.2	0.0226	73	161.00	8	9586.	0.1	0.1	0.0087
19	343.00	8	2548.	0.0	0.0	0.0023	74	160.00	12	50890.	0.4	0.4	0.0556*
20	333.00	10	4563.	0.0	0.0	0.0042	75	159.00	17	333760.	0.4	0.4	0.0306*
21	332.00	12	95852.	0.6	0.6	0.0085	76	154.00	6	3866.	0.0	0.0	0.0035
22	331.00	17	366992.	2.4	2.4	0.3349	77	153.00	12	13390.	0.1	0.1	0.0122
23	330.00	17	304912.	2.0	2.0	0.2783	78	151.00	8	2255.	0.0	0.0	0.0021
24	321.00	10	8822.	0.1	0.1	0.0081	79	150.00	8	14669.	0.1	0.1	0.0134
25	320.00	17	166500.	1.1	1.1	0.1520*	80	149.00	10	60860.	0.4	0.4	0.0555*
26	319.00	25	1456384.	9.6	9.6	1.3292*	81	148.00	10	59130.	0.4	0.4	0.0540
27	318.00	35	12428544.	82.3	82.3	*11.34*	82	147.00	8	18184.	0.1	0.1	0.0166
28	317.00	35	5527808.	36.6	36.6	5.0445*	83	146.00	14	38108.	0.3	0.3	0.0348*
29	316.00	10	30458.	0.2	0.2	0.0278*	84	145.00	17	443104.	2.9	2.9	0.0444
30	311.00	10	2655.	0.0	0.0	0.0024	85	144.00	8	6331.	0.0	0.0	0.0058
31	306.00	8	21803.	0.1	0.1	0.0199	86	143.00	8	31416.	0.2	0.2	0.0287
32	305.00	14	115276.	0.8	0.8	0.1052	87	142.00	8	5560.	0.0	0.0	0.0051
33	304.00	8	9621.	0.1	0.1	0.0086	88	141.00	8	11014.	0.1	0.1	0.0101
34	303.00	10	12560.	0.1	0.1	0.0115	89	140.00	6	1333.	0.0	0.0	0.0012
35	299.00	6	3848.	0.0	0.0	0.0035	90	137.00	8	8448.	0.1	0.1	0.0077
36	298.00	10	3472.	0.0	0.0	0.0032	91	136.00	17	225820.	1.5	1.5	0.2061*
37	291.00	8	8499.	0.1	0.1	0.0078	92	135.00	25	2566528.	17.0	17.0	0.3423
38	290.00	17	219704.	1.5	1.5	0.2005*	93	134.00	12	41890.	0.3	0.3	0.0382*
39	289.00	21	2052480.	13.6	13.6	1.8732	94	133.00	21	289280.	1.9	1.9	0.2640
40	285.00	8	5224.	0.0	0.0	0.0048	95	132.00	21	341520.	2.3	2.3	0.3117
41	284.00	12	1924.	0.0	0.0	0.0018	96	131.00	25	2418496.	16.0	16.0	2.2072*
42	283.00	12	87788.	0.6	0.6	0.0801	97	130.00	10	33853.	0.2	0.2	0.0309*
43	281.00	10	8246.	0.1	0.1	0.0075	98	129.00	14	141388.	0.9	0.9	0.1290*
44	273.00	10	35559.	0.2	0.2	0.0325	99	128.00	14	141388.	0.9	0.9	0.1296*
45	266.00	6	1706.	0.0	0.0	0.0016	100	127.00	10	42329.	0.3	0.3	0.0386*
46	265.00	6	7177.	0.0	0.0	0.0066	101	123.00	8	2459.	0.0	0.0	0.0022
47	264.00	8	5766.	0.0	0.0	0.0053	102	122.00	14	106124.	0.7	0.7	0.0969*
48	257.00	6	1395.	0.0	0.0	0.0013	103	121.00	10	21548.	0.1	0.1	0.0197
49	253.00	8	3692.	0.0	0.0	0.0034*	104	120.00	17	181500.	1.2	1.2	0.1650*
50	252.00	12	8410.	0.1	0.1	0.0077*	105	119.00	29	2065472.	13.7	13.7	1.8850
51	251.00	8	6274.	0.0	0.0	0.0057	106	118.00	25	2592320.	17.2	17.2	2.3659
52	219.00	14	93128.	0.6	0.6	0.0850*	107	117.00	21	663840.	4.4	4.4	0.6058
53	211.00	6	1663.	0.0	0.0	0.0015	108	116.00	21	307168.	2.0	2.0	0.2803*
54	208.00	6	1967.	0.0	0.0	0.0018	109	115.00	21	729760.	4.8	4.8	0.6660
55	207.00	12	55396.	0.4	0.4	0.0506	110	114.00	8	25808.	0.2	0.2	0.0236

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	113.00	21	476880.	3.2	3.2	0.4345	166	55.00	29	1610496.	10.7	10.7	1.4698
112	111.00	6	1034.	0.0	0.0	0.0009	167	54.00	14	97096.	0.6	0.6	0.0000
113	110.00	8	29636.	0.2	0.2	0.0270*	168	53.00	21	295120.	2.0	2.0	0.2693*
114	109.00	12	45981.	0.3	0.3	0.0416*	169	52.00	17	137804.	0.9	0.9	0.1258*
115	108.00	8	34096.	0.2	0.2	0.0311	170	51.00	29	1039904.	6.9	6.9	0.9491
116	107.00	21	724544.	4.8	4.8	0.6612*	171	50.00	17	198208.	1.3	1.3	0.1809*
117	106.00	17	240976.	1.6	1.6	0.2199*	172	45.00	17	84872.	0.6	0.6	0.0775*
118	105.00	25	1454464.	9.6	9.6	1.3274	173	44.00	35	471232.	3.1	3.1	0.4301*
119	104.00	25	1371456.	7.8	7.8	1.0691	174	43.00	35	12961280.	85.8	85.8	*11.82*
120	103.00	25	1164160.	7.7	7.7	1.0625	175	42.00	25	622992.	4.1	4.1	0.5680
121	102.00	21	242216.	1.6	1.6	0.2211*	176	41.00	35	4833536.	32.0	32.0	4.4113*
122	101.00	12	48203.	0.3	0.3	0.0440	177	40.00	21	208292.	1.4	1.4	0.1901*
123	100.00	14	88532.	0.6	0.6	0.0808*	178	39.00	29	1385216.	9.2	9.2	1.2642
124	98.00	8	7478.	0.0	0.0	0.0068	179	38.00	12	38225.	0.3	0.3	0.0349*
125	97.00	10	26653.	0.2	0.2	0.0243	180	37.00	6	1491.	0.0	0.0	0.0014
126	96.00	12	65804.	0.4	0.4	0.0601*	181	36.00	14	26194.	0.2	0.2	0.0239*
127	95.00	21	391200.	2.6	2.6	0.3570							
128	94.00	10	9709.	0.1	0.1	0.0089*							
129	93.00	12	64505.	0.4	0.4	0.0590*							
130	92.00	25	1124544.	7.4	7.4	1.0263							
131	91.00	43	15101696.	100.0	100.0	*13.78*							
132	90.00	29	3590268.	23.8	23.8	3.2766							
133	89.00	25	1471232.	9.7	9.7	1.3427							
134	88.00	14	38900.	0.3	0.3	0.0355*							
135	87.00	8	7318.	0.0	0.0	0.0067							
136	86.00	10	20704.	0.1	0.1	0.0189*							
137	85.00	21	539600.	3.6	3.6	0.4925							
138	84.00	12	31118.	0.2	0.2	0.0284							
139	83.00	17	154348.	1.0	1.0	0.1409*							
140	82.00	12	78376.	0.5	0.5	0.0715*							
141	81.00	12	52498.	0.3	0.3	0.0478*							
142	80.00	8	25280.	0.2	0.2	0.0231*							
143	79.00	21	306368.	2.0	2.0	0.2796							
144	78.00	25	754816.	5.0	5.0	0.6889							
145	77.00	25	1213312.	8.0	8.0	1.1073							
146	76.00	17	192432.	1.3	1.3	0.1756*							
147	75.00	17	134472.	0.9	0.9	0.1227*							
148	74.00	12	22410.	0.1	0.1	0.0205							
149	73.00	8	6883.	0.0	0.0	0.0063							
150	72.00	8	9810.	0.1	0.1	0.0090							
151	71.00	10	56924.	0.4	0.4	0.0520*							
152	70.00	17	165428.	1.1	1.1	0.1510*							
153	69.00	35	1318720.	8.7	8.7	1.2035*							
154	68.00	10	11752.	0.1	0.1	0.0107							
155	67.00	17	148716.	1.0	1.0	0.1357*							
156	66.00	10	38965.	0.3	0.3	0.0356*							
157	65.00	25	650448.	4.3	4.3	0.5936							
158	64.00	21	327872.	2.2	2.2	0.2992*							
159	63.00	21	461680.	3.1	3.1	0.4213*							
160	62.00	14	66940.	0.4	0.4	0.0611*							
161	61.00	10	7651.	0.1	0.1	0.0070							
162	59.00	8	3588.	0.0	0.0	0.0033							
163	58.00	14	64920.	0.4	0.4	0.0592*							
164	57.00	35	1589376.	10.5	10.5	1.4505*							
165	56.00	25	576160.	3.8	3.8	0.5258							

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
166	55.00	29	1610496.	10.7	10.7	1.4698
167	54.00	14	97096.	0.6	0.6	0.0000
168	53.00	21	295120.	2.0	2.0	0.2693*
169	52.00	17	137804.	0.9	0.9	0.1258*
170	51.00	29	1039904.	6.9	6.9	0.9491
171	50.00	17	198208.	1.3	1.3	0.1809*
172	45.00	17	84872.	0.6	0.6	0.0775*
173	44.00	35	471232.	3.1	3.1	0.4301*
174	43.00	35	12961280.	85.8	85.8	*11.82*
175	42.00	25	622992.	4.1	4.1	0.5680
176	41.00	35	4833536.	32.0	32.0	4.4113*
177	40.00	21	208292.	1.4	1.4	0.1901*
178	39.00	29	1385216.	9.2	9.2	1.2642
179	38.00	12	38225.	0.3	0.3	0.0349*
180	37.00	6	1491.	0.0	0.0	0.0014
181	36.00	14	26194.	0.2	0.2	0.0239*

AC11PK.1 [TIC-189522944, 188X-23342888] EI

Cyclohexylphenylacetic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	401.00	10	77904.	0.3	0.3	0.0711	56	132.00	8	9129.	0.0	0.0	0.0083
2	400.00	14	360704.	1.5	1.5	0.3293	57	131.00	21	286512.	1.2	1.2	0.2616
3	329.00	8	1505.	0.0	0.0	0.0014	58	130.00	21	467984.	2.0	2.0	0.4273
4	322.00	6	515.	0.0	0.0	0.0005	59	129.00	21	1005136.	4.3	4.3	0.9177
5	321.00	10	20216.	0.1	0.1	0.0185	60	128.00	25	705360.	3.0	3.0	0.5440
6	320.00	21	278800.	1.2	1.2	0.2546	61	127.00	21	251644.	1.1	1.1	0.2298
7	319.00	25	2875320.	12.3	12.3	2.6253	62	126.00	8	100066.	0.0	0.0	0.0091
8	318.00	51	23342000.	100.0	100.0	*21.31*	63	122.00	8	7425.	0.0	0.0	0.0059
9	317.00	25	171096.	0.7	0.7	0.1562	64	121.00	8	7184.	0.0	0.0	0.0066
10	316.00	8	11038.	0.0	0.0	0.0101	65	120.00	12	45989.	0.2	0.2	0.0420
11	300.00	8	8901.	0.0	0.0	0.0081	66	119.00	25	929000.	0.0	0.0	0.0042
12	299.00	14	163800.	0.7	0.7	0.1496	67	118.00	35	6223104.	4.0	4.0	0.8482
13	290.00	12	50399.	0.2	0.2	0.0460	68	117.00	25	1028000.	4.4	4.4	0.9393
14	289.00	17	487568.	2.1	2.1	0.4452	69	116.00	21	532512.	2.3	2.3	0.4862
15	281.00	8	7350.	0.0	0.0	0.0067	70	115.00	25	1708032.	7.3	7.3	1.5595
16	253.00	8	2951.	0.0	0.0	0.0027	71	114.00	12	12473.	0.1	0.1	0.0114
17	251.00	8	1700.	0.0	0.0	0.0016	72	113.00	21	237472.	1.0	1.0	0.2168
18	219.00	8	6294.	0.0	0.0	0.0057	73	110.00	8	1637.	0.0	0.0	0.0015
19	207.00	8	10524.	0.0	0.0	0.0096	74	109.00	12	40070.	0.2	0.2	0.0366
20	201.00	8	3435.	0.0	0.0	0.0031	75	108.00	12	52739.	0.0	0.0	0.0482
21	200.00	8	14048.	0.1	0.1	0.0128	76	107.00	21	1055744.	4.5	4.5	0.9639
22	199.00	12	34445.	0.1	0.1	0.0315	77	106.00	17	132668.	0.6	0.6	0.1211
23	198.00	6	1666.	0.0	0.0	0.0015	78	105.00	25	748032.	3.2	3.2	0.6830
24	193.00	6	2152.	0.0	0.0	0.0020	79	104.00	21	292656.	1.3	1.3	0.2672
25	183.00	8	1936.	0.0	0.0	0.0018	80	103.00	21	430560.	1.8	1.8	0.3931
26	181.00	8	19355.	0.1	0.1	0.0177	81	102.00	17	204686.	0.9	0.9	0.1869
27	175.00	6	1837.	0.0	0.0	0.0017	82	101.00	10	21104.	0.1	0.1	0.0193
28	174.00	17	228696.	1.0	1.0	0.2088	83	100.00	14	97048.	0.4	0.4	0.0886
29	173.00	25	1765568.	7.6	7.6	1.6121	84	96.00	10	5706.	0.0	0.0	0.0052
30	172.00	10	44746.	0.2	0.2	0.0409	85	95.00	29	526480.	2.3	2.3	0.4807
31	171.00	17	163188.	0.7	0.7	0.1490	86	94.00	17	8155.	0.0	0.0	0.0074
32	169.00	8	18142.	0.1	0.1	0.0166	87	93.00	8	124800.	0.5	0.5	0.1140
33	163.00	8	2391.	0.0	0.0	0.0022	88	92.00	21	759232.	3.3	3.3	0.6932
34	159.00	6	7317.	0.0	0.0	0.0067	89	91.00	35	8933120.	5.7	5.7	1.2079
35	157.00	8	4616.	0.0	0.0	0.0042	90	90.00	25	1322944.	2.7	2.7	0.5843
36	156.00	8	1230.	0.0	0.0	0.0011	91	89.00	21	630904.	1.1	1.1	0.0159
37	155.00	8	10707.	0.0	0.0	0.0098	92	88.00	8	17305.	0.0	0.0	0.0081
38	154.00	8	5840.	0.0	0.0	0.0053	93	87.00	20	8800.	0.1	0.1	0.0142
39	153.00	10	22599.	0.1	0.1	0.0089	94	86.00	8	15553.	0.1	0.1	0.0118
40	152.00	8	9724.	0.0	0.0	0.0045	95	85.00	8	12078.	0.1	0.1	0.0142
41	151.00	8	4953.	0.0	0.0	0.0089	96	84.00	21	581712.	2.5	2.5	0.5311
42	150.00	8	11779.	0.1	0.1	0.0108	97	83.00	35	9784576.	41.9	41.9	8.9338
43	147.00	8	1968.	0.0	0.0	0.0018	98	82.00	25	53384.	2.3	2.3	0.4874
44	145.00	8	7451.	0.0	0.0	0.0068	99	81.00	25	1283520.	5.5	5.5	1.1719
45	144.00	8	29318.	0.1	0.1	0.0268	100	80.00	17	175632.	0.8	0.8	0.1604
46	143.00	17	160344.	0.7	0.7	0.1464	101	79.00	25	1657856.	7.1	7.1	1.5137
47	142.00	12	52900.	0.2	0.2	0.0483	102	78.00	21	464304.	2.0	2.0	0.4239
48	141.00	17	124620.	0.5	0.5	0.1138	103	77.00	25	1010032.	4.3	4.3	0.9222
49	140.00	8	6970.	0.0	0.0	0.0064	104	76.00	17	103480.	0.4	0.4	0.0945
50	139.00	10	5524.	0.0	0.0	0.0050	105	75.00	14	80140.	0.3	0.3	0.0732
51	137.00	8	8188.	0.0	0.0	0.0075	106	74.00	8	12814.	0.1	0.1	0.0177
52	136.00	17	240500.	1.0	1.0	0.2196	107	73.00	8	1678.	0.0	0.0	0.0015
53	135.00	25	3155136.	13.5	13.5	2.8808	108	71.00	8	12080.	0.1	0.1	0.0110
54	134.00	10	25285.	0.1	0.1	0.0231	109	70.00	8	12489.	0.1	0.1	0.0114
55	133.00	17	97780.	0.4	0.4	0.0893	110	69.00	35	1352960.	5.8	5.8	1.2353

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	68.00	17	71788.	0.3	0.3	0.0655*
112	67.00	25	1365824.	5.9	5.9	1.2471
113	66.00	17	140756.	0.6	0.6	0.1285
114	65.00	25	780832.	3.3	3.3	0.7129
115	64.00	21	276464.	1.2	1.2	0.2524*
116	63.00	21	380048.	1.6	1.6	0.3470*
117	62.00	12	55909.	0.2	0.2	0.0510*
118	61.00	6	6701.	0.0	0.0	0.0061
119	59.00	6	1634.	0.0	0.0	0.0015
120	58.00	8	7333.	0.0	0.0	0.0067
121	57.00	12	30528.	0.1	0.1	0.0279*
122	56.00	25	585472.	2.5	2.5	0.5346
123	55.00	35	14222848.	60.9	60.9	*12.98*
124	54.00	25	619008.	2.7	2.7	0.5652
125	53.00	25	686768.	2.9	2.9	0.6271
126	52.00	21	179628.	0.8	0.8	0.1640*
127	51.00	29	1248512.	5.3	5.3	1.1400
128	50.00	21	151200.	0.6	0.6	0.1381*
129	49.00	6	4145.	0.0	0.0	0.0038
130	45.00	14	67280.	0.3	0.3	0.0614*
131	44.00	25	125900.	0.5	0.5	0.1150*
132	43.00	25	459568.	2.0	2.0	0.4196*
133	42.00	21	272896.	1.2	1.2	0.2492*
134	41.00	35	5806336.	24.9	24.9	5.3015
135	40.00	25	177892.	0.8	0.8	0.1624*
136	39.00	29	1531968.	6.6	6.6	1.3988
137	38.00	8	9666.	0.0	0.0	0.0088
138	37.00	12	22345.	0.1	0.1	0.0204*
139	36.00	21	73908.	0.3	0.3	0.0675*

