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ORGANICS IN DRINKING WATER.

PART II.-

MASS SPECTRAL
IDENTIFICATION DATA

Gregor A. Junk

AMES LABORATORY, USERDA
IOWA STATE UNIVERSITY
AMES, IOWA

Date Transmitted: July 1975

PREPARED FOR THE U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
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Gregor A. Junk

Ames Laboratory-ERDA
Iowa State University
Ames, Iowa 50010

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ABSTRACT

The essence of this report is a tabulation, ordered by molecular weight, of the mass/charge ratios and the intensities of the eight most abundant peaks and the parent ions from 352 specific organic chemicals which have been identified in water. This limited bank of mass spectral data is highly useful in water research for the identification of organic contaminants. The tabular format includes provision for adding to the data bank as new chemicals are identified in the future.

DISTRIBUTION LIST

Robert D. Kleopfer, USEPA, Region VII, 25 Funston Rd., Kansas City, Kansas, 66115	1
Fred E. Saalfeld, Naval Research Laboratory, Code 6110, Washington, D. C. 20390	1
Fred W. McLafferty, Dept. of Chemistry, Cornell University, Ithaca, N. Y. 14850	1
Ann Alford, Southeastern Environmental Research Lab, USEPA, College Station Road, Athens, Georgia 30601	1
A. Wayne Garrison, Southeastern Environ- mental Research Center, Water Supply Labora- tory, USEPA, Cincinnati, Ohio 45268	1
Robert G. Tardiff, National Environmental Research Center, Water Supply Laboratory, USEPA, Cincinnati, Ohio 45268	1
Karen M. Slimak, Versar Inc., 6621 Electronic Drive, Springfield, Virginia	1
Michael Avery, Ames Laboratory-ERDA, Iowa State University, Ames, Iowa 50010	1
Harry J. Svec, Ames Laboratory-ERDA, Iowa State University, Ames, Iowa 50010	1
James S. Fritz, Ames Laboratory-ERDA, Iowa State University, Ames, Iowa 50010	1
John J. Richard, Ames Laboratory-ERDA, Iowa State University, Ames, Iowa 50010	1
Ray Vick, Ames Laboratory-ERDA, Iowa State University, Ames, Iowa 50010	1
Thomas Bath, Staff Director, Science Advisory Board, USEPA, Crystal Mall, Bldg. 2, 1921 Jefferson Davis Highway, Arlington, Virginia 20460	1

George G. Hess, Associate Professor of Chemistry, Wright State University, Dayton, Ohio 45431	1
Kurt Grob, GC Laboratory of the University, Raemistrasse 54, 8001 Zürich, Switzerland	1
Betty J. Dowty, Dept. of Biological Sciences, University of New Orleans, New Orleans, Louisiana 70122	1
Larry H. Keith, Southeastern Environmental Research Lab, USEPA, College Station Road, Athens, Georgia 30601	1
William E. Loy, Southeastern Environmental Research Lab, USEPA, College Station Road, Athens, Georgia 30601	1
David Friedman, Division of Chem. Technol. (HFF-424), USDHEW, Public Health Service, Bureau of Foods, USFDA, Washington, D. C. 20204	1
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Organics in Drinking Water. Part II.-

Mass Spectral Identification Data

Gregor A. Junk

The most useful instrumental technique employed for the identification of trace levels of organic components isolated from water is combined gas chromatography-mass spectrometry (GC-MS). This combined technique has been used for the identification of over 300 organic constituents in various waters (1).

The usual procedure is to extract the organic components from the water matrix by methods such as solvent extraction, charcoal adsorption or resin sorption. The extracted material is invariably a complex mixture and some sort of convenient separation is required prior to chemical characterization. Gas chromatography has been and will continue to be the separation scheme most commonly employed. However, gas chromatography excels in separation and quantitation but provides minimal characterization data. Mass spectrometry excels in characterization data and use of the two techniques in combination provides the analyst with a very powerful tool for water research.

The availability of a GC-MS and the expertise in its operation unfortunately does not resolve all of the problems. Such instruments generate vast amounts of mass spectral data and a computerized data system is frequently essential for data logging and data manipulations. These combined GC-MS-computer systems are expensive, costing about \$100,000. After the data have been logged, reduced and properly manipulated, they must be interpreted before identifications can be made. In only a few isolated cases is it possible to efficiently utilize an experienced mass spectrometrists to arrive at a valid identification based solely on inspection of the raw data. The efficient operation involves a comparison, either manually or by computer, of the unknown mass spectrum against one or all of the data bases of authentic mass spectra (2,3,4,5,6). To maximize the reliability of this efficient method of identification-by-comparison requires an extensive data base that includes the mass spectra of all possible organic compounds. Such a data base is not currently available but even the most recent data banks contain the mass spectra of over 35,000 organic compounds which makes the manual comparison very tedious and the computer comparison very costly.

The cost of the computer comparison can be decreased by reducing the data base information and programming the comparisons to reduce the computer time. However many laboratories do not have the computer hardware and/or software

personnel available for programming and the continuous updating of the data base. Yet basic GC-MS equipment is becoming rather commonplace. Some systems include a minicomputer for data logging, data reduction, data manipulation and data display. Whether one has only the basic GC-MS equipped with an oscillographic recorder or a complete GC-MS-computer system, it is helpful to use a reduced data bank which includes only those compounds which previously had been identified in water. The GC-MS data accumulated from the extract of the organic components from any new water supply can then be rapidly searched against this purposefully limited data bank to efficiently and accurately identify many organic components present in the water under investigation.

The data in Table I fill this need of analytical chemists involved in the assay of water for trace organic constituents. With the exception of glucose, fulvic acids and endotoxins, all the organics which so far have been identified in water are gas chromatographable. Thus the reduced mass spectral data from combination GC-MS analyses can be rapidly searched, either manually or by computer, against this limited mass spectral data bank.

The table is ordered by increasing molecular weight with the names and empirical formulae consistent with those given in "Part I-Listing of Identified Chemicals" (1). The molecular weights are calculated from the most abundant isotope. Thus CCl_4 and HCBBr_3 are found at molecular weights of 152 and 250, corresponding to three ^{35}Cl and three ^{79}Br atoms respectively.

The table contains the 8 peak mass spectral data for 352 chemicals which have been identified in water. An additional 27 specific chemicals are also listed for which mass spectral data are not available. The 28 undesignated chemicals listed at the end of the table are included only for informational purposes and to be consistent with the tabulation in Part I (1) which contains 423 entries, 16 being hydrocarbon duplicates.

Additions to the table are allowed within the spacing between entries. This spacing is based on projected additions. Should these projections be in error and an unusually large number of additions occur for a particular molecular weight, then supplementary pages may be designated in the tabulation and added at the end of the table.

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Table I. MASS SPECTRAL DATA FOR ORGANICS FOUND IN DRINKING WATER.