AC9PK.1 [TIC-8ES44968, 188X-22274848] E1

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	357.00	18	5748.	0.0	0.0	0.0067	56	126.00	35	2709760.	12.2	12.2	3.1676*
2	356.00	21	189688.	0.9	0.9	0.2217*	57	125.00	25	332608.	1.5	1.5	0.3888*
3	355.00	21	1809408.	0.1	0.1	2.1152*	58	123.00	8	3851.	0.0	0.0	0.0045
4	354.00	43	12466944.	56.0	56.0	*14.57*	59	122.00	18	10775.	0.0	0.0	0.0126
5	353.00	21	159976.	0.7	0.7	0.1870*	60	119.00	21	301712.	1.4	1.4	0.3527
6	352.00	8	7555.	0.0	0.0	0.0088	61	118.00	18	38268.	0.2	0.2	0.0447
7	351.00	12	69136.	0.3	0.3	0.0008	62	117.00	8	7029.	0.0	0.0	0.0082
8	350.00	17	405104.	0.3	0.3	0.4736	63	116.00	18	19420.	0.1	0.1	0.0227
9	334.00	6	1700.	0.0	0.0	0.0020	64	115.00	21	267856.	1.2	1.2	0.3131
10	336.00	6	3740.	0.0	0.0	0.0044	65	114.00	21	341088.	1.5	1.5	0.3987
11	315.00	14	85320.	0.4	0.4	0.0097	66	113.00	21	212034.	1.0	1.0	0.2479
12	309.00	6	1578.	0.0	0.0	0.0018	67	111.00	18	5131.	0.0	0.0	0.0060
13	281.00	6	2807.	0.0	0.0	0.0033	68	105.00	12	15935.	0.1	0.1	0.0186*
14	271.00	8	12811.	0.1	0.1	0.0150	69	104.00	29	115424.	0.5	0.5	0.1349*
15	251.00	8	3834.	0.0	0.0	0.0045	70	103.00	6	1246.	0.0	0.0	0.0015
16	235.00	12	47072.	0.2	0.2	0.0550	71	102.00	17	143076.	0.6	0.6	0.1673*
17	227.00	6	1128.	0.0	0.0	0.0013	72	101.00	25	1116544.	5.0	5.0	1.3052
18	219.00	6	5993.	0.0	0.0	0.0016	73	100.00	21	420272.	1.9	1.9	0.4913
19	218.00	8	1336.	0.0	0.0	0.0070	74	99.00	21	226500.	1.0	1.0	0.2648
20	217.00	8	16148.	0.1	0.1	0.0019	75	98.00	21	233584.	1.0	1.0	0.2731
21	208.00	6	1137.	0.0	0.0	0.0013	76	95.00	17	152384.	0.7	0.7	0.1781*
22	207.00	6	8642.	0.0	0.0	0.0101	77	93.00	8	24564.	0.1	0.1	0.0287*
23	202.00	8	2863.	0.0	0.0	0.0033	78	89.00	12	59672.	0.3	0.3	0.0698
24	191.00	8	3809.	0.0	0.0	0.0045	79	88.00	17	115744.	0.5	0.5	0.1353*
25	190.00	8	6729.	0.0	0.0	0.0079	80	87.00	21	324928.	1.5	1.5	0.3798
26	189.00	6	967.	0.0	0.0	0.0011	81	86.00	1	157512.	0.7	0.7	0.1841*
27	187.00	8	3227.	0.0	0.0	0.0038	82	85.00	18	17074.	0.1	0.1	0.0200
28	185.00	14	84012.	0.4	0.4	0.0082	83	83.00	18	29541.	0.1	0.1	0.0345
29	181.00	8	1533.	0.0	0.0	0.0018	84	82.00	8	13849.	0.1	0.1	0.0162
30	172.00	8	5516.	0.0	0.0	0.0064	85	81.00	6	1993.	0.0	0.0	0.0023
31	171.00	17	147840.	0.7	0.7	0.1728	86	78.00	43	1845632.	8.3	8.3	2.1575*
32	170.00	21	285136.	1.3	1.3	0.3333	87	77.00	35	2633984.	11.8	11.8	3.0791*
33	169.00	14	80464.	0.4	0.4	0.0941	88	76.00	21	620416.	2.8	2.8	0.7253
34	168.00	8	3641.	0.0	0.0	0.0043	89	75.00	25	1223552.	5.5	5.5	1.4303
35	164.00	6	1350.	0.0	0.0	0.0016	90	74.00	21	770240.	3.5	3.5	0.9004
36	160.00	6	1027.	0.0	0.0	0.0012	91	73.00	18	18423.	0.1	0.1	0.0215*
37	158.00	6	1121.	0.0	0.0	0.0013	92	70.00	6	1474.	0.0	0.0	0.0017
38	157.00	17	181852.	0.8	0.8	0.2126	93	69.00	29	1540736.	6.9	6.9	1.8011
39	156.00	29	2554368.	11.5	11.5	2.9860*	94	68.00	12	25879.	0.1	0.1	0.0303*
40	155.00	59	22274048.	100.0	100.0	*26.03*	95	65.00	8	15148.	0.1	0.1	0.0177
41	154.00	21	274288.	1.2	1.2	0.3206*	96	64.00	35	1757888.	0.1	0.1	2.0549*
42	153.00	12	46925.	0.2	0.2	0.0549	97	63.00	51	3137152.	7.9	7.9	3.6673*
43	150.00	18	6971.	0.0	0.0	0.0081	98	62.00	25	313008.	14.1	14.1	0.3659*
44	147.00	6	790.	0.0	0.0	0.0009	99	61.00	12	62587.	1.4	1.4	0.0732*
45	146.00	6	3328.	0.0	0.0	0.0039	100	57.00	18	3882.	0.3	0.3	0.0732*
46	144.00	6	1737.	0.0	0.0	0.0020	101	53.00	18	19507.	0.0	0.0	0.0045
47	143.00	18	19778.	0.1	0.1	0.0023	102	52.00	17	146284.	0.7	0.7	0.1710*
48	142.00	14	95520.	0.4	0.4	0.1117	103	51.00	29	1447936.	6.5	6.5	1.6926
49	141.00	14	60384.	0.3	0.3	0.0706*	104	50.00	25	618064.	2.8	2.8	0.7225*
50	133.00	8	12838.	0.1	0.1	0.0150	105	49.00	8	2158.	0.0	0.0	0.0025
51	132.00	6	17741.	0.0	0.0	0.0008	106	45.00	12	51626.	0.2	0.2	0.0603*
52	131.00	18	17741.	0.1	0.1	0.0008	107	44.00	21	127540.	0.6	0.6	0.1491*
53	129.00	17	140092.	0.6	0.6	0.0207	108	41.00	6	2056.	0.0	0.0	0.0024
54	128.00	29	2234752.	10.0	10.0	0.1638	109	40.00	12	15851.	0.1	0.1	0.0185*
55	127.00	51	17513472.	78.6	78.6	*20.47*	110	39.00	21	284576.	1.3	1.3	0.3327*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	38.00	12	48031.	0.2	0.2	0.0561*
112	37.00	6	2872.	0.0	0.0	0.0034
113	36.00	12	13271.	0.1	0.1	0.0155*

AV8AV.i [TIC-15717984, 158X-37485696] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	358.00	5	849.	0.1	0.0	0.0005	56	150.00	10	41992.	0.1	0.1	0.0267
2	357.00	14	33041.	0.1	0.1	0.0210*	57	146.00	8	25304.	0.1	0.1	0.0161
3	356.00	17	240148.	0.6	0.6	0.1528*	58	145.00	12	23173.	0.1	0.1	0.0147
4	355.00	35	3046976.	8.1	8.1	1.9385*	59	144.00	10	3145.	0.0	0.0	0.0020
5	354.00	43	24288256.	64.9	64.9	*15.45*	60	143.00	8	10534.	0.0	0.0	0.0067
6	353.00	25	370544.	1.0	1.0	0.2357*	61	142.00	17	126188.	0.3	0.3	0.0803
7	352.00	17	35630.	0.1	0.1	0.0227*	62	141.00	12	74456.	0.2	0.2	0.0474
8	351.00	10	13530.	0.0	0.0	0.0086*	63	139.00	8	3362.	0.0	0.0	0.0021
9	350.00	10	3297.	0.0	0.0	0.0021	64	133.00	10	32069.	0.1	0.1	0.0204
10	349.00	6	1074.	0.0	0.0	0.0007	65	131.00	12	61686.	0.2	0.2	0.0392*
11	337.00	6	13424.	0.0	0.0	0.0085	66	129.00	17	227160.	0.6	0.6	0.1445
12	336.00	14	145808.	0.4	0.4	0.0928	67	128.00	35	3701952.	9.9	9.9	2.3552*
13	335.00	21	936992.	2.5	2.5	0.5961*	68	127.00	59	30084096.	80.4	80.4	*15.13*
14	326.00	8	1550.	0.0	0.0	0.0010	69	126.00	51	5002496.	13.4	13.4	3.1827*
15	315.00	6	1056.	0.0	0.0	0.0007	70	125.00	43	597296.	1.6	1.6	0.3800*
16	309.00	10	13842.	0.0	0.0	0.0088	71	124.00	8	5737.	0.0	0.0	0.0036
17	291.00	10	9205.	0.0	0.0	0.0059	72	123.00	12	18947.	0.1	0.1	0.0121
18	281.00	14	10312.	0.0	0.0	0.0066	73	122.00	12	52011.	0.1	0.1	0.0331
19	271.00	10	21373.	0.1	0.1	0.0136	74	121.00	10	3475.	0.7	0.0	0.0022
20	251.00	8	10703.	0.0	0.0	0.0068	75	120.00	8	10465.	0.0	0.0	0.0067
21	236.00	12	13808.	0.0	0.0	0.0088	76	119.00	21	456064.	1.2	1.2	0.2902
22	235.00	14	127288.	0.3	0.3	0.0810	77	118.00	10	26103.	0.1	0.1	0.0166
23	221.00	6	1857.	0.0	0.0	0.0012	78	117.00	14	137272.	0.4	0.4	0.0873
24	219.00	6	4417.	0.0	0.0	0.0028	79	116.00	8	5377.	0.0	0.0	0.0034
25	217.00	8	1263.	0.0	0.0	0.0008	80	115.00	14	187672.	0.5	0.5	0.1194
26	215.00	8	2242.	0.0	0.0	0.0014	81	114.00	21	342704.	0.9	0.9	0.2180
27	208.00	8	2016.	0.0	0.0	0.0013	82	113.00	21	217980.	0.6	0.6	0.1387
28	207.00	8	10693.	0.0	0.0	0.0068	83	112.00	8	5691.	0.0	0.0	0.0036
29	202.00	8	10003.	0.0	0.0	0.0064	84	111.00	10	30670.	0.1	0.1	0.0195
30	201.00	10	3300.	0.0	0.0	0.0021	85	110.00	10	3431.	0.0	0.0	0.0022
31	195.00	8	2696.	0.0	0.0	0.0017	86	109.00	8	5846.	0.0	0.0	0.0037
32	191.00	10	33369.	0.1	0.1	0.0212	87	107.00	8	4524.	0.0	0.0	0.0029
33	190.00	12	34815.	0.1	0.1	0.0221*	88	106.00	6	1058.	0.0	0.0	0.0007
34	188.00	8	2049.	0.0	0.0	0.0013	89	105.00	21	81552.	0.2	0.2	0.0519*
35	187.00	8	4629.	0.0	0.0	0.0029	90	104.00	59	360672.	1.0	1.0	0.2295*
36	186.00	12	46958.	0.1	0.1	0.0299	91	103.00	10	15195.	0.0	0.0	0.0097*
37	185.00	17	385744.	1.0	1.0	0.2454	92	102.00	21	216984.	0.6	0.6	0.1380*
38	183.00	8	1979.	0.0	0.0	0.0013	93	101.00	25	2004480.	5.4	5.4	1.2753
39	181.00	10	5515.	0.0	0.0	0.0035	94	100.00	25	857312.	2.3	2.3	0.5454
40	177.00	12	17326.	0.0	0.0	0.0110	95	99.00	21	431248.	1.2	1.2	0.2744*
41	173.00	10	17909.	0.0	0.0	0.0114	96	98.00	25	431488.	1.2	1.2	0.2745*
42	172.00	12	24051.	0.1	0.1	0.0158	97	97.00	10	22360.	0.1	0.1	0.0142
43	171.00	17	77484.	0.2	0.2	0.0493	98	96.00	8	5312.	0.0	0.0	0.0034
44	170.00	17	311680.	0.8	0.8	0.1983	99	95.00	17	251176.	0.7	0.7	0.1598
45	169.00	17	219156.	0.6	0.6	0.1394	100	94.00	10	6385.	0.0	0.0	0.0041
46	167.00	6	1200.	0.0	0.0	0.0008	101	93.00	10	34985.	0.1	0.1	0.0223
47	164.00	6	1439.	0.0	0.0	0.0009	102	92.00	17	199628.	0.5	0.5	0.1270
48	160.00	6	2798.	0.0	0.0	0.0018	103	91.00	10	4323.	0.0	0.0	0.0028
49	158.00	8	4369.	0.0	0.0	0.0028	104	89.00	14	99832.	0.3	0.3	0.0635*
50	157.00	21	321072.	0.9	0.9	0.2043*	105	88.00	17	173836.	0.5	0.5	0.1106
51	156.00	35	4383488.	11.7	11.7	2.7888*	106	87.00	21	701088.	1.9	1.9	0.4460
52	155.00	59	37405696.	100.0	100.0	*23.79*	107	86.00	21	323936.	0.9	0.9	0.2061*
53	154.00	35	425360.	1.1	1.1	0.2706*	108	85.00	14	51406.	0.1	0.1	0.0327*
54	153.00	10	33099.	0.1	0.1	0.0211*	109	83.00	12	57522.	0.2	0.2	0.0366
55	152.00	8	5045.	0.0	0.0	0.0032	110	82.00	10	24922.	0.1	0.1	0.0159

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	81.00	8	22839.	0.1	0.1	0.0145
112	80.00	8	4034.	0.0	0.0	0.0026
113	79.00	8	13270.	0.0	0.0	0.0084
114	78.00	29	1063552.	2.8	2.8	0.6766*
115	77.00	59	10355968.	27.7	27.7	6.5886*
116	76.00	29	1177472.	3.1	3.1	0.7491*
117	75.00	29	2292160.	6.1	6.1	1.4583
118	74.00	25	1558976.	4.2	4.2	0.9918
119	73.00	17	77777.	0.2	0.2	0.0492*
120	70.00	8	10168.	0.0	0.0	0.0065
121	69.00	25	2764416.	7.4	7.4	1.7588*
122	68.00	43	150336.	0.4	0.4	0.0956*
123	67.00	21	29287.	0.1	0.1	0.0186*
124	65.00	29	44893.	0.1	0.1	0.0286
125	64.00	17	1049600.	2.8	2.8	0.6678*
126	63.00	71	9315584.	24.9	24.9	5.9267*
127	62.00	43	742832.	2.0	2.0	0.4726*
128	61.00	17	134080.	0.4	0.4	0.0853*
129	57.00	10	12387.	0.0	0.0	0.0079*
130	55.00	8	3817.	0.0	0.0	0.0024
131	53.00	17	94176.	0.3	0.3	0.0599*
132	52.00	25	297392.	0.8	0.8	0.1892*
133	51.00	29	2447232.	6.5	6.5	1.5570
134	50.00	35	1348288.	3.6	3.6	0.8578*
135	49.00	10	25593.	0.1	0.1	0.0163
136	47.00	8	963.	0.0	0.0	0.0006
137	45.00	17	138952.	0.4	0.4	0.0884*
138	44.00	17	146312.	0.4	0.4	0.0931*
139	43.00	8	7313.	0.0	0.0	0.0047
140	41.00	6	4707.	0.0	0.0	0.0030
141	40.00	14	48985.	0.1	0.1	0.0312*
142	39.00	25	509888.	1.4	1.4	0.3244*
143	38.00	21	180728.	0.5	0.5	0.1150*
144	37.00	10	13276.	0.0	0.0	0.0084
145	36.00	14	63591.	0.2	0.2	0.0405*

AG18AV.1 [TIC=97468416, 188X=38921216] EI

1-naphthylacetic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	371.00	6	4702.	0.4	0.4	0.0048	56	132.00	8	2288.	0.0	0.0	0.0023
2	370.00	14	154200.	0.4	0.4	0.1582	57	131.00	12	71776.	0.2	0.2	0.0736
3	369.00	21	1050432.	2.7	2.7	1.0777*	58	129.00	17	185144.	0.5	0.5	0.1900*
4	368.00	51	10732288.	27.6	27.6	*11.01*	59	128.00	21	501312.	1.3	1.3	0.5143
5	367.00	17	60560.	0.2	0.2	0.0621*	60	127.00	17	307072.	0.8	0.8	0.3150
6	366.00	8	2358.	0.0	0.0	0.0024	61	126.00	17	188764.	0.5	0.5	0.1937*
7	350.00	8	12438.	0.0	0.0	0.0128	62	122.00	8	1849.	0.0	0.0	0.0019
8	349.00	12	149892.	0.4	0.4	0.1538*	63	120.00	8	1846.	0.0	0.0	0.0019
9	340.00	8	1266.	0.0	0.0	0.0013	64	119.00	21	598352.	1.5	1.5	0.6139
10	339.00	8	20850.	0.1	0.1	0.0214	65	117.00	8	15435.	0.0	0.0	0.0158
11	330.00	6	756.	0.0	0.0	0.0008	66	116.00	21	805448.	2.1	2.1	0.8274
12	329.00	8	7514.	0.0	0.0	0.0077	67	115.00	35	8830208.	22.7	22.7	9.0596*
13	326.00	10	44555.	0.1	0.1	0.0457	68	114.00	21	421920.	1.1	1.1	0.4329
14	322.00	17	14438.	0.0	0.0	0.0148	69	113.00	25	1093440.	2.8	2.8	1.1218
15	321.00	17	172140.	0.4	0.4	0.1766	70	112.00	8	12026.	0.0	0.0	0.0123
16	307.00	8	5855.	0.0	0.0	0.0060	71	111.00	12	72272.	0.2	0.2	0.0741
17	303.00	8	14515.	0.0	0.0	0.0149	72	110.00	10	14967.	0.0	0.0	0.0154
18	302.00	10	19268.	0.0	0.0	0.0198	73	109.00	8	2793.	0.0	0.0	0.0029
19	301.00	17	194132.	0.5	0.5	0.1992	74	103.00	8	6214.	0.0	0.0	0.0064
20	281.00	6	1899.	0.0	0.0	0.0019	75	102.00	12	233148.	0.6	0.6	0.2392*
21	271.00	6	1021.	0.0	0.0	0.0010	76	101.00	12	66584.	0.2	0.2	0.0683
22	253.00	8	6372.	0.0	0.0	0.0065	77	99.00	21	336816.	0.9	0.9	0.3456
23	249.00	10	27458.	0.1	0.1	0.0282	78	98.00	10	62947.	0.2	0.2	0.0646
24	207.00	8	12661.	0.0	0.0	0.0130	79	95.00	14	72872.	0.2	0.2	0.0748*
25	191.00	8	2392.	0.0	0.0	0.0025	80	95.00	25	464528.	1.2	1.2	0.4766*
26	190.00	8	2347.	0.0	0.0	0.0024	81	94.00	17	59971.	0.2	0.2	0.0615*
27	186.00	6	4635.	0.0	0.0	0.0048	82	93.00	17	40131.	0.1	0.1	0.0412*
28	185.00	17	125324.	0.3	0.3	0.1286	83	92.00	10	2083.	0.0	0.0	0.0021
29	184.00	10	55327.	0.1	0.1	0.0558	84	91.00	21	363838.	0.9	0.9	0.3733
30	183.00	10	28386.	0.1	0.1	0.0291	85	90.00	12	75588.	0.2	0.2	0.0776*
31	181.00	6	3284.	0.0	0.0	0.0034	86	89.00	25	938624.	2.4	2.4	0.9630
32	171.00	10	1976.	0.0	0.0	0.0020	87	88.00	21	297056.	0.8	0.8	0.3048*
33	170.00	6	13953.	0.0	0.0	0.0143	88	87.00	21	408736.	1.1	1.1	0.4194
34	169.00	21	284304.	0.7	0.7	0.0143	89	86.00	17	200412.	0.5	0.5	0.2056*
35	168.00	17	427824.	1.1	1.1	0.4389	90	85.00	17	89356.	0.2	0.2	0.0917*
36	164.00	6	1948.	0.0	0.0	0.0020	91	84.00	8	22282.	0.1	0.1	0.0229
37	161.00	8	2215.	0.0	0.0	0.0023	92	83.00	14	112096.	0.3	0.3	0.1150*
38	159.00	8	38761.	0.1	0.1	0.0398	93	82.00	6	5045.	0.0	0.0	0.0052
39	158.00	8	1281.	0.0	0.0	0.0013	94	81.00	8	13673.	0.0	0.0	0.0140
40	157.00	14	111076.	0.3	0.3	0.1140*	95	78.00	10	20132.	0.1	0.1	0.0207
41	156.00	17	219400.	0.6	0.6	0.2251	96	77.00	17	241520.	0.6	0.6	0.2478*
42	155.00	17	210572.	0.5	0.5	0.2160	97	76.00	21	281584.	0.7	0.7	0.2889
43	154.00	8	2087.	0.0	0.0	0.0021	98	75.00	25	497088.	1.3	1.3	0.5100*
44	153.00	10	2647.	0.0	0.0	0.0027	99	74.00	21	380144.	1.0	1.0	0.3900*
45	152.00	6	4435.	0.0	0.0	0.0046	100	73.00	8	9741.	0.0	0.0	0.0100
46	150.00	10	29720.	0.1	0.1	0.0305	101	71.00	35	2879808.	7.4	7.4	2.9546*
47	144.00	12	5034.	0.0	0.0	0.0052	102	70.00	43	996928.	2.6	2.6	1.0228*
48	142.00	21	303984.	0.8	0.8	0.3119	103	69.00	35	2881856.	7.4	7.4	2.9567*
49	142.00	35	4500848.	11.8	11.8	4.7101*	104	66.00	8	1694.	0.0	0.0	0.0017
50	141.00	71	38921216.	100.0	100.0	*39.93*	105	65.00	21	466208.	1.2	1.2	0.4783*
51	140.00	35	1645120.	4.2	4.2	1.6878*	106	64.00	25	495072.	1.3	1.3	0.5079*
52	139.00	43	3982080.	10.2	10.2	4.0855*	107	63.00	25	1436032.	3.7	3.7	1.4733
53	138.00	25	237904.	0.6	0.6	0.2441*	108	62.00	21	463744.	1.2	1.2	0.4758*
54	137.00	17	100984.	0.3	0.3	0.1036*	109	61.00	14	112960.	0.3	0.3	0.1159*
55	133.00	14	88968.	0.2	0.2	0.0913*	110	58.00	25	781888.	2.0	2.0	0.8022*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	57.00	21	468224.	1.2	1.2	0.4800*
112	56.00	8	4664.	0.0	0.0	0.0008
113	55.00	10	10070.	0.0	0.0	0.0103*
114	54.00	17	32091.	0.1	0.1	0.0329*
115	53.00	10	4830.	0.0	0.0	0.0050
116	52.00	17	151112.	0.4	0.4	0.1550*
117	51.00	29	1932096.	5.0	5.0	1.9823*
118	50.00	25	472112.	1.2	1.2	0.4844
119	49.00	8	15031.	0.0	0.0	0.0154
120	47.00	8	3142.	0.0	0.0	0.0032
121	45.00	17	122524.	0.3	0.3	0.1257*
122	44.00	21	221676.	0.6	0.6	0.2274*
123	43.00	8	8669.	0.0	0.0	0.0089
124	42.00	8	30292.	0.1	0.1	0.0311*
125	41.00	8	16359.	0.0	0.0	0.0168
126	40.00	12	19774.	0.1	0.1	0.0203*
127	39.00	25	744080.	1.9	1.9	0.7634
128	38.00	14	87168.	0.2	0.2	0.0894*
129	37.00	8	6799.	0.0	0.0	0.0070
130	36.00	6	9925.	0.0	0.0	0.0102

AC12PK.1 (TIC-89432649, INX-23678976) EI

Biphenyl-2-carboxylic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester.

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	384.00	10	1789.	0.0	0.0	0.0020	56	138.00	12	11241.	0.0	0.0	0.0127*
2	363.00	14	10290.	0.0	0.0	0.0116*	57	137.00	14	9203.	0.0	0.0	0.0104*
3	382.00	21	18298.	0.0	0.0	0.0069*	58	140.00	8	14003.	0.0	0.1	0.0158
4	381.00	25	1557696.	6.6	6.6	1.7614*	59	131.00	10	44300.	0.2	0.2	0.0502*
5	380.00	35	10801152.	45.6	45.6	*12.21*	60	130.00	17	52249.	0.2	0.2	0.0591*
6	379.00	25	1151936.	4.9	4.9	1.3026*	61	129.00	17	75112.	0.3	0.3	0.0849*
7	378.00	25	129848.	0.5	0.5	0.1468*	62	128.00	17	88364.	0.4	0.4	0.0999*
8	377.00	10	2184.	0.0	0.0	0.0025	63	127.00	21	750144.	3.2	3.2	0.0843
9	363.00	8	29869.	0.1	0.1	0.0338	64	126.00	21	743936.	3.1	3.1	0.0812
10	362.00	10	36967.	0.2	0.2	0.0418*	65	125.00	17	130576.	0.6	0.6	0.1477
11	361.00	17	232060.	1.0	1.0	0.2624	66	124.00	8	5304.	0.0	0.0	0.0860
12	341.00	8	30508.	0.1	0.1	0.0350	67	123.00	12	4020.	0.0	0.0	0.0845
13	321.00	10	1818.	0.0	0.0	0.0021	68	122.00	8	5796.	0.0	0.0	0.0866
14	291.00	8	1215.	0.0	0.0	0.0014	69	120.00	6	892.	0.0	0.0	0.0810
15	261.00	8	16306.	0.1	0.1	0.0184	70	119.00	21	327984.	1.4	1.4	0.0370
16	241.00	6	2513.	0.0	0.0	0.0028	71	116.00	8	20934.	0.1	0.1	0.0237*
17	219.00	8	1221.	0.0	0.0	0.0014	72	115.00	21	335632.	1.4	1.4	0.03795
18	218.00	12	7276.	0.0	0.0	0.0002	73	114.00	17	88424.	0.4	0.4	0.1000
19	217.00	8	1291.	0.0	0.0	0.0015	74	113.00	21	265168.	1.1	1.1	0.02999
20	211.00	9	11225.	0.0	0.0	0.0127	75	112.00	6	6761.	0.0	0.0	0.0076
21	200.00	6	2477.	0.0	0.0	0.0028	76	111.00	12	38715.	0.2	0.2	0.0438*
22	199.00	12	24384.	0.1	0.1	0.0276*	77	110.00	8	7533.	0.0	0.0	0.0085
23	198.00	8	8557.	0.0	0.0	0.0097	78	105.00	12	24426.	0.1	0.1	0.0276*
24	197.00	17	201108.	0.8	0.8	0.2274	79	104.00	10	36517.	0.2	0.2	0.0413
25	196.00	17	309008.	1.6	1.6	0.4399	80	103.00	10	24615.	0.1	0.1	0.0278*
26	195.00	10	19313.	0.1	0.1	0.0218	81	102.00	21	260108.	1.1	1.1	0.02941
27	191.00	6	1516.	0.0	0.0	0.0017	82	101.00	21	237876.	1.0	1.0	0.02690
28	184.00	6	10501.	0.0	0.0	0.0119	83	99.00	21	229448.	1.0	1.0	0.02595
29	183.00	21	269424.	1.1	1.1	0.3047*	84	98.00	17	162760.	0.7	0.7	0.1840
30	182.00	35	3283648.	13.9	13.9	3.7132*	85	98.00	17	131860.	0.6	0.6	0.1491*
31	181.00	71	23678976.	100.0	100.0	*26.77*	86	95.00	17	138476.	0.6	0.6	0.1566
32	180.00	25	373760.	1.5	1.6	0.4226*	87	93.00	12	6268.	0.0	0.0	0.0071*
33	179.00	12	22436.	0.1	0.1	0.0254*	88	92.00	12	11251.	0.0	0.0	0.0127*
34	177.00	6	1026.	0.0	0.0	0.0012	89	91.00	51	3140672.	13.3	13.3	3.5515*
35	171.00	8	4411.	0.0	0.0	0.0050	90	90.00	10	19543.	0.1	0.1	0.0221*
36	170.00	10	14596.	0.1	0.1	0.0165	91	89.00	17	142448.	0.6	0.6	0.1611*
37	169.00	17	115416.	0.5	0.5	0.1305	92	88.00	17	130640.	0.6	0.6	0.1477*
38	168.00	21	266304.	1.1	1.1	0.3011	93	87.00	29	314624.	1.3	1.3	0.3558*
39	167.00	8	7387.	0.0	0.0	0.0004	94	86.00	29	192192.	0.8	0.8	0.2173*
40	166.00	6	4493.	0.0	0.0	0.0051	95	85.00	8	11029.	0.0	0.0	0.0125*
41	165.00	10	15848.	0.1	0.1	0.0051	96	84.00	6	2661.	0.0	0.0	0.0030
42	163.00	6	1448.	0.0	0.0	0.0016	97	83.00	17	80544.	0.3	0.3	0.0911*
43	161.00	10	5681.	0.0	0.0	0.0029	98	82.00	6	7463.	0.0	0.0	0.0004
44	156.00	6	2564.	0.0	0.0	0.0064	99	81.00	6	3499.	0.0	0.0	0.0040
45	155.00	12	69280.	0.3	0.3	0.0703*	100	79.00	6	1503.	0.0	0.0	0.0017
46	154.00	21	970240.	4.1	4.1	1.0972*	101	78.00	17	83816.	0.4	0.4	0.0918*
47	153.00	51	7453440.	31.5	31.5	8.4284*	102	77.00	51	2284208.	9.7	9.7	0.0943*
48	152.00	59	9303552.	39.3	39.3	*10.52*	103	76.00	59	5309312.	22.9	22.9	6.0943*
49	151.00	71	2804224.	11.8	11.8	3.1710*	104	75.00	35	1056320.	4.5	4.5	1.1945*
50	150.00	35	746880.	3.2	3.2	0.8446*	105	74.00	25	446736.	1.9	1.9	0.5052*
51	149.00	21	95568.	0.4	0.4	0.1081*	106	73.00	8	6797.	0.0	0.0	0.0077
52	142.00	12	3386.	0.0	0.0	0.0030	107	70.00	6	9179.	0.0	0.0	0.0104
53	141.00	17	161392.	0.7	0.7	0.1825	108	69.00	25	1324288.	5.6	5.6	1.4975
54	140.00	17	122844.	0.5	0.5	0.1289	109	66.00	6	2079.	0.0	0.0	0.0024
55	139.00	21	385712.	1.6	1.6	0.4362	110	65.00	17	81586.	0.3	0.3	0.0923*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	64.00	25	270336.	1.1	1.1	0.3057*
112	63.00	35	1026544.	4.3	4.3	1.1608*
113	62.00	25	240136.	1.0	1.0	0.2715*
114	61.00	10	14859.	0.1	0.1	0.0168
115	57.00	8	4845.	0.0	0.0	0.0055
116	55.00	10	11517.	0.0	0.0	0.0130*
117	53.00	8	30355.	0.1	0.1	0.0343
118	52.00	17	146783.	0.6	0.6	0.1660
119	51.00	29	1348756.	5.7	5.7	1.5252
120	50.00	25	545760.	2.3	2.3	0.6171
121	49.00	17	3504.	0.0	0.0	0.0040
122	45.00	12	37991.	0.2	0.2	0.0430*
123	44.00	17	69976.	0.3	0.3	0.0791*
124	41.00	8	5878.	0.0	0.0	0.0066
125	40.00	10	18282.	0.1	0.1	0.0207*
126	39.00	25	497088.	2.1	2.1	0.5621
127	38.00	17	67092.	0.3	0.3	0.0759*
128	36.00	10	9835.	0.0	0.0	0.0111*