MWt.	FORMULA	COMPOUND NAME	PARENT†	MASS SPECTRA							
16	CH ₄	methane	16 100	15 82	14 13	13 6					
31	CH ₅ N	*methylamine	30 100	31 75	28 51	29 12	27 8	15 7	32 3	17 2	
32	CH ₄ O	methanol	31 100	32 71	29 46	15 18	30 7	28 6	14 3	33 3	
43	CHON	isocyanic acid									

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA						
44	CO ₂	carbon dioxide		44	28	16	12	22	45	
				100	10	10	9	2	1	
44	C ₂ H ₄ O	acetaldehyde		29	44	43	15	28	42	14
				100	89	47	34	26	13	11
										41
										5
45	C ₂ H ₇ N	*dimethylamine		44	28	45	15	42	18	43
				100	68	51	20	19	16	14
										30
45	C ₂ H ₇ N	ethylamine		30	28	44	45	18	27	15
				100	29	20	19	13	13	10
										42
										9
46	CH ₂ O ₂	*formic acid		29	46	45	28	17	44	16
				100	61	48	17	17	10	5
										12
										3
46	C ₂ H ₆ O	methylether		45	46	29	15	31	14	43
				100	61	39	24	3	2	1
										47
										1

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
46	C ₂ H ₆ O	ethanol		31 100	45 44	27 20	29 19	46 19	43 8	15 8	26 6
50	CH ₃ Cl	chloromethane (methylchloride)		50 100	15 83	52 32	49 10	47 8	14 8	13 6	35 6
53	C ₃ H ₃ N	*acrylonitrile		53 100	26 93	52 79	51 30	27 12	50 7	25 5	54 5
58	C ₃ H ₆ O	acetone		43 100	58 33	15 27	42 11	27 5	39 4	29 4	26 3

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
59	C ₃ H ₉ N	propylamine		30 100	28 21	27 9	59 9	42 4	26 4	29 4	39 3
60	C ₃ H ₈ O	propanol		31 100	27 14	29 13	59 9	42 8	28 5	41 5	60 5
60	C ₂ H ₄ O ₂	methylformate		31 100	29 78	32 33	60 32	28 12	30 8	44 2	45 1
60	C ₃ H ₈ O	isopropanol	0.3	45 100	43 18	27 17	29 11	41 7	31 6	39 6	42 4
60	C ₂ HCl	acetylene chloride		60 100	62 32	28 26	25 23	59 13	44 9	24 9	47 8
60	C ₂ H ₄ O	acetic acid		43 100	45 92	60 59	15 45	18 27	42 13	29 11	28 10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
61	$\text{CH}_3\text{O}_2\text{N}$	nitromethane		30	15	61	46	14	29	27	45
				100	53	53	36	8	8	6	6
61	CNCI	cyanogen chloride		61	63	35	26	28	30	12	37
				100	32	11	7	4	4	4	4
62	$\text{C}_2\text{H}_3\text{Cl}$	vinyl chloride		27	62	28	26	64	25	61	35
				100	89	37	34	27	13	8	8
64	$\text{C}_2\text{H}_5\text{Cl}$	chloroethane		64	28	29	27	66	26	49	51
				100	90	34	74	32	28	25	8

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
66	C ₅ H ₆	cyclopentadiene		66	65	39	40	38	63	62	41
				100	57	45	37	14	10	7	7
68	C ₅ H ₈	cyclopentene		67	68	39	53	41	40	27	42
				100	42	37	23	19	16	15	8
70	C ₅ H ₁₀	pentene		42	55	41	39	27	70	29	40
				100	60	44	35	32	31	27	9

Mwt.	FORMULA	COMPOUND NAME	PARENT		MASS SPECTRA						
70	C ₄ H ₆ O	crotonaldehyde (2-butenal)	41 100	39 90	70 83	69 40	29 24	27 24	38 21	42 16	
70	C ₅ H ₁₀	cyclopentane	42 100	70 29	55 29	41 29	39 21	27 15	40 7	29 5	
72	C ₄ H ₈ O	tetrahydrofuran	42 100	41 44	72 39	71 36	28 27	43 20	27 15	39 13	
72	C ₄ H ₈ O	butanal (n-butyraldehyde)	27 100	29 94	44 84	43 79	41 64	72 47	39 40	28 28	
72	C ₄ H ₈ O	butanone (methylethylketone)	43 100	29 24	72 17	27 16	57 6	26 5	42 5	28 3	
72	C ₅ H ₁₂	pentane	43 100	42 58	41 40	27 35	29 24	39 14	57 12	72 9	
72	C ₄ H ₈ O	2-methylpropanal (isobutyraldehyde) (isobutanal)	43 100	41 56	27 50	72 32	29 21	39 18	42 11	28 10	

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
73	C ₄ H ₁₁ N	*diethylamine		58 100	30 80	73 37	44 31	72 19	29 18	28 14	59 13
74	C ₃ H ₆ O ₂	*methylacetate		43 100	15 25	74 15	42 8	59 5	29 3	44 3	31 2
74	C ₃ H ₆ O ₂	*propanoic acid		28 100	29 91	74 79	45 55	73 47	57 22	30 14	55 11
74	C ₄ H ₁₀ O	*t-butyl alcohol	0.0	59 100	31 27	41 17	57 10	43 10	29 7	39 5	27 4
74	C ₄ H ₁₀ O	diethylether (ethylether)		31 100	29 43	59 43	45 37	74 25	27 16	41 8	28 6

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
76	C ₃ H ₅ Cl	1-chloropropene		41 100	39 56	76 56	78 18	40 14	38 10	37 8	75 8
76	CS ₂	carbon disulfide		76 100	32 22	44 17	78 9	38 6	28 5	77 3	64 1
76	C ₃ H ₈ O ₂	dimethoxymethane	1.5	45 100	29 46	75 44	31 13	47 4	30 3	28 3	44 2
78	C ₃ H ₇ Cl	chloropropane 1-chloro assumed	6.0	42 100	29 46	27 37	41 23	28 15	43 14	39 12	63 6
78	C ₂ H ₆ OS	dimethylsulfoxide		63 100	78 77	45 31	47 21	61 19	46 15	62 12	48 8
78	C ₆ H ₆	benzene		78 100	52 19	77 18	51 16	39 13	50 13	79 7	76 6

MWt.	FORMULA	COMFOUND NAME	PARENT	MASS SPECTRA							
80	C ₂ H ₅ OC1	chlchromethylether	0.6	45 100	29 43	15 39	49 14	14 9	51 5	30 5	35 3
82	C ₅ H ₆ O	*3-methylfuran		53 100	82 88	39 74	81 66	27 55	54 27	28 20	51 20
82	C ₆ H ₁₀	cyclohexene		67 100	54 76	82 40	41 37	39 36	27 20	53 12	81 12