AY12AV.1 [TIC-155254784, 180X-36184192] EI

PAGE 2													
PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
1	386.00	6	374.	0.0	0.0	0.0002	56	153.00	51	11970560.	33.2	33.2	7.7103*
2	384.00	6	487.	0.0	0.0	0.0003	57	152.00	59	16352512.	45.3	45.3	*10.53*
3	383.00	10	34376.	0.1	0.1	0.0021	58	151.00	59	4830720.	13.4	13.4	3.1115*
4	382.00	25	437504.	1.2	1.2	0.0218*	59	150.00	51	1305472.	3.6	3.6	0.8409*
5	381.00	25	2940800.	8.1	8.1	1.8942*	60	149.00	29	206996.	0.6	0.6	0.1333*
6	380.00	43	23648256.	65.5	65.5	*15.23*	61	147.00	8	3688.	0.0	0.0	0.0024
7	379.00	25	320992.	0.9	0.9	0.0268*	62	141.00	12	49017.	0.1	0.1	0.0320*
8	378.00	12	31912.	0.1	0.1	0.0206*	63	140.00	14	70268.	0.2	0.2	0.0453
9	377.00	8	8622.	0.0	0.0	0.0056	64	139.00	17	158716.	0.4	0.4	0.1022*
10	376.00	8	2449.	0.0	0.0	0.0016	65	138.00	10	5884.	0.0	0.0	0.0038
11	363.00	10	7440.	0.0	0.0	0.0048	66	137.00	8	10009.	0.0	0.0	0.0064
12	362.00	14	156680.	0.4	0.4	0.1012	67	133.00	10	29137.	0.1	0.1	0.0188
13	361.00	21	927440.	2.6	2.6	0.0574	68	132.00	6	1552.	0.0	0.0	0.0010
14	360.00	6	628.	0.0	0.0	0.0004	69	131.00	21	107520.	0.3	0.3	0.0693*
15	359.00	6	1887.	0.0	0.0	0.0012	70	130.00	43	224092.	0.6	0.6	0.1443*
16	335.00	8	21241.	0.1	0.1	0.0051	71	129.00	35	207712.	0.6	0.6	0.1338*
17	317.00	10	7892.	0.0	0.0	0.0059	72	128.00	21	185024.	0.5	0.5	0.1192*
18	316.00	8	1399.	0.0	0.0	0.0009	73	127.00	25	1541120.	4.3	4.3	0.9926*
19	303.00	8	2144.	0.0	0.0	0.0014	74	126.00	25	1192064.	3.3	3.3	0.7678*
20	281.00	8	9228.	0.0	0.0	0.0059	75	125.00	17	258612.	0.7	0.7	0.1666
21	262.00	12	9828.	0.0	0.0	0.0063	76	124.00	10	3532.	0.0	0.0	0.0023
22	261.00	14	125312.	0.3	0.3	0.0087	77	123.00	8	19981.	0.1	0.1	0.0129*
23	243.00	6	1271.	0.0	0.0	0.0008	78	122.00	12	22007.	0.1	0.1	0.0142
24	241.00	8	2199.	0.0	0.0	0.0014	79	120.00	6	2046.	0.0	0.0	0.0013
25	217.00	12	43047.	0.1	0.1	0.0277	80	119.00	21	407920.	1.1	1.1	0.2627
26	216.00	10	9356.	0.0	0.0	0.0060	81	116.00	10	25503.	0.1	0.1	0.0164
27	213.00	8	1913.	0.0	0.0	0.0012	82	115.00	21	289520.	0.8	0.8	0.1865*
28	211.00	10	56997.	0.2	0.2	0.0367	83	114.00	14	125896.	0.3	0.3	0.0811
29	209.00	8	2186.	0.0	0.0	0.0014	84	113.00	21	304272.	0.8	0.8	0.1960
30	208.00	6	4081.	0.0	0.0	0.0026	85	112.00	12	15922.	0.0	0.0	0.0103*
31	207.00	12	80188.	0.2	0.2	0.0568	86	111.00	17	71728.	0.2	0.2	0.0462*
32	203.00	6	1838.	0.0	0.0	0.0012	87	110.00	12	21014.	0.1	0.1	0.0135
33	201.00	6	758.	0.0	0.0	0.0005	88	106.00	10	21366.	0.1	0.1	0.0138
34	198.00	10	12270.	0.0	0.0	0.0079	89	105.00	17	105248.	0.3	0.3	0.0678*
35	197.00	14	89652.	0.2	0.2	0.0577*	90	104.00	8	8327.	0.0	0.0	0.0054
36	196.00	17	237948.	0.7	0.7	0.1533	91	103.00	17	134340.	0.4	0.4	0.0865*
37	195.00	12	27293.	0.1	0.1	0.0176	92	102.00	21	926160.	2.6	2.6	0.5965*
38	193.00	6	1578.	0.0	0.0	0.0010	93	101.00	21	408400.	1.3	1.3	0.2953
39	190.00	8	23819.	0.1	0.1	0.0153	94	100.00	21	400928.	1.1	1.1	0.2582*
40	189.00	6	1145.	0.0	0.0	0.0007	95	99.00	17	237332.	0.7	0.7	0.1529
41	184.00	10	13556.	0.0	0.0	0.0007	96	98.00	17	215044.	0.6	0.6	0.1385
42	183.00	21	384512.	1.1	1.1	0.2477*	97	97.00	8	6492.	0.0	0.0	0.0042
43	182.00	43	5189888.	14.4	14.4	3.3428*	98	96.00	8	5036.	0.0	0.0	0.0032
44	181.00	59	36104192.	100.0	100.0	*23.25*	99	95.00	21	223420.	0.6	0.6	0.1439*
45	180.00	29	184820.	0.5	0.5	0.1190*	100	93.00	8	4589.	0.0	0.0	0.0030
46	179.00	17	108996.	0.3	0.3	0.0702*	101	92.00	6	2249.	0.0	0.0	0.0014
47	170.00	12	13263.	0.0	0.0	0.0085	102	91.00	35	1057472.	2.9	2.9	0.6811*
48	169.00	17	176476.	0.5	0.5	0.1137*	103	90.00	51	7678720.	21.3	21.3	4.9459*
49	168.00	17	138476.	0.4	0.4	0.0892	104	89.00	25	250648.	0.7	0.7	0.1614*
50	167.00	17	130656.	0.4	0.4	0.0842	105	88.00	21	181164.	0.5	0.5	0.1167*
51	166.00	8	8456.	0.0	0.0	0.0054	106	87.00	43	552752.	1.5	1.5	0.3560*
52	165.00	10	28898.	0.1	0.1	0.0186	107	86.00	59	408224.	1.1	1.1	0.2629*
53	156.00	6	3094.	0.0	0.0	0.0020	108	85.00	17	62241.	0.2	0.2	0.0401*
54	155.00	14	115008.	0.3	0.3	0.0746*	109	84.00	12	3070.	0.0	0.0	0.0020
55	154.00	25	1517120.	4.2	4.2	0.9772*	110	83.00	12	61826.	0.2	0.2	0.0398

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. MREF	X TOT. ION
111	82.00	6	5502.	0.0	0.0	0.0042
112	81.00	8	6354.	0.0	0.0	0.0041
113	79.00	10	19950.	0.1	0.1	0.0128*
114	78.00	17	176328.	0.5	0.5	0.1136*
115	77.00	35	1738176.	4.8	4.8	1.1196*
116	76.00	71	12473344.	34.5	34.5	8.0341*
117	75.00	59	3407232.	9.4	9.4	2.1946*
118	74.00	25	852768.	2.4	2.4	0.5493*
119	73.00	12	40338.	0.1	0.1	0.0260*
120	70.00	8	1064.	0.0	0.0	0.0007
121	69.00	29	1984704.	0.0	0.0	1.2784*
122	66.00	6	1997.	0.0	0.0	0.0013
123	65.00	21	131492.	0.4	0.4	0.0047*
124	64.00	25	394240.	1.1	1.1	0.2539*
125	63.00	43	2030592.	5.6	5.6	1.3079*
126	62.00	25	428112.	1.2	1.2	0.2757*
127	61.00	17	70680.	0.2	0.2	0.0455*
128	57.00	10	7642.	0.0	0.0	0.0049
129	55.00	6	4733.	0.0	0.0	0.0030
130	53.00	14	79736.	0.2	0.2	0.0514*
131	52.00	25	335824.	0.9	0.9	0.2163*
132	51.00	29	2218624.	6.1	6.1	1.4290
133	50.00	25	1182464.	3.3	3.3	0.7616
134	49.00	10	19932.	0.1	0.1	0.0128*
135	45.00	12	85912.	0.2	0.2	0.0553
136	44.00	17	119436.	0.3	0.3	0.0769*
137	43.00	6	2772.	0.0	0.0	0.0018
138	42.00	6	2268.	0.0	0.0	0.0015
139	41.00	10	14376.	0.0	0.0	0.0093*
140	40.00	14	34821.	0.1	0.1	0.0224*
141	39.00	25	721840.	2.6	2.6	0.4643
142	38.00	17	149880.	0.4	0.4	0.0965*
143	37.00	10	10210.	0.0	0.0	0.0066*
144	36.00	12	48622.	0.1	0.1	0.0313*
145	35.00	8	2944.	0.0	0.0	0.0019

AG11AV.1 [TIC-82272256, 100X-29554688] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	409.00	10	68112.	0.2	0.2	0.0828	56	131.00	12	70188.	0.2	0.2	0.0853*
2	408.00	17	385136.	1.3	1.3	0.4681	57	129.00	12	38289.	0.1	0.1	0.0465*
3	393.00	8	8678.	0.0	0.0	0.0105	58	128.00	17	178264.	0.6	0.6	0.2167*
4	366.00	10	2144.	0.0	0.0	0.0026	59	127.00	17	121028.	0.4	0.4	0.1471*
5	365.00	10	63002.	0.2	0.2	0.0766	60	126.00	14	106328.	0.4	0.4	0.1292*
6	361.00	8	10843.	0.0	0.0	0.0132	61	125.00	10	3098.	0.0	0.0	0.0038
7	330.00	8	4027.	0.0	0.0	0.0049	62	120.00	8	3736.	0.0	0.0	0.0045
8	311.00	10	14418.	0.0	0.0	0.0175	63	119.00	21	611136.	2.1	2.1	0.7428
9	303.00	10	5464.	0.0	0.0	0.0066	64	118.00	8	1783.	0.0	0.0	0.0022
10	290.00	6	1717.	0.0	0.0	0.0021	65	116.00	10	42235.	0.1	0.1	0.0513*
11	289.00	10	39383.	0.1	0.1	0.0479	66	115.00	21	551104.	1.9	1.9	0.6699
12	283.00	10	25055.	0.1	0.1	0.0305	67	114.00	12	44340.	0.2	0.2	0.0539*
13	209.00	8	9704.	0.0	0.0	0.0118	68	113.00	21	521984.	1.8	1.8	0.6345
14	208.00	8	31388.	0.1	0.1	0.0382	69	111.00	8	12474.	0.0	0.0	0.0152
15	207.00	12	54817.	0.2	0.2	0.0666*	70	107.00	6	1644.	0.0	0.0	0.0020
16	195.00	12	2661.	0.0	0.0	0.0032	71	106.00	8	12831.	0.0	0.0	0.0156
17	194.00	10	4120.	0.0	0.0	0.0050	72	105.00	21	507968.	1.7	1.7	0.6174
18	193.00	6	4071.	0.0	0.0	0.0049	73	104.00	25	765312.	2.6	2.6	0.9302
19	191.00	6	2005.	0.0	0.0	0.0024	74	103.00	35	7689472.	26.0	26.0	9.3464*
20	185.00	6	1311.	0.0	0.0	0.0016	75	102.00	21	519104.	1.8	1.8	0.6310
21	184.00	8	1760.	0.0	0.0	0.0021	76	101.00	17	128460.	0.4	0.4	0.1561*
22	183.00	21	320944.	1.1	1.1	0.3901*	77	100.00	17	130920.	0.0	0.0	0.1591*
23	182.00	35	4346112.	14.7	14.7	5.2826*	78	99.00	10	8797.	0.0	0.0	0.0107*
24	181.00	59	29554688.	100.0	100.0	35.92*	79	98.00	10	5159.	0.0	0.0	0.0063
25	180.00	29	830768.	2.8	2.8	1.0098*	80	95.00	21	321344.	1.1	1.1	0.3906
26	179.00	35	1637376.	5.5	5.5	1.9902*	81	92.00	8	2899.	0.0	0.0	0.0035
27	178.00	35	1468160.	5.0	5.0	1.7845*	82	91.00	25	293696.	1.0	1.0	0.3570*
28	177.00	29	311152.	1.1	1.1	0.3782*	83	90.00	35	508304.	1.7	1.7	0.6178*
29	176.00	21	262528.	0.9	0.9	0.3191*	84	89.00	29	878944.	3.0	3.0	1.0683*
30	175.00	10	17826.	0.1	0.1	0.0217*	85	88.00	17	148112.	0.5	0.5	0.1800*
31	174.00	6	1624.	0.0	0.0	0.0020	86	87.00	14	81068.	0.3	0.3	0.0985*
32	169.00	8	24369.	0.1	0.1	0.0296	87	86.00	18	25988.	0.1	0.1	0.0316
33	168.00	10	28648.	0.1	0.1	0.0348	88	84.00	12	64466.	0.2	0.2	0.0784*
34	167.00	21	561008.	1.9	1.9	0.6819*	89	83.00	43	1351488.	4.6	4.6	1.6427*
35	166.00	35	4030208.	13.7	13.7	4.9083*	90	82.00	29	545264.	1.8	1.8	0.6628*
36	165.00	43	5356544.	18.1	18.1	6.5108*	91	81.00	29	45896.	0.2	0.2	0.0558*
37	164.00	35	477456.	1.6	1.6	0.5803*	92	79.00	17	102328.	0.3	0.3	0.1244*
38	163.00	21	240688.	0.8	0.8	0.2926*	93	78.00	25	659264.	2.2	2.2	0.8013
39	162.00	10	12585.	0.0	0.0	0.0153*	94	77.00	35	3619200.	12.2	12.2	4.3991*
40	155.00	8	21083.	0.1	0.1	0.0256	95	76.00	25	590512.	2.0	2.0	0.7178*
41	154.00	17	137692.	0.5	0.5	0.1674*	96	75.00	21	288624.	1.0	1.0	0.3500*
42	153.00	35	614368.	2.1	2.1	0.7467*	97	74.00	17	147788.	0.5	0.5	0.1796*
43	152.00	35	768800.	2.6	2.6	0.9345*	98	73.00	8	4391.	0.0	0.0	0.0053
44	151.00	21	236900.	0.8	0.8	0.2879*	99	70.00	21	77564.	0.3	0.3	0.0943*
45	150.00	14	97464.	0.3	0.3	0.1185*	100	69.00	25	1722624.	5.8	5.8	2.0938*
46	149.00	6	2294.	0.0	0.0	0.0028	101	66.00	8	4547.	0.0	0.0	0.0055
47	147.00	8	3479.	0.0	0.0	0.0042	102	65.00	17	222464.	0.8	0.8	0.2704*
48	142.00	8	18366.	0.0	0.0	0.0042	103	64.00	17	261136.	0.9	0.9	0.3174
49	141.00	17	234532.	0.1	0.1	0.0223	104	63.00	21	513904.	1.7	1.7	0.6246
50	140.00	10	27190.	0.1	0.1	0.0330*	105	62.00	14	82248.	0.3	0.3	0.1000*
51	139.00	17	333056.	1.1	1.1	0.4048*	106	61.00	8	6357.	0.0	0.0	0.0077
52	138.00	8	6593.	0.0	0.0	0.0080	107	59.00	6	1726.	0.0	0.0	0.0021
53	137.00	8	3669.	0.0	0.0	0.0045	108	58.00	8	2766.	0.0	0.0	0.0034
54	133.00	14	106552.	0.4	0.4	0.1295	109	53.00	17	158984.	0.5	0.5	0.1932*
55	132.00	14	115752.	0.4	0.4	0.1407*	110	52.00	21	269440.	0.9	0.9	0.3275

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	51.00	35	292480.	9.9	9.9	3.5546
112	50.00	21	368368.	1.2	1.2	0.4477*
113	49.00	6	1552.	0.0	0.0	0.0019
114	45.00	14	63433.	0.2	0.2	0.0771*
115	44.00	17	121156.	0.4	0.4	0.1473*
116	43.00	17	134780.	0.5	0.5	0.1638*
117	41.00	10	24159.	0.1	0.1	0.0294*
118	40.00	12	40751.	0.1	0.1	0.0495*
119	39.00	25	525136.	1.8	1.8	0.6383*
120	38.00	8	23730.	0.1	0.1	0.0288*
121	37.00	6	1709.	0.0	0.0	0.0021
122	36.00	6	4650.	0.0	0.0	0.0057

3PK8L7.1 [TIC=112885128.188X=36616192] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	468.00	8	607.	0.0	0.0	0.0005	56	267.00	10	4170.	0.0	0.0	0.0037
2	434.00	8	295.	0.0	0.0	0.0003	57	265.00	6	910.	0.0	0.0	0.0008
3	429.00	8	1302.	0.0	0.0	0.0012	58	263.00	8	1256.	0.0	0.0	0.0011
4	428.00	6	567.	0.0	0.0	0.0005	59	261.00	8	918.	0.0	0.0	0.0008
5	427.00	8	1525.	0.0	0.0	0.0014	60	253.00	8	1006.	0.0	0.0	0.0009
6	426.00	8	1907.	0.0	0.0	0.0017	61	249.00	8	1669.	0.0	0.0	0.0015
7	425.00	14	19356.	0.1	0.1	0.0173*	62	245.00	8	843.	0.0	0.0	0.0008
8	424.00	21	97236.	0.3	0.3	0.0688*	63	243.00	8	2229.	0.0	0.0	0.0020
9	423.00	35	737228.	2.8	2.8	0.0893*	64	242.00	17	59874.	0.2	0.2	0.0535*
10	422.00	59	33055.	0.1	0.1	0.0295*	65	241.00	6	957.	0.0	0.0	0.0009
11	421.00	29	18956.	0.1	0.1	0.0169*	66	240.00	8	1093.	0.0	0.0	0.0010
12	420.00	12	5128.	0.0	0.0	0.0046*	67	239.00	8	7519.	0.0	0.0	0.0067
13	419.00	10	8867.	0.0	0.0	0.0079	68	227.00	8	2584.	0.0	0.0	0.0023
14	418.00	12	1524.	0.0	0.0	0.0014	69	226.00	12	1933.	0.0	0.0	0.0017
15	417.00	8	1217.	0.0	0.0	0.0011	70	225.00	8	4440.	0.0	0.0	0.0040
16	416.00	8	10037.	0.0	0.0	0.0050	71	224.00	17	57843.	0.2	0.2	0.0516
17	415.00	10	1555.	0.0	0.0	0.0014	72	223.00	21	298944.	0.8	0.8	0.2669
18	414.00	8	5846.	0.0	0.0	0.0052	73	222.00	17	67484.	0.2	0.2	0.0603
19	394.00	10	1373.	0.0	0.0	0.0012	74	221.00	17	39468.	0.1	0.1	0.0352
20	393.00	6	12697.	0.0	0.0	0.0113	75	220.00	8	3955.	0.0	0.0	0.0035
21	385.00	10	998.	0.0	0.0	0.0009	76	219.00	10	8734.	0.0	0.0	0.0078
22	384.00	6	1383.	0.0	0.0	0.0012	77	218.00	12	3415.	0.0	0.0	0.0030
23	383.00	8	3796.	0.0	0.0	0.0034	78	215.00	8	592.	0.0	0.0	0.0005
24	381.00	6	2059.	0.0	0.0	0.0018	79	212.00	17	31624.	0.1	0.1	0.0282*
25	380.00	10	13173.	0.0	0.0	0.0118	80	211.00	25	167640.	0.5	0.5	0.1497*
26	379.00	10	1022.	0.0	0.0	0.0009	81	209.00	8	10514.	0.0	0.0	0.0094
27	376.00	12	11400.	0.0	0.0	0.0102	82	208.00	17	27904.	0.1	0.1	0.0249
28	375.00	12	10352.	0.0	0.0	0.0092	83	207.00	14	34113.	0.1	0.1	0.0305
29	363.00	12	84112.	0.2	0.2	0.0358	84	206.00	21	147816.	0.4	0.4	0.1320
30	362.00	17	432160.	1.2	1.2	0.0817	85	205.00	10	8723.	0.0	0.0	0.0078
31	361.00	21	1949.	0.0	0.0	0.0017	86	204.00	14	25705.	0.1	0.1	0.0229
32	359.00	12	7828.	0.0	0.0	0.0070	87	203.00	10	2079.	0.0	0.0	0.0019
33	355.00	8	3313.	0.0	0.0	0.0030	88	202.00	12	17367.	0.0	0.0	0.0155*
34	351.00	8	778.	0.0	0.0	0.0007	89	201.00	21	39721.	0.1	0.1	0.0355*
35	347.00	8	3281.	0.0	0.0	0.0062	90	199.00	17	50596.	0.1	0.1	0.0452*
36	343.00	8	1994.	0.0	0.0	0.0018	91	198.00	10	9675.	0.0	0.0	0.0086*
37	342.00	12	13676.	0.0	0.0	0.0122	92	197.00	14	44587.	0.1	0.1	0.0398
38	341.00	12	1797.	0.0	0.0	0.0016	93	196.00	10	2048.	0.0	0.0	0.0018
39	340.00	8	29099.	0.1	0.1	0.0260	94	195.00	17	34218.	0.1	0.1	0.0306
40	339.00	14	1126.	0.0	0.0	0.0034	95	194.00	17	43588.	0.1	0.1	0.0389
41	327.00	6	3773.	0.0	0.0	0.0058	96	193.00	25	189296.	0.5	0.5	0.1690
42	323.00	8	6538.	0.0	0.0	0.0019	97	192.00	25	207456.	0.6	0.6	0.1852*
43	322.00	10	1263.	0.0	0.0	0.0013	98	191.00	25	396400.	1.1	1.1	0.3539*
44	321.00	12	1451.	0.0	0.0	0.0014	99	190.00	35	235772.	0.3	0.3	0.0921*
45	311.00	8	2172.	0.0	0.0	0.0032	100	189.00	29	144800.	0.6	0.6	0.2105*
46	303.00	8	3635.	0.0	0.0	0.0070	101	188.00	29	268144.	0.7	0.7	0.2394*
47	291.00	6	7822.	0.0	0.0	0.0019	102	187.00	25	42431.	0.1	0.1	0.0379*
48	285.00	8	821.	0.0	0.0	0.0007	103	186.00	17	39437.	0.0	0.0	0.0352*
49	283.00	8	821.	0.0	0.0	0.0007	104	185.00	10	7062.	0.0	0.0	0.0063
50	282.00	6	30773.	0.1	0.1	0.0275	105	184.00	8	2644.	0.0	0.0	0.0024
51	281.00	14	1991.	0.0	0.0	0.0018	106	183.00	14	29064.	0.1	0.1	0.0259*
52	269.00	8	2952.	0.0	0.0	0.0026	107	182.00	35	42776.	1.2	1.2	0.3819*
53	268.00	8					108	181.00	43	5585152.	15.3	15.3	4.9865*
54							109		59	36616192.	100.0	100.0	*32.69*
55							110						

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	180.00	71	4657152.	12.7	12.7	4.1580*	166	122.00	17	29862.	0.1	0.1	0.0267*
112	179.00	51	3871616.	10.6	10.6	3.4566*	167	121.00	10	3237.	0.0	0.0	0.0029
113	178.00	71	3419456.	9.3	9.3	3.0529*	168	120.00	10	11238.	0.0	0.0	0.0100
114	177.00	59	647616.	1.8	1.8	0.5782*	169	119.00	25	367616.	1.0	1.0	0.3282
115	176.00	59	551904.	1.5	1.5	0.4927*	170	118.00	12	3570.	0.0	0.0	0.0032*
116	175.00	59	149880.	0.4	0.4	0.1339*	171	117.00	14	17521.	0.0	0.0	0.0156*
117	174.00	35	61299.	0.2	0.2	0.0547*	172	116.00	21	94596.	0.3	0.3	0.0845*
118	173.00	21	18953.	0.1	0.1	0.0169*	173	115.00	29	817920.	2.2	2.2	0.7303*
119	172.00	14	14551.	0.0	0.0	0.0138*	174	114.00	21	59592.	0.2	0.2	0.0532*
120	171.00	14	16674.	0.0	0.0	0.0149*	175	113.00	25	275184.	0.8	0.8	0.2457*
121	170.00	14	19019.	0.1	0.1	0.0170*	176	112.00	29	131008.	0.4	0.4	0.1170*
122	169.00	17	51059.	0.1	0.1	0.0456*	177	111.00	35	206312.	0.6	0.6	0.1842*
123	168.00	29	155796.	0.4	0.4	0.1391*	178	110.00	17	32762.	0.1	0.1	0.0293*
124	167.00	51	1353664.	3.7	3.7	1.2086*	179	109.00	14	20833.	0.1	0.1	0.0186*
125	166.00	51	6791680.	18.5	18.5	6.0637*	180	108.00	12	3814.	0.0	0.0	0.0034
126	165.00	71	7509504.	20.5	20.5	6.7046*	181	107.00	6	1788.	0.0	0.0	0.0016
127	164.00	71	836240.	2.3	2.3	0.7466*	182	106.00	8	2208.	0.0	0.0	0.0020
128	163.00	51	376432.	1.0	1.0	0.3361*	183	105.00	8	4908.	0.0	0.0	0.0044
129	162.00	35	78148.	0.2	0.2	0.0698*	184	104.00	10	12312.	0.0	0.0	0.0110*
130	161.00	25	39732.	0.1	0.1	0.0355*	185	103.00	25	79292.	0.2	0.2	0.0708*
131	160.00	12	10432.	0.0	0.0	0.0093*	186	102.00	21	108076.	0.3	0.3	0.0965*
132	159.00	17	14409.	0.0	0.0	0.0129*	187	101.00	21	107544.	0.3	0.3	0.0960*
133	158.00	17	19329.	0.1	0.1	0.0173*	188	100.00	25	141044.	0.4	0.4	0.1259*
134	157.00	12	7852.	0.0	0.0	0.0078*	189	99.00	17	47555.	0.1	0.1	0.0425
135	156.00	21	32935.	0.1	0.1	0.0294*	190	98.00	25	79096.	0.2	0.2	0.0706*
136	155.00	35	239632.	0.7	0.7	0.2139*	191	97.00	43	307808.	0.8	0.8	0.2748*
137	154.00	51	1237248.	3.4	3.4	1.1046*	192	96.00	43	259588.	0.7	0.7	0.2318*
138	153.00	71	1626176.	4.4	4.4	1.4519*	193	95.00	43	387248.	1.1	1.1	0.3457*
139	152.00	87	2070336.	5.7	5.7	1.8484*	194	94.00	51	199116.	0.5	0.5	0.1778*
140	151.00	71	672464.	1.8	1.8	0.6004*	195	93.00	25	35591.	0.1	0.1	0.0318*
141	150.00	51	284720.	0.8	0.8	0.2542*	196	92.00	10	2484.	0.0	0.0	0.0022
142	149.00	43	66192.	0.2	0.2	0.0591*	197	91.00	29	100680.	0.3	0.3	0.0899*
143	148.00	12	10161.	0.0	0.0	0.0091*	198	90.00	35	232840.	0.6	0.6	0.2079*
144	147.00	14	11618.	0.0	0.0	0.0104*	199	89.00	59	1224768.	3.3	3.3	1.0935*
145	146.00	8	3986.	0.0	0.0	0.0036	200	88.00	51	349696.	1.0	1.0	0.3122*
146	145.00	6	1438.	0.0	0.0	0.0013	201	87.00	35	145492.	0.4	0.4	0.1299*
147	143.00	17	20352.	0.1	0.1	0.0182*	202	86.00	21	47029.	0.1	0.1	0.0420*
148	142.00	21	170312.	0.5	0.5	0.1521	203	85.00	14	19674.	0.1	0.1	0.0176*
149	141.00	35	1107904.	3.0	3.0	0.9892*	204	84.00	10	22250.	0.1	0.1	0.0199
150	140.00	25	102164.	0.3	0.3	0.0912*	205	83.00	51	593360.	1.6	1.6	0.5298*
151	139.00	25	481776.	1.3	1.3	0.4301*	206	82.00	59	794000.	2.2	2.2	0.7089*
152	138.00	21	43976.	0.1	0.1	0.0393*	207	81.00	43	183384.	0.5	0.5	0.1637*
153	137.00	17	37512.	0.1	0.1	0.0335	208	80.00	21	38254.	0.1	0.1	0.0342*
154	134.00	8	1787.	0.0	0.0	0.0016	209	79.00	29	46101.	0.1	0.1	0.0412*
155	133.00	21	78132.	0.2	0.2	0.0698	210	78.00	103	179736.	0.5	0.5	0.1605*
156	132.00	8	5013.	0.0	0.0	0.0045	211	77.00	87	332704.	0.9	0.9	0.2970*
157	131.00	21	57930.	0.2	0.2	0.0517*	212	76.00	51	706528.	1.9	1.9	0.6308*
158	130.00	35	52861.	0.1	0.1	0.0472*	213	75.00	43	272800.	0.7	0.7	0.2436*
159	129.00	35	132260.	0.4	0.4	0.1181*	214	74.00	25	105956.	0.3	0.3	0.0946*
160	128.00	29	395456.	1.1	1.1	0.3531*	215	73.00	17	35578.	0.1	0.1	0.0318*
161	127.00	29	247948.	0.7	0.7	0.2214*	216	71.00	10	9961.	0.3	0.3	0.0089
162	126.00	25	192484.	0.5	0.5	0.1719*	217	70.00	35	77484.	0.2	0.2	0.0692*
163	125.00	21	41738.	0.1	0.1	0.0373*	218	69.00	51	1399616.	3.8	3.8	1.2496*
164	124.00	8	5077.	0.0	0.0	0.0045	219	68.00	17	17399.	0.0	0.0	0.0153*
165	123.00	14	17351.	0.0	0.0	0.0155	220	67.00	21	58400.	0.2	0.2	0.0521

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	66.00	14	10871.	0.0	0.0	0.0097
222	65.00	25	136964.	0.4	0.4	0.1223*
223	64.00	29	183444.	0.5	0.5	0.1638*
224	63.00	29	351200.	1.0	1.0	0.3136*
225	62.00	21	88404.	0.2	0.2	0.0789*
226	61.00	25	98384.	0.3	0.3	0.0878
227	60.00	17	42451.	0.1	0.1	0.0379
228	59.00	14	15092.	0.0	0.0	0.0135*
229	58.00	10	5288.	0.0	0.0	0.0047
230	57.00	25	47257.	0.1	0.1	0.0422*
231	56.00	12	11752.	0.0	0.0	0.0105
232	55.00	21	64011.	0.2	0.2	0.0572*
233	54.00	12	16692.	0.0	0.0	0.0149
234	53.00	25	221476.	0.6	0.6	0.1977
235	52.00	21	57801.	0.2	0.2	0.0516*
236	51.00	29	1090624.	3.0	3.0	0.9737
237	50.00	25	146704.	0.4	0.4	0.1310
238	49.00	14	21089.	0.1	0.1	0.0188
239	47.00	12	5766.	0.0	0.0	0.0051
240	46.00	8	1321.	0.0	0.0	0.0012
241	45.00	29	156896.	0.4	0.4	0.1401
242	44.00	35	303856.	0.8	0.8	0.2713
243	43.00	35	1266240.	3.5	3.5	1.1305
244	42.00	35	1120576.	3.1	3.1	1.0005*
245	41.00	29	211880.	0.6	0.6	0.1892
246	40.00	21	35210.	0.1	0.1	0.0314*
247	39.00	29	328784.	0.9	0.9	0.2935
248	38.00	25	48933.	0.1	0.1	0.0437*
249	37.00	10	7403.	0.0	0.0	0.0066
250	36.00	21	57083.	0.2	0.2	0.0510*
251	35.00	8	3573.	0.0	0.0	0.0032

EWSPK.1 [TIC-51577856, 188X-15643456] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	428.00	6	778.	0.0	0.0	0.0015	56	166.00	35	1456000.	13.7	13.7	2.8229*
2	395.00	10	7830.	0.1	0.1	0.0152	57	165.00	59	10643455.	100.0	100.0	*20.63*
3	394.00	21	131532.	1.2	1.2	0.2550*	58	164.00	51	2860544.	26.9	26.9	5.5461*
4	393.00	25	661536.	6.2	6.2	0.2026*	59	163.00	51	2083392.	19.6	19.6	4.0393*
5	392.00	59	6990532.	65.7	65.7	*13.55*	60	162.00	43	341616.	3.2	3.2	0.6623*
6	391.00	21	96324.	0.9	0.9	0.1868*	61	161.00	25	114184.	1.1	1.1	0.2214*
7	390.00	8	8896.	0.1	0.1	0.0172	62	160.00	10	15342.	0.1	0.1	0.0297*
8	389.00	12	3716.	0.0	0.0	0.0072*	63	159.00	6	1148.	0.0	0.0	0.0022
9	388.00	8	871.	0.0	0.0	0.0017	64	158.00	8	2085.	0.0	0.0	0.0040
10	387.00	8	317.	0.0	0.0	0.0017	65	157.00	8	3182.	0.0	0.0	0.0062
11	386.00	6	894.	0.0	0.0	0.0006	66	156.00	6	649.	0.0	0.0	0.0013
12	375.00	6	894.	0.0	0.0	0.0017	67	155.00	8	995.	0.0	0.0	0.0019
13	374.00	14	54045.	0.5	0.5	0.1048	68	154.00	21	127052.	1.2	1.2	0.2463
14	373.00	21	227584.	2.1	2.1	0.4412	69	153.00	35	1107840.	10.4	10.4	2.1479*
15	353.00	10	17587.	0.2	0.2	0.0341	70	152.00	35	670032.	6.3	6.3	1.2991*
16	330.00	10	1768.	0.0	0.0	0.0034	71	151.00	29	191292.	1.6	1.6	0.3709*
17	329.00	17	53586.	0.5	0.5	0.1035*	72	150.00	25	92528.	0.9	0.9	0.1794*
18	323.00	6	1170.	0.0	0.0	0.0023	73	149.00	8	3425.	0.0	0.0	0.0066
19	310.00	8	2531.	0.0	0.0	0.0049	74	147.00	8	696.	0.0	0.0	0.0013
20	309.00	10	23232.	0.2	0.2	0.0450*	75	145.00	8	4283.	0.0	0.0	0.0083
21	289.00	8	834.	0.0	0.0	0.0016	76	142.00	6	1418.	0.0	0.0	0.0027
22	282.00	8	1584.	0.0	0.0	0.0031	77	141.00	8	10070.	0.1	0.1	0.0195*
23	281.00	10	25726.	0.2	0.2	0.0499	78	140.00	21	77972.	0.7	0.7	0.1512*
24	273.00	12	26148.	0.2	0.2	0.0507	79	139.00	25	493664.	4.6	4.6	0.9571*
25	269.00	8	928.	0.0	0.0	0.0018	80	138.00	21	122824.	1.2	1.2	0.2381
26	267.00	8	2148.	0.0	0.0	0.0042	81	137.00	21	144724.	1.4	1.4	0.2806
27	265.00	8	3768.	0.0	0.0	0.0073	82	136.00	10	6593.	0.1	0.1	0.0128*
28	229.00	8	1698.	0.0	0.0	0.0033	83	135.00	8	5996.	0.1	0.1	0.0116
29	228.00	8	1314.	0.0	0.0	0.0025	84	134.00	8	4046.	0.0	0.0	0.0078
30	224.00	8	1064.	0.0	0.0	0.0021	85	133.00	8	22897.	0.2	0.2	0.0444*
31	223.00	12	4248.	0.0	0.0	0.0082*	86	131.00	17	41680.	0.4	0.4	0.0808
32	211.00	17	62100.	0.6	0.6	0.1204	87	129.00	8	596.	0.0	0.0	0.0012
33	210.00	35	582960.	5.5	5.5	1.1303*	88	127.00	14	48375.	0.5	0.5	0.0938*
34	209.00	35	4121152.	38.7	38.7	7.9902*	89	126.00	17	77036.	0.7	0.7	0.1494*
35	208.00	21	70876.	0.7	0.7	0.1374*	90	125.00	8	7873.	0.1	0.1	0.0153
36	207.00	17	100120.	0.9	0.9	0.1941	91	124.00	8	2158.	0.0	0.0	0.0042
37	196.00	14	30679.	0.3	0.3	0.0595*	92	123.00	8	6198.	0.1	0.1	0.0120
38	195.00	12	12171.	0.1	0.1	0.0236	93	122.00	8	5986.	0.1	0.1	0.0116
39	194.00	21	219704.	2.1	2.1	0.4260	94	120.00	8	2072.	0.0	0.0	0.0040
40	193.00	35	1657728.	15.6	15.6	3.2140*	95	119.00	25	202624.	1.9	1.9	0.3929
41	192.00	35	1334976.	12.5	12.5	2.5883*	96	117.00	6	1867.	0.0	0.0	0.0036
42	191.00	17	15149.	0.1	0.1	0.0294*	97	116.00	14	39703.	0.4	0.4	0.0770*
43	186.00	17	61171.	0.6	0.6	0.1186*	98	115.00	29	361632.	3.4	3.4	0.7011*
44	184.00	8	3626.	0.0	0.0	0.0070	99	114.00	14	48452.	0.5	0.5	0.0939*
45	183.00	17	56599.	0.5	0.5	0.1097*	100	113.00	25	231972.	2.2	2.2	0.4498
46	182.00	12	37762.	0.4	0.4	0.0732	101	112.00	21	61316.	0.6	0.6	0.1189*
47	181.00	21	191072.	1.8	1.8	0.3705	102	111.00	29	113276.	1.1	1.1	0.2196*
48	180.00	14	41591.	0.4	0.4	0.0806*	103	110.00	17	47372.	0.4	0.4	0.0918*
49	179.00	14	46242.	0.4	0.4	0.0897	104	109.00	8	1661.	0.0	0.0	0.0032
50	178.00	8	12882.	0.1	0.1	0.0250	105	107.00	6	1705.	0.0	0.0	0.0033
51	177.00	8	9566.	0.1	0.1	0.0185	106	103.00	8	3020.	0.0	0.0	0.0059
52	176.00	8	1654.	0.0	0.0	0.0032	107	102.00	12	31298.	0.3	0.3	0.0607*
53	170.00	8	1366.	0.0	0.0	0.0026	108	101.00	10	19707.	0.2	0.2	0.0382*
54	169.00	14	30384.	0.3	0.3	0.0589*	109	100.00	21	127696.	1.2	1.2	0.2476
55	167.00	17	93776.	0.9	0.9	0.1818*	110	99.00	17	61251.	0.6	0.6	0.1188