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
83	C ₅ H ₉ N	2-methylpropyl nitrile (isobutylnitrile)	0.1	43 100	41 61	27 18	39 14	68 7	29 5	28 4	40 4
84	C ₆ H ₁₂	methylcyclopentane		56 100	41 64	29 32	42 29	55 25	39 25	27 24	84 16
84	CH ₂ Cl ₂	dichloromethane (methylenechloride)		49 100	84 57	86 36	51 30	47 18	35 12	48 9	88 6
84	C ₆ H ₁₂	cyclohexane		56 100	84 71	41 68	55 34	42 31	27 30	39 28	69 22
85	C ₅ H ₁₁ N	piperidine		84 100	28 55	56 52	85 48	29 47	57 42	30 38	44 34

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
86	C ₅ H ₁₀ O	3-methylbutanal (methylbutyraldehyde)	10	41 100	43 87	58 67	29 66	56 50	27 46	57 45	39 35
86	C ₅ H ₁₀ O	3-methyl-2-butanone (methylisopropylketone)		43 100	27 13	41 13	86 10	39 7	42 6	71 4	28 2
88	C ₄ H ₈ O ₂	*butyric acid 1-butanolic acid	7.0	43 100	41 30	73 22	27 22	42 9	58 8	45 8	39 7
88	C ₄ H ₈ O ₂	*isobutyric acid		43 100	41 46	73 32	27 28	45 14	88 12	39 12	42 11
88	C ₄ H ₈ O ₂	ethylacetate	4.0	43 100	29 25	27 13	45 13	61 10	42 6	70 5	26 4
88	C ₅ H ₁₂ O	pentanol 1-isomer assumed	0.0	42 100	31 68	29 65	41 60	55 60	70 37	43 28	57 22
88	C ₅ H ₁₂ O	*2-methyl-2-butanol	0.0	59 100	73 52	43 38	31 33	55 32	27 20	29 19	41 18
88	C ₄ H ₈ O ₂	*dioxane 1-4 assumed		28 100	29 37	88 31	58 24	15 17	31 17	27 15	30 13
88	C ₄ H ₈ O ₂	*2-methyldioxalone MS cf dioxolane	0.49	73 100	43 72	45 65	29 51	28 36	58 30	27 29	31 13

MWt.	FORMULA	COMFOUND NAME	PARENT	MASS SPECTRA							
92	C ₇ H ₈	toluene		91 100	92 65	65 11	39 9	63 6	51 5	93 5	45 4
93	C ₆ H ₇ N	*aniline		93 100	66 33	65 18	39 18	92 11	46.5 9	28 8	38 7
94	C ₆ H ₆ O	phenol		94 100	66 29	65 23	39 20	40 13	55 9	47 7	38 6
94	C ₂ H ₆ S ₂	dimethyldisulfide		45 100	94 66	79 52	46 45	47 34	64 24	61 19	48 15
94	C ₃ H ₇ OCl	2-chloroethylmethylether									
94	C ₃ H ₇ OCl	chlchromethylethylether									
94	CH ₃ Br	bromomethane (methylbromide)		15 100	94 92	96 80	79 14	81 14	95 13	93 11	14 10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
96	C ₂ H ₂ Cl ₂	acetylenedichloride (1,2-dichloroethylene)		61 100	96 86	98 55	63 32	60 18	100 9	62 8	48 4
96	C ₂ H ₂ Cl ₂	trans-1,2-dichloroethylene		61 100	96 62	98 40	26 36	63 32	60 27	25 17	35 12
96	C ₂ H ₂ Cl ₂	cis-1,2-dichloroethylene		61 100	96 65	98 41	26 33	63 32	60 22	35 20	25 16
96	C ₂ H ₂ Cl ₂	1,1-dichloroethylene (vinylidene chloride)		61 100	96 81	98 53	63 29	60 13	26 11	100 8	62 6
97	C ₆ H ₁₁ N	2-methylbutylnitrile (isoamyl nitrile)	0.0	55 100	41 35	43 34	57 24	54 24	82 14	27 13	29 12

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
98	C ₂ H ₄ Cl ₂	1,2-dichloroethane	10	62 100	27 86	49 37	64 32	26 29	63 17	51 11	61 11
98	C ₂ H ₄ Cl ₂	1,1-dichloroethane	6.5	63 100	27 73	65 32	26 24	83 13	35 10	61 8	85 8
98	C ₇ H ₁₄	methylcyclohexane		83 100	55 85	41 60	98 42	42 35	56 30	27 29	39 28
100	C ₅ H ₈ O ₂	methylethylmethacrylate		41 100	69 79	39 31	100 28	15 17	99 14	59 9	40 8

MWt.	FORMULA	COMPCUND NAME	PARENT	MASS SPECTRA							
102	C ₅ H ₁₀ O ₂	*valeric acid (pentanoic acid)	0.5	60 100	43 35	41 26	87 21	45 19	27 13	74 12	39 10
102	C ₅ H ₁₀ O ₂	*isovaleric acid	0.0	60 100	43 61	41 54	27 33	45 31	29 27	39 24	74 24
102	C ₄ H ₆ O ₃	acetic anhydride	0.1	43 100	15 12	42 6	45 4	14 3	44 3	60 2	41 1
102	C ₆ H ₁₄ O	3-methyl-3-pentanol									
104	C ₈ H ₈	styrene (vinylbenzene)		104 100	103 38	78 27	51 25	77 17	50 9	52 9	105 9
104	C ₂ HBr	acetylene bromide									

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
106	C ₈ H ₁₀	1,2-dimethylbenzene (o-xylene)		91 100	106 58	105 24	39 17	51 16	77 13	27 11	50 8
106	C ₈ H ₁₀	1,3-dimethylbenzene (m-xylene)		91 100	106 63	105 28	39 19	51 15	77 13	27 10	52 8
106	C ₈ H ₁₀	1,4-dimethylbenzene (p-xylene)		91 100	106 62	105 30	39 16	51 16	77 14	27 12	50 8
106	C ₈ H ₁₀	dimethylbenzene (mixture)		91 100	106 46	105 17	63 11	79 10	27 10	77 10	92 10
106	C ₈ H ₁₀	ethylbenzene		91 100	106 30	51 13	39 10	65 9	77 8	92 8	78 8
106	C ₇ H ₆ O	benzaldehyde		105 100	106 99	77 94	51 33	18 16	50 15	17 13	28 12
108	C ₄ H ₉ OC1	chloroethylether 2-chloro-assumed									
108	C ₇ H ₈ O	o-cresol (2-methylphenol)		108 100	107 89	79 52	77 46	39 42	51 32	90 29	50 25