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	98.00	17	79760.	0.7	0.7	0.1546*
112	97.00	25	216220.	2.0	2.0	0.4192*
113	96.00	71	2105664.	19.8	19.8	4.0825*
114	95.00	29	185368.	1.7	1.7	0.3594*
115	94.00	6	5057.	0.0	0.0	0.0098
116	93.00	8	3988.	0.0	0.0	0.0077
117	91.00	10	17888.	0.2	0.2	0.0347
118	90.00	10	7902.	0.1	0.1	0.0153
119	89.00	25	177900.	1.7	1.7	0.3449*
120	88.00	21	116568.	1.1	1.1	0.2260*
121	87.00	25	300064.	2.9	2.9	0.5973
122	86.00	21	137164.	1.3	1.3	0.2659*
123	85.00	8	18419.	0.2	0.2	0.0357
124	83.00	25	294576.	2.8	2.8	0.5711
125	82.00	71	3118784.	29.3	29.3	6.0467*
126	81.00	71	1032000.	9.7	9.7	2.0010*
127	80.00	8	6117.	0.1	0.1	0.0119*
128	78.00	10	2140.	0.0	0.0	0.0041
129	77.00	17	52730.	0.5	0.5	0.1022*
130	76.00	21	90748.	0.9	0.9	0.1759
131	75.00	25	202884.	1.9	1.9	0.3934
132	74.00	21	163092.	1.5	1.5	0.3162
133	73.00	12	23064.	0.2	0.2	0.0447*
134	72.00	6	1673.	0.0	0.0	0.0032
135	71.00	14	4833.	0.0	0.0	0.0034*
136	70.00	25	100064.	0.9	0.9	0.1940*
137	69.00	71	1703296.	16.0	16.0	3.3824*
138	68.00	12	33356.	0.3	0.3	0.0647*
139	65.00	17	69608.	0.7	0.7	0.1350*
140	64.00	21	161716.	1.5	1.5	0.3135*
141	63.00	29	433760.	4.1	4.1	0.8410
142	62.00	25	160496.	1.5	1.5	0.3112*
143	61.00	14	26785.	0.3	0.3	0.0519*
144	58.00	8	1171.	0.0	0.0	0.0023
145	57.00	10	7739.	0.1	0.1	0.0150
146	56.00	14	17967.	0.2	0.2	0.0348*
147	55.00	8	7988.	0.1	0.1	0.0155
148	53.00	6	2552.	0.0	0.0	0.0049
149	52.00	10	17703.	0.2	0.2	0.0343
150	51.00	35	452864.	4.3	4.3	0.8780
151	50.00	25	180736.	1.7	1.7	0.3504*
152	49.00	10	3373.	0.0	0.0	0.0065
153	47.00	8	5159.	0.0	0.0	0.0100
154	45.00	17	52148.	0.5	0.5	0.1011*
155	44.00	21	83340.	0.8	0.8	0.1616*
156	43.00	12	6101.	0.1	0.1	0.0118*
157	42.00	6	1556.	0.0	0.0	0.0030
158	40.00	10	4510.	0.0	0.0	0.0087*
159	39.00	25	226036.	2.1	2.1	0.4382*
160	38.00	21	62927.	0.6	0.6	0.1220*
161	37.00	10	10107.	0.1	0.1	0.0196
162	36.00	17	61172.	0.6	0.6	0.1186*
163	35.00	8	4246.	0.0	0.0	0.0082

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	407.00	8	4350.	0.1	0.1	0.0159	56	151.00	21	567376.	10.9	10.9	2.0715
2	406.00	17	105568.	2.0	2.0	0.3854*	57	150.00	25	331936.	6.4	6.4	1.2119
3	405.00	25	808272.	15.5	15.5	2.9510*	58	149.00	17	75332.	1.4	1.4	0.2750
4	404.00	35	4725248.	90.4	90.4	*17.25*	59	147.00	8	4006.	0.1	0.1	0.0146
5	403.00	17	47094.	0.9	0.9	0.1719*	60	139.00	10	14154.	0.3	0.3	0.0517
6	402.00	6	1486.	0.0	0.0	0.0054	61	137.00	10	8480.	0.2	0.2	0.0310*
7	401.00	6	660.	0.0	0.0	0.0024	62	133.00	10	11703.	0.2	0.2	0.0427
8	386.00	10	10538.	0.2	0.2	0.0385	63	131.00	10	11945.	0.2	0.2	0.0436
9	385.00	12	59474.	1.1	1.1	0.2171	64	129.00	8	1478.	0.6	0.6	0.0054
10	366.00	10	22494.	0.4	0.4	0.0821	65	127.00	17	33350.	0.6	0.6	0.2586*
11	365.00	17	106848.	2.0	2.0	0.3901	66	126.00	21	70820.	1.4	1.4	0.1311*
12	355.00	8	5461.	0.1	0.1	0.0199	67	125.00	14	35919.	0.7	0.7	0.0457*
13	341.00	12	12011.	0.2	0.2	0.0439	68	123.00	8	12522.	0.7	0.7	0.0282
14	335.00	6	1966.	0.0	0.0	0.0072	69	122.00	10	7711.	0.1	0.1	0.0282
15	321.00	6	2133.	0.0	0.0	0.0078	70	119.00	21	81012.	1.5	1.5	0.2958
16	295.00	8	1317.	0.0	0.0	0.0048	71	115.00	6	9423.	0.2	0.2	0.0344
17	285.00	8	4628.	0.1	0.1	0.0169	72	113.00	17	50218.	1.0	1.0	0.1833
18	283.00	8	4638.	0.1	0.1	0.0169	73	112.00	8	1631.	0.0	0.0	0.0060
19	282.00	10	7925.	0.2	0.2	0.0289	74	111.00	12	20948.	0.4	0.4	0.0765
20	281.00	12	49865.	1.0	1.0	0.1821	75	110.00	10	14948.	0.3	0.3	0.0546
21	267.00	6	2451.	0.0	0.0	0.0089	76	105.00	6	1600.	0.0	0.0	0.0058
22	249.00	8	1846.	0.0	0.0	0.0067	77	104.00	10	13753.	0.3	0.3	0.0502*
23	240.00	8	1408.	0.0	0.0	0.0051	78	103.00	43	886288.	17.0	17.0	3.2358*
24	235.00	10	2892.	0.1	0.1	0.0106	79	102.00	17	4704.	0.1	0.1	0.0172
25	222.00	10	9683.	0.2	0.2	0.0354*	80	101.00	17	23274.	0.4	0.4	0.0850*
26	221.00	14	45570.	0.9	0.9	0.1664	81	100.00	17	64687.	1.2	1.2	0.2362
27	220.00	17	81736.	1.6	1.6	0.2984	82	99.00	17	50668.	1.0	1.0	0.1850*
28	209.00	14	19625.	0.4	0.4	0.0717*	83	98.00	17	56120.	1.1	1.1	0.2049
29	208.00	14	43519.	0.8	0.8	0.1589*	84	97.00	6	1906.	0.0	0.0	0.0070
30	207.00	21	274128.	5.2	5.2	1.0008	85	96.00	8	11928.	0.2	0.2	0.0435
31	205.00	25	840272.	16.1	16.1	3.0678*	86	95.00	14	41512.	0.8	0.8	0.1516
32	204.00	43	5227008.	100.0	100.0	*19.08*	87	90.00	6	2626.	0.1	0.1	0.0096
33	204.00	14	32551.	0.6	0.6	0.1188*	88	89.00	51	1493952.	28.6	28.6	5.4544*
34	203.00	17	19289.	0.4	0.4	0.0704*	89	88.00	59	1751744.	33.5	33.5	6.3956*
35	202.00	17	119916.	2.3	2.3	0.4378	90	87.00	21	160684.	3.1	3.1	0.5867*
36	194.00	12	25144.	0.5	0.5	0.0918*	91	86.00	12	37045.	0.7	0.7	0.1353
37	193.00	17	94192.	1.8	1.8	0.3439	92	86.00	6	2225.	0.0	0.0	0.0081
38	192.00	12	14053.	0.3	0.3	0.0513	93	82.00	17	23590.	0.5	0.5	0.0861*
39	191.00	14	35384.	0.7	0.7	0.1288	94	77.00	17	41027.	0.8	0.8	0.1498*
40	180.00	6	986.	0.0	0.0	0.0036	95	76.00	29	113484.	2.2	2.2	0.4143*
41	179.00	17	71196.	1.4	1.4	0.2599	96	75.00	25	338080.	6.5	6.5	1.2343*
42	178.00	25	726624.	13.9	13.9	2.6529*	97	74.00	29	37720.	1.9	1.9	0.3568*
43	177.00	43	3469632.	66.4	66.4	*12.66*	98	73.00	25	37720.	0.8	0.8	0.1529*
44	176.00	51	1830976.	35.0	35.0	6.16848*	99	69.00	25	350480.	6.7	6.7	1.2796*
45	175.00	35	302592.	5.8	5.8	1.1048*	100	64.00	12	25627.	0.5	0.5	0.0936
46	174.00	21	151932.	2.9	2.9	0.5547	101	63.00	21	78140.	1.5	1.5	0.2853*
47	169.00	8	10953.	0.2	0.2	0.0400	102	62.00	14	43418.	0.8	0.8	0.1585*
48	166.00	10	7822.	0.1	0.1	0.0286	103	61.00	6	3735.	0.1	0.1	0.0136
49	165.00	17	83544.	1.6	1.6	0.3050*	104	51.00	25	207268.	4.0	4.0	0.7567*
50	164.00	17	127260.	2.4	2.4	0.4646	105	50.00	17	50926.	1.0	1.0	0.1859*
51	163.00	21	107360.	2.1	2.1	0.3920	106	45.00	6	1399.	0.0	0.0	0.0051
52	162.00	8	10780.	0.2	0.2	0.0394	107	44.00	17	41494.	0.8	0.8	0.1515*
53	154.00	8	3264.	0.1	0.1	0.0119	108	41.00	6	2757.	0.1	0.1	0.0101
54	153.00	17	31550.	0.6	0.6	0.1152*	109	40.00	8	7508.	0.1	0.1	0.0274
55	152.00	21	96692.	1.8	1.8	0.3530*	110	39.00	14	38196.	0.7	0.7	0.1395

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	38.00	8	4941.	0.1	0.1	0.0180
112	36.00	6	3169.	0.1	0.1	0.0116

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	429.00	8	4218.	0.1	0.1	0.0104	56	267.00	12	24325.	0.4	0.4	0.0597
2	419.00	6	1443.	0.0	0.0	0.0035	57	265.00	10	1137.	0.0	0.0	0.0028
3	415.00	6	654.	0.0	0.0	0.0016	58	253.00	6	1247.	0.0	0.0	0.0031
4	413.00	8	1204.	0.0	0.0	0.0030	59	252.00	8	5855.	0.1	0.1	0.0144
5	412.00	8	1137.	0.0	0.0	0.0028	60	251.00	10	6604.	0.1	0.1	0.0162
6	410.00	6	447.	0.0	0.0	0.0011	61	249.00	8	2888.	0.0	0.0	0.0071
7	408.00	10	941.	0.0	0.0	0.0023	62	241.00	8	2342.	0.0	0.0	0.0057
8	407.00	12	15138.	0.2	0.2	0.0372*	63	240.00	10	14648.	0.2	0.2	0.0360
9	406.00	21	68404.	1.0	1.0	0.1679*	64	239.00	8	2123.	0.0	0.0	0.0052
10	405.00	35	1195584.	17.5	17.5	2.9346*	65	238.00	8	4943.	0.1	0.1	0.0121
11	404.00	43	6425600.	94.3	94.3	*15.77*	66	237.00	6	2388.	0.0	0.0	0.0070
12	403.00	25	75888.	1.1	1.1	0.1863*	67	236.00	10	2710.	0.0	0.0	0.0067
13	402.00	12	11678.	0.2	0.2	0.0287*	68	235.00	14	24873.	0.4	0.4	0.0611
14	401.00	17	14864.	0.2	0.2	0.0365*	69	227.00	10	5035.	0.1	0.1	0.0124
15	400.00	14	7106.	0.1	0.1	0.0174*	70	226.00	6	659.	0.0	0.0	0.0016
16	399.00	8	2168.	0.0	0.0	0.0053	71	225.00	6	2167.	0.0	0.0	0.0053
17	398.00	8	771.	0.0	0.0	0.0019	72	223.00	8	2784.	0.0	0.0	0.0058
18	387.00	8	2302.	0.0	0.0	0.0057	73	222.00	14	21461.	0.3	0.3	0.0027
19	386.00	14	42847.	0.6	0.6	0.1052	74	221.00	21	84796.	1.2	1.2	0.2081
20	385.00	17	192548.	2.8	2.8	0.04726	75	220.00	17	98888.	1.5	1.5	0.2427
21	384.00	6	942.	0.0	0.0	0.0023	76	219.00	8	7917.	0.1	0.1	0.0194
22	383.00	8	912.	0.0	0.0	0.0022	77	218.00	14	2798.	0.0	0.0	0.0069*
23	381.00	6	455.	0.0	0.0	0.0016	78	217.00	14	2285.	0.0	0.0	0.0056
24	377.00	6	652.	0.0	0.0	0.0011	79	212.00	8	1687.	0.0	0.0	0.0041
25	376.00	10	2923.	0.0	0.0	0.0072	80	211.00	10	3303.	0.0	0.0	0.0081
26	375.00	8	1066.	0.0	0.0	0.0026	81	210.00	6	1242.	0.0	0.0	0.0030
27	366.00	12	15674.	0.2	0.2	0.0385	82	209.00	14	37564.	0.6	0.6	0.0022
28	365.00	12	41360.	0.6	0.6	0.1015	83	208.00	17	61230.	0.5	0.5	0.1503
29	361.00	6	335.	0.0	0.0	0.0008	84	207.00	25	353152.	5.2	5.2	0.8668
30	359.00	8	2712.	0.0	0.0	0.0067	85	206.00	35	1097216.	16.1	16.1	2.6932*
31	358.00	10	2039.	0.0	0.0	0.0050	86	205.00	51	6813952.	100.0	100.0	*16.72*
32	357.00	12	16285.	0.2	0.2	0.0400	87	204.00	29	80628.	1.2	1.2	0.1979*
33	355.00	10	4815.	0.1	0.1	0.0118	88	203.00	17	45583.	0.7	0.7	0.1119*
34	341.00	10	10954.	0.2	0.2	0.0269	89	202.00	25	90392.	1.3	1.3	0.2219*
35	340.00	6	918.	0.0	0.0	0.0023	90	201.00	10	5786.	0.1	0.1	0.0142
36	337.00	6	1110.	0.0	0.0	0.0027	91	199.00	8	1165.	0.0	0.0	0.0029
37	327.00	6	1650.	0.0	0.0	0.0040	92	196.00	12	10000.	0.1	0.1	0.0245
38	322.00	10	4176.	0.1	0.1	0.0103	93	195.00	14	8186.	0.1	0.1	0.0201
39	321.00	12	24413.	0.4	0.4	0.0599	94	194.00	14	6180.	0.1	0.1	0.0152
40	317.00	6	1173.	0.0	0.0	0.0029	95	193.00	14	25880.	0.4	0.4	0.0635*
41	302.00	8	935.	0.0	0.0	0.0023	96	192.00	14	27790.	0.4	0.4	0.0682*
42	301.00	8	2006.	0.0	0.0	0.0049	97	191.00	21	58892.	0.9	0.9	0.1446
43	288.00	8	1778.	0.0	0.0	0.0044	98	190.00	6	2396.	0.0	0.0	0.0059
44	287.00	8	1425.	0.0	0.0	0.0035	99	189.00	12	13900.	0.2	0.2	0.0341*
45	286.00	10	2442.	0.0	0.0	0.0060	100	188.00	14	2740.	0.0	0.0	0.0067*
46	285.00	14	20648.	0.3	0.3	0.0507	101	187.00	10	2510.	0.0	0.0	0.0062
47	284.00	6	1831.	0.0	0.0	0.0045	102	182.00	6	1455.	0.0	0.0	0.0036
48	283.00	12	4133.	0.1	0.1	0.0101	103	181.00	12	22673.	0.3	0.3	0.0557
49	282.00	14	16772.	0.2	0.2	0.0412*	104	180.00	10	8389.	0.1	0.1	0.0206
50	281.00	17	45295.	0.7	0.7	0.1112	105	179.00	21	99912.	1.5	1.5	0.2452*
51	275.00	6	591.	0.0	0.0	0.0015	106	178.00	35	997200.	14.6	14.6	2.4477*
52	271.00	10	5194.	0.1	0.1	0.0127	107	177.00	51	5873920.	86.2	86.2	*14.41*
53	270.00	8	2294.	0.0	0.0	0.0056	108	176.00	59	2509504.	36.8	36.8	6.1597*
54	269.00	10	5734.	0.1	0.1	0.0141	109	175.00	59	565728.	8.3	8.3	1.3886*
55	268.00	10	4101.	0.1	0.1	0.0101	110	174.00	35	237328.	3.5	3.5	0.5825*

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	173.00	17	27249.	0.4	0.4	0.0669*	166	110.00	12	28951.	0.4	0.4	0.0711*
112	172.00	10	5304.	0.1	0.1	0.0130*	167	109.00	10	10572.	0.2	0.2	0.0259
113	171.00	8	1170.	0.0	0.0	0.0029	168	106.00	8	3052.	0.0	0.0	0.0075
114	170.00	8	1428.	0.0	0.0	0.0035	169	105.00	25	27148.	0.4	0.4	0.0666*
115	169.00	17	17985.	0.3	0.3	0.0441*	170	104.00	51	56880.	1.0	1.0	0.1642*
116	168.00	10	2024.	0.0	0.0	0.0050	171	103.00	51	672192.	9.9	9.9	1.6499*
117	167.00	6	1041.	0.0	0.0	0.0026	172	102.00	35	968448.	14.2	14.2	2.3771*
118	166.00	14	22686.	0.3	0.3	0.0557*	173	101.00	21	58748.	0.9	0.9	0.1442*
119	165.00	21	108892.	1.6	1.6	0.2673	174	100.00	21	102948.	1.5	1.5	0.2527
120	164.00	21	122852.	1.8	1.8	0.3015	175	99.00	21	87600.	1.3	1.3	0.2150
121	163.00	21	117236.	1.7	1.7	0.2878	176	98.00	21	106880.	1.6	1.6	0.2623
122	162.00	14	17702.	0.3	0.3	0.0435*	177	97.00	17	97382.	0.3	0.3	0.0581*
123	161.00	12	14973.	0.2	0.2	0.0369*	178	96.00	21	53498.	0.8	0.8	0.1313*
124	159.00	8	3427.	0.1	0.1	0.0084	179	95.00	21	131356.	1.9	1.9	0.3224
125	156.00	8	1133.	0.0	0.0	0.0028	180	94.00	10	11820.	0.2	0.2	0.0290*
126	155.00	12	6663.	0.1	0.1	0.0164	181	90.00	8	4510.	0.1	0.1	0.0111
127	154.00	29	41559.	0.6	0.6	0.1020*	182	89.00	35	354576.	5.2	5.2	0.0703*
128	153.00	51	103668.	1.5	1.5	0.2545*	183	88.00	87	3828480.	56.2	56.2	9.3971*
129	152.00	35	148908.	2.2	2.2	0.3655*	184	87.00	59	472928.	6.9	6.9	1.1608*
130	151.00	29	816496.	12.0	12.0	2.0041*	185	86.00	25	73808.	1.1	1.1	0.1812*
131	150.00	29	512192.	7.5	7.5	1.2572*	186	85.00	17	32107.	0.5	0.5	0.0788*
132	149.00	25	113652.	1.7	1.7	0.2790*	187	84.00	10	1409.	0.0	0.0	0.0035
133	148.00	10	9694.	0.1	0.1	0.0238	188	83.00	17	46429.	0.7	0.7	0.1140
134	147.00	12	13714.	0.2	0.2	0.0337*	189	82.00	25	53225.	0.8	0.8	0.1306*
135	146.00	8	8230.	0.1	0.1	0.0202	190	81.00	25	39598.	0.6	0.6	0.0972*
136	145.00	10	1264.	0.0	0.0	0.0031	191	79.00	10	13236.	0.2	0.2	0.0325
137	143.00	6	1093.	0.0	0.0	0.0027	192	78.00	12	11545.	0.2	0.2	0.0283*
138	142.00	10	2881.	0.0	0.0	0.0071	193	77.00	29	110796.	1.6	1.6	0.2720*
139	140.00	10	1928.	0.0	0.0	0.0047	194	76.00	35	152108.	2.2	2.2	0.3734*
140	139.00	14	40285.	0.6	0.6	0.0989	195	75.00	51	526384.	7.7	7.7	1.2320*
141	138.00	10	9271.	0.1	0.1	0.0228	196	74.00	35	186472.	2.7	2.7	0.4577*
142	137.00	12	25889.	0.4	0.4	0.0635	197	73.00	21	53474.	0.8	0.8	0.1313*
143	135.00	10	1663.	0.0	0.0	0.0041	198	70.00	8	3800.	0.1	0.1	0.0095*
144	135.00	10	8274.	0.1	0.1	0.0203*	199	69.00	29	529408.	7.8	7.8	1.2395*
145	134.00	10	5906.	0.1	0.1	0.0145	200	68.00	8	1300.	0.0	0.0	0.0032
146	133.00	14	36217.	0.5	0.5	0.0889	201	67.00	10	4197.	0.1	0.1	0.0103
147	132.00	6	738.	0.0	0.0	0.0018	202	65.00	12	21145.	0.3	0.3	0.0519*
148	131.00	17	22293.	0.3	0.3	0.0547*	203	64.00	21	75560.	1.1	1.1	0.1855*
149	129.00	12	9641.	0.1	0.1	0.0237*	204	63.00	21	150744.	2.2	2.2	0.3700
150	128.00	14	10918.	0.2	0.2	0.0268*	205	62.00	17	100844.	1.5	1.5	0.2475*
151	127.00	21	58209.	0.9	0.9	0.1429*	206	61.00	14	19059.	0.3	0.3	0.0468*
152	126.00	21	112732.	1.7	1.7	0.2757	207	59.00	8	4501.	0.1	0.1	0.0110
153	125.00	17	48265.	0.7	0.7	0.1185	208	57.00	8	13396.	0.2	0.2	0.0329
154	124.00	14	30458.	0.4	0.4	0.0748	209	56.00	10	11600.	0.2	0.2	0.0285*
155	123.00	17	38509.	0.6	0.6	0.0945	210	55.00	8	12222.	0.2	0.2	0.0300
156	122.00	17	38060.	0.6	0.6	0.0934	211	53.00	6	4208.	0.1	0.1	0.0103
157	121.00	6	3461.	0.1	0.1	0.0085	212	52.00	12	26473.	0.4	0.4	0.0650
158	120.00	8	2743.	0.0	0.0	0.0067	213	51.00	29	346384.	5.1	5.1	0.8502*
159	119.00	21	112600.	1.7	1.7	0.2764	214	50.00	21	97868.	1.4	1.4	0.2402
160	117.00	8	3412.	0.1	0.1	0.0064	215	49.00	12	3607.	0.1	0.1	0.0089
161	115.00	12	15028.	0.2	0.2	0.0369*	216	46.00	6	2813.	0.0	0.0	0.0059
162	114.00	8	3952.	0.1	0.1	0.0097	217	45.00	17	37648.	0.6	0.6	0.0924*
163	113.00	21	80376.	1.2	1.2	0.1973	218	44.00	25	72840.	1.1	1.1	0.1788
164	112.00	12	11061.	0.2	0.2	0.0271	219	43.00	12	8332.	0.1	0.1	0.0205
165	111.00	21	53504.	0.8	0.8	0.1313*	220	42.00	10	1430.	0.0	0.0	0.0035

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
221	41.00	10	6782.	0.1	0.1	0.0166
222	40.00	8	2013.	0.0	0.0	0.0049
223	39.00	17	65122.	1.0	1.0	0.1598
224	38.00	17	27409.	0.4	0.4	0.0673*
225	37.00	8	1598.	0.0	0.0	0.0039
226	36.00	17	35661.	0.5	0.5	0.0875

HEP3PK.1 [TIC=3537152, 100%-509552] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	418.00	8	1307.	0.3	0.3	0.0370	56	95.00	21	222984.	43.8	43.8	6.3041
2	417.00	12	18750.	3.7	3.7	0.5301	57	94.00	10	11187.	2.2	2.2	0.3163
3	416.00	17	108996.	21.4	21.4	3.0815	58	93.00	14	38223.	7.5	7.5	1.0806
4	414.00	6	864.	0.2	0.2	0.0244	59	92.00	25	236412.	46.4	46.4	6.6837*
5	398.00	8	1120.	0.2	0.2	0.0317	60	91.00	8	7152.	1.4	1.4	0.2022
6	397.00	12	19800.	3.9	3.9	0.5620	61	83.00	12	12225.	2.4	2.4	0.3456
7	347.00	10	7963.	1.6	1.6	0.2251	62	82.00	10	3837.	0.8	0.8	0.1085
8	320.00	8	1275.	0.3	0.3	0.0360	63	81.00	12	24973.	4.9	4.9	0.7060
9	304.00	10	2788.	0.5	0.5	0.0788	64	80.00	14	18620.	3.7	3.7	0.5264*
10	303.00	12	21738.	4.3	4.3	0.6146	65	79.00	6	4114.	0.8	0.8	0.1163
11	291.00	10	2534.	0.5	0.5	0.0716	66	78.00	5	1612.	0.3	0.3	0.0456
12	277.00	8	1733.	0.3	0.3	0.0490	67	77.00	12	17301.	3.4	3.4	0.4891
13	269.00	8	977.	0.2	0.2	0.0276	68	76.00	14	27120.	5.3	5.3	0.7667
14	263.00	12	9106.	1.8	1.8	0.2574*	69	75.00	17	51129.	10.0	10.0	1.4455*
15	219.00	12	7700.	1.5	1.5	0.2177	70	74.00	10	11008.	2.2	2.2	0.3112
16	218.00	14	51249.	10.1	10.1	0.4489*	71	73.00	8	1311.	0.3	0.3	0.0371
17	217.00	29	509552.	100.0	100.0	*14.40*	72	71.00	6	1133.	0.2	0.2	0.0320
18	216.00	10	4911.	1.0	1.0	0.1388	73	69.00	29	449312.	88.2	88.2	*12.70*
19	193.00	8	1884.	0.4	0.4	0.0533	74	67.00	8	1492.	0.3	0.3	0.0422
20	190.00	12	33635.	6.6	6.6	0.9509	75	66.00	8	5567.	1.1	1.1	0.1574
21	189.00	21	232416.	45.6	45.6	6.5707*	76	65.00	17	39393.	7.7	7.7	1.1137*
22	187.00	8	3148.	0.6	0.6	0.0890	77	64.00	25	139056.	27.3	27.3	3.9313
23	183.00	10	11952.	2.3	2.3	0.3379	78	63.00	25	130988.	25.7	25.7	3.7032
24	181.00	6	1134.	0.2	0.2	0.0321	79	62.00	14	22509.	4.4	4.4	0.6364
25	177.00	8	1174.	0.2	0.2	0.0332	80	61.00	14	8825.	1.7	1.7	0.2495
26	169.00	12	6951.	1.4	1.4	0.1965	81	57.00	17	10114.	2.0	2.0	0.2859*
27	161.00	6	640.	0.1	0.1	0.0181	82	56.00	8	1827.	0.4	0.4	0.0517
28	159.00	8	1545.	0.3	0.3	0.0437	83	55.00	12	4970.	1.0	1.0	0.1405*
29	150.00	6	1472.	0.3	0.3	0.0416	84	54.00	6	2871.	0.6	0.6	0.0812
30	149.00	12	12270.	2.4	2.4	0.3469	85	53.00	12	16891.	3.3	3.3	0.4775*
31	145.00	8	1930.	0.4	0.4	0.0546	86	52.00	10	12193.	2.4	2.4	0.3447
32	139.00	10	13907.	2.7	2.7	0.3932	87	51.00	21	55709.	10.9	10.9	1.5750*
33	137.00	6	998.	0.2	0.2	0.0282	88	50.00	17	64659.	12.7	12.7	1.8280*
34	135.00	8	1147.	0.2	0.2	0.0324	89	45.00	12	7056.	1.4	1.4	0.1995*
35	133.00	10	4932.	1.0	1.0	0.1394	90	44.00	10	14065.	2.8	2.8	0.3976
36	131.00	8	6300.	1.2	1.2	0.1783	91	43.00	8	5749.	1.1	1.1	0.1625
37	127.00	10	3354.	0.7	0.7	0.0948	92	42.00	8	2678.	0.5	0.5	0.0757
38	125.00	8	1662.	0.3	0.3	0.0470	93	41.00	8	8004.	1.6	1.6	0.2263
39	124.00	12	7064.	1.4	1.4	0.0470	94	39.00	14	34693.	6.8	6.8	0.9808
40	123.00	21	142736.	28.0	28.0	4.0353	95	38.00	21	60327.	11.8	11.8	1.7055*
41	122.00	12	7866.	1.5	1.5	0.2224	96	37.00	14	4720.	0.9	0.9	0.1334
42	121.00	25	231016.	45.3	45.3	6.5311	97	36.00	12	21036.	4.1	4.1	0.5947
43	120.00	12	35489.	7.0	7.0	1.0033							
44	119.00	12	21948.	4.3	4.3	0.6205							
45	113.00	10	2032.	0.4	0.4	0.0574							
46	111.00	8	3267.	0.6	0.6	0.0924							
47	108.00	8	1164.	0.2	0.2	0.0329							
48	107.00	8	1973.	0.4	0.4	0.0558							
49	106.00	8	7088.	1.4	1.4	0.2004							
50	105.00	17	10229.	2.0	2.0	0.2892							
51	104.00	12	3828.	0.8	0.8	0.1082							
52	101.00	10	16552.	3.2	3.2	0.4679*							
53	100.00	12	26948.	5.3	5.3	0.7619*							
54	97.00	17	16396.	3.2	3.2	0.4635							
55	96.00	8											

1PKBL7.1 [TIC-68448256, 188X-21272576] EI

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	511.00	8	2113.	0.0	0.0	0.0031	56	275.00	8	1486.	0.0	0.0	0.0022
2	486.00	6	353.	0.0	0.0	0.0005	57	272.00	14	21083.	0.1	0.1	0.0308
3	485.00	10	3377.	0.0	0.0	0.0049	58	264.00	14	26823.	0.1	0.1	0.0392
4	458.00	6	1030.	0.0	0.0	0.0015	59	263.00	21	225764.	1.1	1.1	0.3298*
5	438.00	6	670.	0.0	0.0	0.0010	60	259.00	10	2720.	0.0	0.0	0.0040
6	437.00	6	527.	0.0	0.0	0.0008	61	258.00	14	26196.	0.1	0.1	0.0383
7	419.00	12	8446.	0.0	0.0	0.0123*	62	253.00	10	4766.	0.0	0.0	0.0070
8	418.00	21	56775.	0.3	0.3	0.0829*	63	251.00	8	1165.	0.0	0.0	0.0017
9	417.00	25	259808.	1.2	1.2	0.3796*	64	249.00	8	1621.	0.0	0.0	0.0024
10	416.00	51	4807936.	22.6	22.6	7.0242*	65	247.00	14	25258.	0.1	0.1	0.0369
11	415.00	29	169844.	0.8	0.8	0.2481*	66	245.00	8	2250.	0.0	0.0	0.0033
12	414.00	14	14833.	0.1	0.1	0.0217*	67	243.00	8	753.	0.0	0.0	0.0011
13	413.00	21	3641.	0.0	0.0	0.0053*	68	237.00	10	6150.	0.0	0.0	0.0090
14	412.00	8	1712.	0.0	0.0	0.0025	69	236.00	6	707.	0.0	0.0	0.0010
15	411.00	8	2870.	0.0	0.0	0.0042	70	235.00	10	4467.	0.0	0.0	0.0065
16	399.00	8	8578.	0.0	0.0	0.0125	71	234.00	8	2144.	0.0	0.0	0.0031
17	398.00	14	60602.	0.3	0.3	0.0885	72	233.00	17	2179.	0.0	0.0	0.0032*
18	397.00	25	447296.	2.1	2.1	0.6535*	73	231.00	8	1116.	0.0	0.0	0.0016
19	396.00	8	6382.	0.0	0.0	0.0093	74	227.00	6	935.	0.0	0.0	0.0014
20	395.00	8	1459.	0.0	0.0	0.0021	75	224.00	10	3286.	0.0	0.0	0.0048
21	391.00	8	529.	0.0	0.0	0.0008	76	222.00	12	1590.	0.0	0.0	0.0023
22	387.00	6	2403.	0.0	0.0	0.0035	77	221.00	8	2455.	0.0	0.0	0.0036
23	377.00	10	4075.	0.0	0.0	0.0060	78	220.00	21	22886.	0.1	0.1	0.0334*
24	376.00	8	1109.	0.0	0.0	0.0015	79	219.00	29	213028.	1.0	1.0	0.3112*
25	372.00	6	1019.	0.0	0.0	0.0015	80	218.00	43	1925952.	9.1	9.1	2.8137*
26	370.00	14	12507.	0.1	0.1	0.0183	81	217.00	71	21272576.	0.5	0.5	0.1646*
27	369.00	17	76180.	0.4	0.4	0.1113	82	216.00	35	112664.	0.2	0.2	0.0671*
28	365.00	10	19871.	0.1	0.1	0.0290	83	215.00	29	45933.	0.1	0.1	0.0235*
29	354.00	8	2993.	0.0	0.0	0.0044	84	214.00	21	16083.	0.0	0.0	0.0088*
30	353.00	17	54133.	0.3	0.3	0.0791	85	213.00	17	6030.	0.0	0.0	0.0022
31	352.00	8	9459.	0.0	0.0	0.0138	86	211.00	6	1525.	0.0	0.0	0.0027
32	349.00	6	2135.	0.0	0.0	0.0031	87	208.00	6	1860.	0.0	0.0	0.0084
33	347.00	10	8314.	0.0	0.0	0.0121	88	207.00	10	5747.	0.0	0.0	0.0085*
34	341.00	8	1511.	0.0	0.0	0.0022	89	205.00	10	5816.	0.0	0.0	0.0087
35	325.00	12	8009.	0.0	0.0	0.0117	90	204.00	12	5922.	0.0	0.0	0.0083
36	321.00	10	2457.	0.0	0.0	0.0036	91	203.00	8	5683.	0.0	0.0	0.0029*
37	320.00	12	11096.	0.1	0.1	0.0162	92	202.00	12	1972.	0.0	0.0	0.0187*
38	319.00	14	59729.	0.3	0.3	0.0873	93	200.00	14	12805.	0.1	0.1	0.017
39	307.00	6	1093.	0.0	0.0	0.0016	94	199.00	6	1140.	0.0	0.0	0.0017
40	305.00	12	4911.	0.0	0.0	0.0072*	95	197.00	8	1179.	0.0	0.0	0.0017
41	304.00	17	54911.	0.3	0.3	0.0802	96	193.00	8	2428.	0.0	0.0	0.0035
42	303.00	25	498192.	2.3	2.3	0.7278*	97	192.00	6	996.	0.0	0.0	0.0015
43	302.00	17	57291.	0.3	0.3	0.0837*	98	191.00	17	33279.	0.2	0.2	0.0486
44	301.00	14	1976.	0.0	0.0	0.0029	99	190.00	29	355184.	1.7	1.7	0.5189*
45	300.00	12	10945.	0.1	0.1	0.0160	100	189.00	51	4231680.	19.9	19.9	6.1823*
46	298.00	12	10854.	0.1	0.1	0.0159	101	188.00	25	69124.	0.3	0.3	0.1010*
47	297.00	21	114476.	0.5	0.5	0.1672	102	187.00	8	1875.	0.0	0.0	0.0027
48	293.00	8	1602.	0.0	0.0	0.0023	103	185.00	6	870.	0.0	0.0	0.0013
49	292.00	14	25406.	0.1	0.1	0.0371	104	184.00	12	3961.	0.0	0.0	0.0058*
50	291.00	21	233096.	1.1	1.1	0.3405*	105	183.00	21	86444.	0.4	0.4	0.1263
51	290.00	8	2799.	0.0	0.0	0.0041	106	182.00	6	390.	0.0	0.0	0.0006
52	283.00	8	2413.	0.0	0.0	0.0035	107	177.00	17	41826.	0.2	0.2	0.0611
53	281.00	8	2350.	0.0	0.0	0.0034	108	176.00	8	10230.	0.0	0.0	0.0149
54	279.00	6	1905.	0.0	0.0	0.0028	109	175.00	8	4969.	0.0	0.0	0.0073
55	277.00	12	26839.	0.1	0.1	0.0392	110	173.00	8	1611.	0.0	0.0	0.0024