MWt.	FORMULA	COMFOUND NAME	PARENT	MASS SPECTRA							
110	$C_3H_4Cl_2$	3,3-dichloropropene	3.4	75 100	39 38	77 36	49 15	38 11	36 8	37 8	27 8
		1,3-dichloropropene		75 100	39 55	77 32	49 26	110 20	38 14	112 13	36 10
112	C_6H_5Cl	chlorobenzene		112 100	77 48	114 32	51 16	50 14	38 9	113 7	74 6
112	$C_7H_{12}O$	cycloheptanone		55 100	68 90	41 61	112 55	56 51	69 42	84 41	42 37
112	$C_3H_6Cl_2$	dichloropropane (unknown isomer) MS of 1,3 isomer	1.7	76 100	41 48	78 33	27 22	39 12	49 12	63 11	40 6
112	$C_3H_6Cl_2$	1,3-dichloropropane	1.7	76 100	41 48	78 33	27 22	39 12	49 12	63 11	40 6

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
113	C ₅ H ₄ NC1	3-chloropyridine		113	78	115	18	51	50	86	114
				100	49	32	24	24	12	8	7
113	C ₆ H ₁₁ ON	ε-caprolactam		30	55	56	85	42	113	41	84
				100	89	65	46	46	43	37	32
114	C ₈ H ₁₈	2-ethylhexane MS of 3-ethyl	1.6	43	85	84	41	27	29	71	57
				100	29	23	23	22	20	13	12
114	C ₈ H ₁₈	octane n-assumed	6.7	43	41	29	57	85	27	71	56
				100	38	35	34	30	29	23	18

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
116	C ₉ H ₈	indene		116 100	115 85	63 14	39 11	57.5 11	89 10	117 10	58 9
116	C ₆ H ₁₂ O ₂	cis-2-ethyl-4-methyl-1,3-dioxolane(?)	0.2	87 100	59 77	31 44	41 43	57 36	29 19	72 18	42 15
116	C ₆ H ₁₂ O ₂	trans-2-ethyl-4-methyl-1,3-dioxolane(?)	0.3	87 100	59 62	31 58	41 51	29 34	57 29	72 24	42 23
116	C ₆ H ₁₂ O ₂	*caproic acid (hexanoic acid)	0.2	60 100	73 44	41 20	43 16	87 13	27 12	61 11	45 11
118	C ₉ H ₁₀	indan (indane) (2,3-dihydroindene)		117 100	118 78	115 28	39 22	91 20	116 17	58 14	63 13
118	CHCl ₃	chloroform	2.4	83 100	85 65	47 20	87 11	48 10	49 7	50 3	82 3

MWt.	FORMULA	COMPOUND NAME	PARENT		MASS SPECTRA						
120	C ₉ H ₁₂	C ₃ -benzene isopropyl assumed	105 100	120 26	77 13	79 12	51 11	106 9	103 8	39 6	
120	C ₉ H ₁₂	isopropyl benzene (cumene)	105 100	120 27	77 12	79 10	51 10	106 9	103 8	91 5	
120	C ₉ H ₁₂	propylbenzene n-assumed	91 100	120 21	92 10	65 9	39 9	78 6	51 6	27 5	
120	C ₉ H ₁₂	1,2,3-trimethylbenzene	105 100	120 53	119 10	77 9	106 9	91 8	39 7	51 6	
120	C ₉ H ₁₂	1,2,4-trimethylbenzene	105 100	120 59	119 16	39 14	77 12	27 10	51 10	91 9	
120	C ₉ H ₁₂	1,3,5-trimethylbenzene	105 100	120 67	119 16	39 15	77 13	27 10	51 10	91 9	
120	C ₉ H ₁₂	o-ethyltoluene	105 100	120 31	77 10	91 10	106 9	79 9	44 7	103 6	
120	C ₉ H ₁₂	p-ethyltoluene	91 100	90 90	89 73	119 64	120 63	92 31	63 18	51 15	
120	C ₈ H ₈ O	acetophenone	105 100	77 81	51 29	120 23	43 18	50 12	78 8	28 5	
120	C ₉ H ₁₂	m-ethyltoluene	105 100	120 32	91 10	77 9	106 9	79 6	103 5	39 5	

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
121	C ₈ H ₁₁ N	*2-methyl-5-ethylpyridine		106 100	121 54	39 21	77 18	120 16	27 15	79 14	51 12
122	C ₈ H ₁₀ O	2,4-dimethylphenol		122 100	107 90	121 55	39 28	77 28	51 19	91 18	79 14
122	C ₈ H ₁₀ O	*p-ethylphenol		107 100	122 32	77 12	108 8	39 4	121 3	91 3	51 3
122	C ₈ H ₁₀ O	methylphenylcarbinol (phenylmethylcarbinol) (α-methylbenzylalcohol)		107 100	79 97	77 57	122 30	78 25	105 13	108 9	63 7
122	C ₇ H ₅ O ₂	benzoic acid		105 100	122 77	77 75	51 46	50 29	39 11	38 10	74 10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
123	$C_6H_5O_2N$	nitrobenzene		77 100	51 59	123 42	50 25	30 16	65 13	39 10	93 9
124	$C_6H_3ON_2$	2-hydroxyadiponitrile									
124	$C_7H_8O_2$	guaiacol (o-methoxyphenol)		109 100	124 86	81 50	27 20	39 17	52 15	51 13	50 9
126	$C_8H_{14}O$	isocctenone									

MWt.	FORMULA	COMFOUND NAME	PARENT	MASS SPECTRA							
128	C ₁₀ H ₈	naphthalene		128 100	127 12	129 11	64 7	51 7	126 6	102 6	63 4
128	C ₉ H ₂₀	n-nonane	6.4	43 100	57 67	41 41	29 37	27 29	85 23	71 20	56 17
130	C ₂ HCl ₃	1,1,2-trichloroethylene		95 100	130 99	132 95	97 64	60 56	35 31	134 30	25 28
130	C ₈ H ₁₈ O	C ₈ -sat. alcohol 1-octanol assumed	0.0	56 100	55 82	41 69	70 67	43 66	69 63	84 55	42 51
130	C ₁₀ H ₁₀	methylindene MS cf isomer mixture		130 100	115 77	129 70	128 38	51 19	127 17	63 16	39 13
130	C ₈ H ₁₈ O	2-ethylhexanol	0.0	57 100	41 40	43 38	29 27	55 25	27 22	56 20	70 18

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
132	C ₂ H ₃ Cl ₃	1,1,2-trichloroethane	9.0	97 100	83 95	99 62	85 60	61 58	26 23	96 21	63 19
132	C ₂ H ₃ Cl ₃	1,1,1-trichloroethane	0.0	97 100	99 65	61 50	117 19	119 19	63 17	101 10	62 8
132	C ₁₀ H ₁₂	*tetralin (1,2,3,4-tetrahydronaphthalene)		104 100	91 58	132 43	39 22	51 21	65 17	27 16	77 14
132	C ₆ H ₁₂ O ₃	paraldehyde	0.3	45 100	43 51	89 16	87 11	117 10	15 5	29 5	131 4
132	C ₁₀ H ₁₂	methyl-2,3-dihydroindene (methylinan)		117 100	132 25	115 24	91 13	39 12	51 11	131 11	118 10
132	C ₁₀ H ₁₂	dicyclopentadiene		66 100	132 12	67 9	39 8	65 5	40 4	51 3	91 3
134	C ₂ H ₂ Cl ₂ F ₂	dichlorodifluoroethane 1,1-2,2 isomer assumed		83 100	85 67	134 24	136 15	51 12	87 11	49 10	133 9
134	C ₁₀ H ₁₄	propyltoluene m-n-propyl assumed		119 100	134 28	91 15	120 10	117 8	77 5	115 4	65 4

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
134	C ₁₀ H ₁₄	diethylbenzene 1,3-isomer assumed		119 100	105 92	134 43	91 19	27 16	39 16	77 15	51 12
134	C ₁₀ H ₁₄	tetramethyl benzene 1,2,3,4-isomer assumed		119 100	134 50	91 13	120 9	133 9	77 8	39 8	117 6
134	C ₁₀ H ₁₄	butylbenzene tert-butyl assumed		119 100	91 46	134 26	41 17	79 10	77 9	120 9	51 8
134	C ₁₀ H ₁₄	C ₄ -benzene t-butyl assumed		119 100	97 46	134 26	41 17	79 10	77 9	120 9	51 8
134	C ₈ H ₅ S	benzothiophene (thianaphthane)		134 100	89 12	135 10	63 9	69 9	90 9	45 8	67 8
135	C ₇ H ₅ NS	benzothiazole		135 100	108 35	69 27	63 13	45 12	82 12	136 9	54 9
136	CCl ₃ F	trichlorofluoromethane (Freon-11)	0.0	101 100	103 60	35 16	66 15	47 12	31 10	105 10	37 5

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
136	C ₉ H ₁₂ O	*C ₃ -substituted phenols p-isopropyl assumed		121 100	136 30	77 13	103 12	91 10	122 9	39 5	65 5
136	C ₉ H ₁₂ O	*isopropylphenol para isomer assumed		121 100	136 30	77 13	103 12	91 10	122 9	39 5	65 5
136	C ₈ H ₈ O ₂	phenylacetic acid		91 100	136 35	92 17	65 12	39 6	63 4	51 3	137 3
136	C ₈ H ₈ O ₂	methylbenzoate		105 100	77 65	51 36	136 32	50 18	106 8	78 5	74 5
136	C ₁₀ H ₁₆	limonene	12	68 100	67 58	93 55	94 25	79 22	92 19	121 16	107 16
136	C ₄ H ₉ Br	butylbromide (2-bromo-2-methyl-propane) (tert-butylbromide)	0.0	57 100	41 48	29 28	27 7	55 4	97 2	56 2	42 2
138	C ₈ H ₁₀ O ₂	*veratrole (1,2-dimethoxybenzene)		138 100	95 61	123 41	77 36	52 35	51 25	65 23	41 22
138	C ₈ H ₁₀ O ₂	dimethoxybenzene (probably veratrole)		138 100	95 61	123 41	77 36	52 35	51 25	65 23	41 22
138	C ₉ H ₁₄ O	isophorone(isoacetophorone) (3,5,5-trimethyl-2-cyclohexen-1-one)		82 100	39 28	138 17	27 17	41 13	54 13	53 9	29 7

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
142	C ₁₁ H ₁₀	2-methylnaphthalene		142	141	115	143	139	63	71	58
				100	72	25	12	10	8	8	7
142	C ₁₁ H ₁₀	methylnaphthalene 1-methyl assumed		142	141	115	71	57.5	63	143	39
				100	69	26	15	12	12	11	10
142	C ₁₀ H ₂₂	isodecane (2-methylnonane)	1.4	43	57	41	29	71	42	27	56
				100	84	43	30	29	28	27	17
142	C ₄ H ₈ OC ₂	bis(2-chloroethyl ether)	1.6	93	63	27	95	65	31	49	28
				100	74	38	32	24	9	4	4
142	C ₁₀ H ₂₂	n-decane	6.7	43	57	41	29	71	27	85	56
				100	82	43	38	30	28	21	18

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
143	C ₁₀ H ₉ N	*naphthylamine α-isomer assumed		143 100	115 45	116 25	144 14	71.5 8	89 8	63 7	142 6
144	C ₉ H ₂₀ O	*diisobutyl carbinol (2,6-dimethyl-4-heptanol)	0.0	69 100	87 49	45 43	43 42	41 18	57 15	70 9	44 7
146	C ₃ H ₅ Cl ₃	1,1,1-trichloropropane	0.0	111 100	113 78	75 62	29 61	39 44	27 28	36 22	117 21
146	C ₃ H ₅ Cl ₃	1,2,3-trichloropropane	1.2	75 100	110 37	77 32	61 29	49 26	39 26	112 24	97 23
146	C ₁₁ H ₁₄	ethylindane (ethylindan) 1-ethyl assumed		131 100	146 40	145 16	115 15	91 11	39 10	132 8	129 7
146	C ₆ H ₄ Cl ₂	1,2-dichlorobenzene (o-dichlorobenzene)		146 100	148 65	111 36	75 20	113 12	150 11	74 11	50 10

MWt.	FORMULA	COMFOUND NAME	PARENT	MASS SPECTRA							
146	C ₆ H ₄ Cl ₂	1,3-dichlorobenzene (m-dichlorobenzene)		146 100	148 65	111 32	75 17	150 10	74 10	113 10	50 9
146	C ₆ H ₄ Cl ₂	1,4-dichlorobenzene (p-dichlorobenzene)		146 100	148 65	111 32	75 19	74 12	150 11	113 10	73 8
146	C ₂ HOC1 ₃	chlcral	4.6	82 100	84 66	111 35	83 32	29 31	47 28	113 22	85 21
148	C ₈ H ₄ O ₃	phthalic anhydride		104 100	76 89	50 60	74 24	38 23	37 22	75 14	148 13
148	C ₉ H ₈ S	methyl benzothiophene (methyl thianaphthene)		147 100	148 83	149 13	45 11	69 10	74 10	39 9	63 8
148	C ₈ H ₁₇ Cl	5-methyl assumed octylchloride 1-chloro assumed	0.1	91 100	41 83	43 76	27 62	29 56	55 55	39 34	57 32
148	C ₁₀ H ₁₂ O	ethyl acetophenone para isomer assumed		133 100	148 27	105 25	79 13	77 12	134 10	43 9	103 8
148	C ₁₁ H ₁₆	C ₅ -benzene n-pentyl assumed		91 100	92 58	148 21	39 13	65 12	41 11	105 9	51 7