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
111	172.00	14	21718.	0.1	0.1	0.0317	166	112.00	25	18545.	0.1	0.1	0.0271*
112	171.00	14	31398.	0.1	0.1	0.0459	167	111.00	21	91072.	0.4	0.4	0.1331
113	169.00	14	50120.	0.2	0.2	0.0732	168	110.00	17	13134.	0.1	0.1	0.0192*
114	167.00	10	11410.	0.1	0.1	0.0167	169	109.00	17	86448.	0.4	0.4	0.1263
115	166.00	17	7134.	0.0	0.0	0.0104*	170	108.00	21	153032.	0.7	0.7	0.2236
116	165.00	43	77472.	0.4	0.4	0.1132*	171	107.00	17	64616.	0.3	0.3	0.0944
117	164.00	29	58008.	0.3	0.3	0.0859*	172	106.00	10	2563.	0.0	0.0	0.0037
118	163.00	14	24463.	0.1	0.1	0.0357*	173	105.00	17	51455.	0.2	0.2	0.0752
119	162.00	17	68732.	0.3	0.3	0.1004	174	104.00	21	171296.	0.8	0.8	0.2503
120	161.00	29	898512.	4.2	4.2	1.3127*	175	103.00	21	209516.	1.0	1.0	0.3061
121	160.00	14	27227.	0.1	0.1	0.0398	176	102.00	6	1550.	0.0	0.0	0.0023
122	159.00	12	6774.	0.0	0.0	0.0099*	177	101.00	17	23420.	0.1	0.1	0.0342
123	158.00	8	2931.	0.0	0.0	0.0041	178	100.00	21	131100.	0.6	0.6	0.1915
124	157.00	8	1302.	0.0	0.0	0.0020	179	99.00	17	28751.	0.1	0.1	0.0420
125	156.00	8	1141.	0.0	0.0	0.0017	180	98.00	17	8000.	0.0	0.0	0.0117
126	155.00	8	2504.	0.0	0.0	0.0037	181	97.00	25	428656.	2.0	2.0	0.6262
127	154.00	8	4705.	0.0	0.0	0.0069	182	96.00	21	190236.	0.9	0.9	0.2779*
128	153.00	6	618.	0.0	0.0	0.0009	183	95.00	43	3047232.	14.3	14.3	4.4519*
129	152.00	10	2375.	0.1	0.1	0.0035	184	94.00	25	91440.	0.4	0.4	0.1336*
130	151.00	14	24507.	0.1	0.1	0.0358	185	93.00	25	235548.	1.1	1.1	0.3441*
131	150.00	12	22660.	0.1	0.1	0.0331*	186	92.00	43	2529216.	11.9	11.9	3.6951*
132	149.00	10	12688.	0.1	0.1	0.0185	187	91.00	21	108576.	0.5	0.5	0.1586*
133	148.00	10	2445.	0.0	0.0	0.0036	188	90.00	10	8040.	0.0	0.0	0.0117
134	147.00	12	7887.	0.0	0.0	0.00115	189	89.00	6	1345.	0.0	0.0	0.0020
135	146.00	6	523.	0.0	0.0	0.0008	190	88.00	8	3933.	0.0	0.0	0.0057
136	145.00	17	22714.	0.1	0.1	0.0332*	191	87.00	8	3278.	0.0	0.0	0.0048
137	143.00	8	1968.	0.0	0.0	0.0029	192	86.00	10	1860.	0.0	0.0	0.0027
138	142.00	10	9081.	0.0	0.0	0.0133	193	85.00	21	97656.	0.5	0.5	0.1427*
139	141.00	14	29086.	0.1	0.1	0.0425	194	84.00	12	12097.	0.1	0.1	0.0177*
140	140.00	21	26305.	0.1	0.1	0.0384	195	83.00	21	221056.	1.0	1.0	0.3230
141	139.00	25	395504.	1.9	1.9	0.5778*	196	82.00	21	64446.	0.3	0.3	0.0942*
142	138.00	25	35130.	0.2	0.2	0.0513*	197	81.00	29	439280.	2.1	2.1	0.6418*
143	137.00	29	48977.	0.2	0.2	0.0716*	198	80.00	25	217612.	1.0	1.0	0.3179
144	136.00	17	34234.	0.2	0.2	0.0500*	199	79.00	21	73792.	0.3	0.3	0.1078
145	135.00	8	4373.	0.1	0.1	0.0064	200	78.00	21	68440.	0.3	0.3	0.1000*
146	134.00	12	25449.	0.1	0.1	0.0372	201	77.00	21	108916.	0.5	0.5	0.1591
147	133.00	25	303392.	1.4	1.4	0.4432*	202	76.00	25	488272.	2.3	2.3	0.7133
148	132.00	14	36474.	0.2	0.2	0.0533	203	75.00	35	1547840.	7.3	7.3	2.2613*
149	131.00	14	35570.	0.2	0.2	0.0520	204	74.00	29	334000.	1.6	1.6	0.4880*
150	129.00	6	1282.	0.0	0.0	0.0019	205	73.00	21	46961.	0.2	0.2	0.0686*
151	128.00	12	15891.	0.1	0.1	0.0232	206	72.00	17	4081.	0.0	0.0	0.0060*
152	127.00	12	18813.	0.1	0.1	0.0275	207	71.00	14	19832.	0.1	0.1	0.0290*
153	126.00	14	22293.	0.1	0.1	0.0326*	208	70.00	21	70316.	0.3	0.3	0.1027*
154	125.00	10	4529.	0.0	0.0	0.0066	209	69.00	51	711808.	33.5	33.5	*0.39*
155	124.00	10	2231.	0.0	0.0	0.0033	210	68.00	25	28159.	0.1	0.1	0.0411*
156	123.00	14	27787.	0.1	0.1	0.0466*	211	67.00	21	84324.	0.4	0.4	0.1232*
157	122.00	10	10034.	0.0	0.0	0.0147	212	66.00	25	193316.	0.9	0.9	0.2824
158	121.00	21	135764.	0.6	0.6	0.1983*	213	65.00	25	303280.	1.4	1.4	0.4431*
159	120.00	35	804480.	3.8	3.8	1.1753*	214	64.00	35	2216000.	10.4	10.4	3.2375*
160	119.00	25	637856.	3.0	3.0	0.9319*	215	63.00	43	1879744.	8.8	8.8	2.7462*
161	118.00	25	24737.	0.1	0.1	0.0361*	216	62.00	21	421696.	2.0	2.0	0.6161*
162	116.00	10	8140.	0.0	0.0	0.0119*	217	61.00	21	100444.	0.5	0.5	0.1467
163	115.00	12	7133.	0.0	0.0	0.0104*	218	60.00	25	19336.	0.1	0.1	0.0282*
164	114.00	25	62059.	0.3	0.3	0.0907*	219	59.00	25	15026.	0.1	0.1	0.0220*
165	113.00	59	651808.	3.1	3.1	0.9669*	220	57.00	21	51421.	0.2	0.2	0.0751

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT BASE	% INT. NREF	% TOT. ION
221	56.00	17	24995.	0.1	0.1	0.0365*
222	55.00	14	31720.	0.1	0.1	0.0463
223	54.00	17	37290.	0.2	0.2	0.0545
224	53.00	29	209052.	1.0	1.0	0.3054*
225	52.00	35	435344.	2.0	2.0	0.6360*
226	51.00	29	616752.	2.9	2.9	0.9010*
227	50.00	29	761984.	3.6	3.6	1.1132
228	49.00	25	34339.	0.2	0.2	0.0502*
229	48.00	8	2607.	0.0	0.0	0.0038
230	47.00	17	20294.	0.1	0.1	0.0296*
231	46.00	17	37401.	0.2	0.2	0.0546
232	45.00	21	78960.	0.4	0.4	0.1154*
233	44.00	29	134220.	0.6	0.6	0.1961*
234	43.00	10	7770.	0.0	0.0	0.0114*
235	42.00	10	8798.	0.0	0.0	0.0129*
236	41.00	14	10726.	0.1	0.1	0.0157*
237	40.00	10	6265.	0.0	0.0	0.0092*
238	39.00	29	204412.	1.0	1.0	0.2986*
239	38.00	35	765088.	3.6	3.6	1.1178*
240	37.00	21	118852.	0.6	0.6	0.1736*
241	36.00	25	65059.	0.3	0.3	0.0950
242	35.00	14	11045.	0.1	0.1	0.0161*

AY9AV.1 [TIC-89198488, 188X-51734528] EI

9-xanthenecarboxylic acid,
2,2,3,3,4,4,4-heptafluorobutyl ester

PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION	PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	% INT. BASE	% INT. NREF	% TOT. ION
1	410.00	10	9708.	0.0	0.0	0.0109	56	128.00	25	126316.	0.2	0.2	0.1416*
2	409.00	12	114276.	0.2	0.2	0.1281	57	127.00	35	804032.	1.6	1.6	0.9015*
3	408.00	17	707568.	1.4	1.4	0.7933	58	126.00	25	780912.	1.5	1.5	0.8756*
4	407.00	10	174252.	0.3	0.3	0.1954	59	125.00	14	124552.	0.2	0.2	0.1336*
5	406.00	12	8297.	0.0	0.0	0.0093	60	124.00	8	3314.	0.0	0.0	0.0037
6	389.00	8	3766.	0.0	0.0	0.0042	61	123.00	10	7155.	0.0	0.0	0.0080
7	388.00	10	2192.	0.0	0.0	0.0025	62	122.00	10	4445.	0.0	0.0	0.0050
8	379.00	10	6618.	0.0	0.0	0.0074	63	121.00	8	1864.	0.0	0.0	0.0021
9	363.00	8	6095.	0.0	0.0	0.0068	64	120.00	6	1233.	0.0	0.0	0.0014
10	362.00	12	67280.	0.1	0.1	0.0754	65	119.00	21	423392.	0.8	0.8	0.4747
11	361.00	17	333584.	0.6	0.6	0.3740	66	118.00	8	5461.	0.0	0.0	0.0061
12	281.00	8	12981.	0.0	0.0	0.0146	67	115.00	14	62458.	0.1	0.1	0.0700*
13	225.00	8	3275.	0.0	0.0	0.0037	68	114.00	14	125560.	0.2	0.2	0.1408
14	208.00	10	9485.	0.0	0.0	0.0106	69	113.00	21	576544.	1.1	1.1	0.6469*
15	208.00	12	23277.	0.0	0.0	0.0261*	70	112.00	12	1848.	0.0	0.0	0.0021*
16	207.00	12	51406.	0.1	0.1	0.0576	71	111.00	17	31291.	0.1	0.1	0.0351
17	208.00	6	2784.	0.0	0.0	0.00931	72	110.00	12	20107.	0.0	0.0	0.00225
18	199.00	12	39559.	0.1	0.1	0.0444	73	109.00	6	2735.	0.0	0.0	0.0031
19	197.00	14	60946.	0.1	0.1	0.0683	74	105.00	12	21847.	0.0	0.0	0.0245*
20	196.00	17	186240.	0.4	0.4	0.2088	75	104.00	8	11088.	0.0	0.0	0.0124
21	195.00	12	20655.	0.0	0.0	0.0232*	76	103.00	14	41636.	0.1	0.1	0.0467
22	193.00	6	1329.	0.0	0.0	0.0015	77	102.00	17	216196.	0.4	0.4	0.2424*
23	191.00	6	1475.	0.0	0.0	0.0017	78	101.00	17	225172.	0.4	0.4	0.2525*
24	187.00	12	26687.	0.1	0.1	0.0299	79	100.00	17	209280.	0.4	0.4	0.2346*
25	183.00	25	584048.	1.1	1.1	0.6548*	80	98.00	17	134228.	0.3	0.3	0.1505
26	182.00	35	7158528.	13.8	13.8	0.0261*	81	98.00	14	98964.	0.2	0.2	0.1110
27	181.00	59	51734528.	100.0	100.0	*58.00*	82	96.00	6	3144.	0.0	0.0	0.0035
28	180.00	35	1246912.	2.4	2.4	1.3980*	83	95.00	21	327840.	0.6	0.6	0.3676*
29	179.00	25	259776.	0.5	0.5	0.2913*	84	94.00	10	1920.	0.0	0.0	0.0022
30	178.00	14	26013.	0.1	0.1	0.0292*	85	93.00	8	1897.	0.0	0.0	0.0021
31	177.00	10	1175.	0.0	0.0	0.0013	86	92.00	6	5237.	0.0	0.0	0.0059
32	170.00	8	6687.	0.0	0.0	0.0075	87	91.00	17	275360.	0.5	0.5	0.3087*
33	169.00	12	43864.	0.1	0.1	0.0492*	88	90.00	29	1850944.	3.6	3.6	2.0753*
34	168.00	17	102628.	0.2	0.2	0.1151	89	89.00	17	123632.	0.2	0.2	0.1386*
35	165.00	10	12702.	0.0	0.0	0.0142	90	88.00	17	95684.	0.2	0.2	0.1075
36	164.00	10	3927.	0.0	0.0	0.0044	91	87.00	17	232800.	0.5	0.5	0.2610*
37	163.00	12	10308.	0.0	0.0	0.0116	92	86.00	14	113912.	0.2	0.2	0.1277
38	155.00	10	43134.	0.1	0.1	0.0484	93	85.00	12	13644.	0.0	0.0	0.0153*
39	154.00	17	29040.	0.1	0.1	0.0326	94	84.00	8	6663.	0.0	0.0	0.0075
40	153.00	21	645664.	1.2	1.2	0.7239	95	83.00	17	95304.	0.2	0.2	0.1069*
41	152.00	35	4945920.	9.6	9.6	5.5454*	96	82.00	6	8936.	0.0	0.0	0.0100
42	151.00	35	1542208.	3.0	3.0	1.7291*	97	81.00	8	6494.	0.0	0.0	0.0073
43	150.00	35	669504.	1.3	1.3	0.7506*	98	80.00	8	6901.	0.0	0.0	0.0077
44	149.00	17	55592.	0.1	0.1	0.0623*	99	79.00	14	10851.	0.0	0.0	0.0122
45	144.00	6	2315.	0.0	0.0	0.0026	100	78.00	14	66924.	0.1	0.1	0.0750*
46	143.00	8	1779.	0.0	0.0	0.0020	101	77.00	35	689040.	1.3	1.3	0.7725*
47	142.00	10	24616.	0.0	0.0	0.0276	102	76.00	35	1729056.	3.3	3.3	1.9395*
48	141.00	10	3533.	0.0	0.0	0.0040	103	75.00	35	822560.	1.6	1.6	0.9223*
49	140.00	10	19645.	0.0	0.0	0.0220	104	74.00	17	347984.	0.7	0.7	0.3902*
50	139.00	14	96276.	0.2	0.2	0.1079	105	73.00	14	21679.	0.0	0.0	0.0243*
51	137.00	8	11914.	0.0	0.0	0.0134	106	70.00	12	8066.	0.0	0.0	0.0090
52	133.00	14	57526.	0.1	0.1	0.0645	107	69.00	29	1618880.	3.1	3.1	1.8151
53	132.00	6	618.	0.0	0.0	0.0007	108	65.00	14	41948.	0.1	0.1	0.0470
54	131.00	12	74504.	0.1	0.1	0.0835*	109	64.00	21	325152.	0.6	0.6	0.3646*
55	129.00	14	21860.	0.0	0.0	0.0245*	110	63.00	29	937024.	1.8	1.8	1.0506*

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PEAK NO.	MEASURED MASS	NO. POINTS	ABSOLUTE INTENSITY	X INT. BASE	X INT. NREF	X TOT. ION
111	62.00	21	198752.	0.4	0.4	0.2228*
112	61.00	10	30859.	0.1	0.1	0.0346*
113	57.00	10	6101.	0.0	0.0	0.0068
114	55.00	10	33937.	0.1	0.1	0.0381*
115	53.00	14	48716.	0.1	0.1	0.0546*
116	52.00	17	106524.	0.2	0.2	0.1194*
117	51.00	35	2159616.	4.2	4.2	2.4214
118	50.00	21	444240.	0.9	0.9	0.4981*
119	49.00	8	13123.	0.0	0.0	0.0147
120	45.00	17	93936.	0.2	0.2	0.1053*
121	44.00	21	182480.	0.4	0.4	0.2046*
122	43.00	8	2365.	0.0	0.0	0.0027
123	41.00	8	4488.	0.0	0.0	0.0050
124	40.00	12	40040.	0.1	0.1	0.0449*
125	39.00	21	525552.	1.0	1.0	0.5892*
126	38.00	17	103124.	0.2	0.2	0.1156*
127	37.00	8	1783.	0.0	0.0	0.0020
128	35.00	14	32952.	0.1	0.1	0.0369*

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