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
149	C ₈ H ₇ NS	methylbenzothiazole 2-methyl assumed		148 100	103 32	69 29	149 17	63 16	82 11	45 11	150 11
150	C ₆ H ₁₁ O ₂ Cl	*butylchloroacetate n-butyl assumed	0.0	56 100	57 79	41 75	29 70	77 52	27 26	49 25	28 25
150	C ₁₀ H ₁₄ O	*p-tert-butyl-phenol		135 100	107 27	41 24	150 20	39 20	28 18	95 17	77 13
150	C ₁₀ H ₁₄ O	3,5,5-trimethyl-bicyclo(4,1,0) heptene-2-one									
152	C ₁₀ H ₁₆ O	dihydrocarvone	29	67 100	95 76	41 72	68 67	81 49	82 48	55 41	69 35
152	CCl ₄	carbon tetrachloride	0.0	117 100	119 96	47 48	35 44	82 30	121 30	84 19	49 15

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
152	C ₁₀ H ₁₆ O	camphor	29	126 100	95 97	41 79	81 71	39 48	69 43	108 39	83 37
152	C ₁₂ H ₈	acenaphthylene		152 100	76 17	151 17	153 16	150 11	63 7	75 5	154 3
153	C ₇ H ₇ O ₃ N	nitroanisoie o-assumed		77 100	153 82	106 80	91 55	123 40	64 30	63 28	78 21
154	C ₁₀ H ₁₈ O	borneol (bornyl alcohol)	1.7	95 100	110 22	93 8	139 7	121 6	69 5	96 5	71 5
154	C ₁₀ H ₁₈ O	isoborneol	0.7	95 100	41 42	27 25	43 24	39 23	93 22	55 20	29 19
154	C ₁₀ H ₁₈ O	p-menth-1-en-8-ol (α-terpineol)	0.5	59 100	43 74	93 72	121 52	68 44	136 42	41 39	81 32
154	C ₁₀ H ₁₈ O	1,8-cineole (eucalyptol)	46	81 100	71 95	108 75	43 75	84 65	69 65	93 60	111 55
154	C ₁₂ H ₁₀	biphenyl		154 100	153 35	152 22	155 13	76 7	151 6	77 4	128 3

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
154	C ₁₂ H ₁₀	acenaphthene		154 100	153 95	152 53	76 26	151 16	155 12	63 12	77 11
156	C ₁₁ H ₂₄	n-undecane	3.8	43 100	57 85	41 43	29 39	71 36	27 23	85 21	42 16
156	C ₁₁ H ₂₄	undecane isomer 4-methyl assumed	1.8	43 100	71 78	57 65	41 51	29 41	27 38	70 32	55 22
156	C ₁₁ H ₂₄	isoundecane (2-methyldecane)	1.0	43 100	57 68	41 50	71 37	42 25	85 17	39 17	56 15
156	C ₁₂ H ₁₂	dimethyl naphthalene 1,2-isomer assumed		156 100	141 94	155 19	115 16	157 13	142 11	76 10	153 10
156	C ₆ H ₅ Br	bromobenzene		77 100	156 94	158 92	50 17	78 11	38 9	51 7	74 7

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
157	$C_{10}H_{23}N$	*decylamine	0.9	30 100	41 11	29 8	27 8	43 8	28 7	18 7	45 5
157	$C_6H_4O_2NCl$	*nitrochlorobenzene para-isomer assumed		157 100	111 94	75 91	127 40	99 30	50 28	113 27	159 25
157	$C_6H_4O_2NCl$	m-chloronitrobenzene		111 100	157 73	75 52	113 32	159 23	74 10	29 10	76 8
158	$C_6H_6O_3S$	benzenesulfonic acid		158 100	77 90	94 75	51 40	65 20	141 10	93 8	66 7
160	$C_{12}H_{16}$	1-isopropenyl-4-isopropyl- benzene		145 100	160 43	105 16	117 13	146 12	91 11	41 11	147 9

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
162	C ₁₀ H ₁₄ N ₂	nicotine		84	133	42	162	161	28	39	51
				100	27	20	19	18	17	9	7
162	C ₁₂ H ₁₈	C ₆ -benzene		147	133	162	105	91	27	29	39
		1,3,5-triethyl assumed		100	81	58	25	20	19	17	14
162	C ₆ H ₄ OC1 ₂	2,4-dichlorophenol		162	164	63	98	126	166	100	99
				100	63	30	27	11	10	9	9
162	CHCl ₂ Br	bromodichloromethane	0.6	83	85	129	47	127	87	48	79
				100	66	17	16	13	11	11	7
162	C ₈ H ₁₈ O ₃	bis-(2-ethoxyethyl) ether	0.0	45	59	72	31	43	73	29	28
				100	53	45	45	43	43	25	15
163	CO ₂ NC1 ₃	chloropicrin (nitrotrichloromethane)	0.0	117	119	30	82	121	47	84	35
				100	96	45	32	31	27	20	13

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
164	C ₂ Cl ₄	tetrachloroethylene		166	164	129	131	168	94	133	96
				100	78	64	62	48	21	20	14
164	C ₁₁ H ₁₆ O	*2-tert-butyl- ^L methyl phenol MS of 2-5 isomer		149	121	164	91	28	41	116	77
				100	52	30	14	8	8	7	7
166	C ₆ H ₈ OC1 ₂	1,1-dichloro-2-hexanone									
166	C ₂ H ₂ Cl ₄	tetrachloroethane (1,1-2,2-tetrachloroethane)	6.2	83	85	95	87	61	60	168	131
				100	63	11	10	8	8	8	8
166	C ₂ H ₂ Cl ₄	1,1,1,2-(tetrachloroethane)	0.1	131	133	117	119	95	135	121	97
				100	96	76	73	34	31	23	23
168	C ₁₁ H ₂₀ O	*2-methyl-isoborneol	0.0	107	41	79	93	94	95	135	91
				100	67	54	51	50	35	34	34
168	C ₁₃ H ₁₂	metnylbiphenyl 2-isomer assumed		168	167	165	153	152	83	169	166
				100	84	31	29	22	14	13	10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
169	C ₁₂ H ₁₁ N	diphenylamine		169 100	168 36	167 26	82.5 21	170 13	51 13	77 12	66 9
170	C ₁₂ H ₁₀ O	phenyl ether (diphenylether)		170 100	51 56	77 53	141 34	39 29	142 20	169 18	50 15
170	C ₁₃ H ₁₄	*C ₃ -naphthalene 2-isopropyl assumed		155 100	170 33	128 15	156 14	153 10	127 9	152 9	115 9
170	C ₁₂ H ₂₆	n-dodecane	4.3	43 100	57 92	41 47	71 43	29 41	27 26	85 25	55 16
170	C ₁₁ H ₂₂ O	*diamylketone	0.0	43 100	71 84	58 50	29 35	41 30	27 27	53 25	55 17
170	C ₁₂ H ₁₀ O	diphenyl ether		170 100	51 74	141 65	77 65	142 38	115 25	50 21	65 17

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
170	$C_6H_{12}CCl_2$	bis(2-chloroisopropyl ether)	0.0	45 100	43 36	41 34	77 19	121 15	79 12	27 11	39 7
170	$C_{12}H_{10}O$	o-phenylphenol (2-hydroxybiphenyl)		170 100	169 60	141 24	115 15	171 13	142 8	139 6	63 4
171	$C_6H_9O_3N_3$	trimethylisocyanurate (trimethyltrioxohexahydro- triazine)		58 100	171 97	55 40	28 33	143 26	29 15	57 14	15 11
171	$C_7H_3NCl_2$	*2,6-dichlorobenzonitrile (2,6-dichlorobenzenecarbo- nitrile)		171 100	173 60	135 18	100 13	75 10	175 10	172 8	50 8
178	$C_{14}H_{10}$	phenanthrene		178 100	176 18	179 16	89 13	76 12	88 10	151 7	152 7
178	$C_{14}H_{10}$	*anthracene		178 100	176 17	179 16	89 14	76 11	88 9	151 6	152 6
178	$C_{11}H_{14}O_2$	*butyl benzoate n-butyl assumed	2.0	105 100	123 68	77 38	56 19	122 17	106 8	41 6	124 5

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
180	C ₆ H ₃ Cl ₃	1,2,3-trichlorobenzene		180	182	184	145	147	109	74	75
				100	97	31	26	16	15	12	7
180	C ₆ H ₃ Cl ₃	trichlorobenzene 1,3,5-assumed		180	182	184	145	147	109	74	73
				100	96	31	22	74	12	12	7
180	C ₆ H ₃ Cl ₃	1,3,4-trichlorobenzene same as 1,2,4 isomer		180	182	184	145	147	109	74	73
				100	97	30	23	15	14	12	7
180	C ₁₀ H ₁₂ O ₃	*3,4-dimethoxyacetophenone (acetoveratrone)		165	180	137	166	77	43	79	122
				100	51	11	10	10	10	8	6
180	C ₁₀ H ₁₂ O ₃	dimethoxyacetophenone 3,4 assumed		165	180	137	166	77	43	79	122
				100	51	11	10	10	10	8	6
180	C ₅ H ₁₂ O ₆	*glucose (dextrose)									

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
181	C ₈ H ₇ NS ₂	2-thiomethylbenzothiazole (2-methylthiobenzothiazole)		181 100	148 77	108 39	180 28	69 21	45 18	136 18	135 13
182	C ₇ H ₆ O ₄ N ₂	dinitrotoluene 3,5-assumed		30 100	89 99	182 68	90 61	136 55	106 43	64 17	51 15
182	C ₁₂ H ₂₂ O	geosmin (trans-1,10-dimethyl-9-decalol)	7.0	112 100	41 80	149 62	55 62	67 49	43 47	93 46	81 44
184	C ₁₃ H ₂₈	n-tridecane	4.8	43 100	57 87	41 52	29 49	71 43	27 27	85 26	55 19
184	C ₁₃ H ₁₂ O	unknown									
184	C ₁₃ H ₁₂ O	2-methoxybiphenyl 3-methoxy assumed		184 100	141 26	115 22	154 20	185 14	153 12	155 10	152 9
184	C ₁₄ H ₁₆	*C ₄ -naphthalene 2-tert-butyl assumed		184 100	141 88	128 49	41 48	129 43	152 34	76 28	153 25

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
184	C ₁₂ H ₁₂ N ₂	diphenylhydrazine	2.0	169 100	168 52	167 30	84 21	41 21	170 20	77 18	66 12
184	C ₁₂ H ₁₂ N ₂	*benzidine		184 100	92 15	183 12	185 12	156 6	167 5	182 4	166 4
184	C ₈ H ₁₂ O ₃ N ₂	barbital (5,5-diethylbarbituric acid) (veronal)	8.0	156 100	141 90	41 85	39 83	55 63	155 45	44 36	83 33
186	C ₆ H ₁₂ Cl ₂	triglycodichloride [1,2-bis(2-chloroethoxy) ethane]	0.0	63 100	27 43	93 43	18 33	65 32	28 27	45 25	31 19

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
187 ^a	C ₆ H ₁₀ N ₅ Cl	deethyl atrazine (2-chloro-4-amino-5-iso- propylamino- <u>s</u> -triazine)	30	43	172	69	58	68	42	104	174
				100	98	68	58	56	44	37	35
190	C ₁₄ H ₂₂	*diisopropyl-p-xylene 2,5-isomer assumed		175	190	176	133	147	119	191	91
				100	24	15	14	6	5	4	4
190	C ₆ H ₄ ClBr	bromochlorobenzene 1,3-isomer assumed		192	190	111	75	194	113	28	50
				100	78	61	26	24	19	16	13
191	C ₆ H ₉ O ₆ N	*nitrilotriacetic acid (NTA)									
192	C ₁₅ H ₁₂	*C ₁ -anthracene 2-methyl assumed		192	191	189	193	178	165	82.5	96
				100	34	22	17	15	12	11	10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
194	C ₁₀ H ₁₀ O ₄	dimethyl phthalate	3.0	163 100	77 14	164 10	133 7	135 7	76 4	92 4	104 3
194	C ₃ H ₂ OC1 ₄	1,1,3,3-tetrachloroacetone (1,1,3,3-tetrachloro-2-propanone)		83 100	85 65	111 22	113 14	87 11	196 4	194 3	115 2
196	C ₆ H ₃ OC1 ₃	2,4,6-trichlorophenol		196 100	198 96	200 31	132 28	97 25	134 18	160 13	99 12

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
198	C ₁₄ H ₃₀	tetradecane n-isomer assumed	5.0	43 100	57 89	41 59	71 48	85 30	55 23	42 17	56 16
198	C ₁₃ H ₁₀ O ₂	phenylbenzoate		105 100	77 38	51 10	50 9	106 8	198 5	39 3	78 3
199	C ₆ H ₅ O ₅ N ₃	4,6-dinitro-2-aminophenol									
200	C ₁₂ H ₂₄ O ₂	*lauric acid	2.7	60 100	73 84	43 61	37 38	41 36	55 35	18 27	71 23
200	C ₂ HCl ₅	pentachloroethane	1.3	117 100	119 96	167 95	95 93	165 74	169 46	83 38	121 31

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
201	C ₇ H ₁₂ N ₅ Cl	simazine [2-chloro-4,6-di(ethyl- amino)- <u>s</u> -triazine]		201 100	44 78	186 49	43 46	173 36	203 36	68 27	55 23
202	C ₁₆ H ₁₀	pyrene		202 100	101 26	100 17	203 17	200 15	201 12	88 6	100.5 5
202	C ₁₆ H ₁₀	*fluoranthene		202 100	101 23	203 17	200 15	100 14	88 9	201 8	87 4
206	C ₁₆ H ₁₄	*C ₂ anthracene 2-ethyl assumed		206 100	191 84	189 23	207 18	192 15	165 13	190 10	89 10
206	CHClBr ₂	chlorodibromomethane (bromodichloromethane)	7.1	129 100	127 78	131 25	208 14	210 10	48 9	47 9	93 8

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
208	C ₂ Cl ₃ Br	bromotrichloroethylene									
210	CHCl ₂ I	dichloriodomethane		83 100	85 63	127 35	48 23	47 20	210 13	175 11	87 11
210	C ₁₁ H ₈ Cl ₂	naphthyldichloromethane (1 or 2-isomer)									
211	C ₁₁ H ₁₄ ONCl	*propachlor	3.0	120 100	77 46	93 38	43 26	176 24	57 23	51 15	41 13

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
212	C ₁₅ H ₃₂	n-pentadecane	4.4	43 100	57 90	41 85	71 49	85 32	55 25	42 16	56 16
213	C ₁₀ H ₁₅ O ₂ NS	butylbenzenesulfonamide (n-butyl assumed)	6.8	77 100	170 99	141 98	51 20	30 11	158 10	78 10	171 9
214	C ₆ H ₂ Cl ₄	1,2,3,4-tetrachlorobenzene		216 100	214 79	218 48	179 16	181 16	108 12	220 10	109 8

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
215	$C_3H_{14}N_5Cl$	atrazine		200 100	58 79	215 59	43 58	68 46	202 35	69 34	173 33
217	$C_{11}H_{23}ONS$	*sutan									
220	$C_{15}H_{24}O$	* p-nonylphenol	4.0	135 100	107 32	149 31	121 30	136 10	163 8	41 7	191 5
220	$C_{14}H_{20}O_2$	2,6-di-t-butyl-p- benzoquinone 2,5-mass spectrum		203 100	163 83	220 77	177 66	41 58	135 35	43 32	149 29
220	$C_{15}H_{24}O$	2,6-di-t-butyl-p-cresol (ionol)		205 100	57 32	220 22	41 18	206 15	145 12	81 11	29 11

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
220	$C_8H_6O_3Cl_2$	*2,4-D (2,4-dichlorophenoxyacetic acid)		162 100	220 78	164 64	222 49	161 29	175 27	163 26	177 17
222	$C_{12}H_{14}O_4$	diethylphthalate	3.0	149 100	177 28	150 13	176 9	65 8	105 8	76 6	29 6
226	$C_{16}H_{34}$	hexadecane	3.8	43 100	57 90	41 58	71 50	85 33	55 26	42 16	56 16

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
228	C ₁₄ H ₂₈ O ₂	*myristic acid ? (mixture)	23	73 100	60 92	57 92	43 75	41 57	55 42	129 44	71 33
228	C ₁₂ H ₂₀ O ₄	*dibutyl maleate	2.2	99 100	57 55	117 36	41 21	43 21	29 21	56 19	100 18
228	C ₁₈ H ₁₂	*chrysene		228 100	226 25	229 20	113 18	114 17	101 10	227 9	100 8
228	C ₁₈ H ₁₂	*1,2-benzanthracene		228 100	229 19	226 19	114 18	113 13	101 7	100 6	112 5
229	C ₉ H ₁₆ N ₅ Cl	prcpazine [2-chloro-4,6-di(isopropyl- amino)1,3,5-triazine]		214 100	58 84	229 82	172 51	43 41	187 36	216 32	41 28

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
230	C ₁₈ H ₁₄	o-terphenyl		230	229	228	215	231	114	226	101
				100	53	30	27	18	16	14	14
230	C ₆ H ₂ OC ₁₄	tetrachlorophenol 2,3,4,6 isomer assumed		232	230	234	131	133	194	196	96
				100	78	46	25	12	11	10	9
232	C ₁₃ H ₉ O ₂ Cl	chlorohydroxybenzophenone 3,4 isomer assumed		155	232	105	77	157	234	51	197
				100	58	57	32	32	18	11	10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
234	C ₂ Cl ₆	hexachloroethane	0.0	117 100	119 96	201 83	203 54	199 53	165 41	164 32	121 31
234	C ₁₅ H ₂₆ O	2,6-di-t-butyl-4ethylphenol		219 100	234 24	220 17	57 12	88 6	159 6	41 5	235 4
234	C ₆ H ₄ Br ₂	dibromobenzene o-isomer assumed		236 100	234 51	238 49	155 30	157 29	75 18	50 13	76 12
236	C ₁₅ H ₂₄ O ₂	*2,6-di-t-butyl-4-methoxyphenol									
238	C ₁₇ H ₃₄	1-heptadecene	8.8	41 100	43 96	55 87	57 72	83 70	97 67	29 66	69 59
238	C ₈ H ₅ O ₂ Cl ₃	*Fenac (2,3,6-trichlorophenoxyacetic acid)									

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA								
240	C ₉ H ₁₃ N ₆ Cl	Bladex [2-(4-chloro-6-ethylamino- s-triazin-2ylamino)-2- methylpropionitrile]	29	68 100	44 83	225 64	43 60	173 51	198 49	145 47	172 45	
240	C ₁₇ H ₃₅	heptadecane	3.4	43 100	57 94	41 56	71 54	85 36	55 26	56 15	42 15	
248	C ₁₂ H ₉ Br	bromophenylphenyl ether isomer unknown		248 100	250 99	141 45	77 32	169 24	51 19	249 16	168 14	
248	C ₁₃ H ₂₈ O ₄	*dibutoxyethoxyethoxymethane										

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
250	C ₁₄ H ₁₈ O ₄	dipropyl phthalate n-propyl assumed	0.3	149 100	150 9	209 8	191 8	43 7	41 6	104 5	76 4
250	CHBr ₃	bromoform	3.9	173 100	171 50	175 49	93 22	91 22	79 18	81 17	92 13
252	C ₂₀ H ₁₂	3,4-benzopyrene		252 100	126 23	253 21	250 16	125 15	113 9	112 7	124 7
252	C ₂₀ H ₁₂	benzopyrene isomers M.S of 1,2-isomer		252 100	250 26	253 23	126 20	125 20	124 10	251 10	248 9
252	C ₂₀ H ₁₂	*3,4-benzofluoranthene		252 100	126 23	253 22	250 17	125 15	113 8	112 7	248 5
252	C ₂₀ H ₁₂	*4,5-benzofluoranthene									
252	C ₂₀ H ₁₂	*10,11-benzofluoranthene (benzo[j]fluoranthene)		252 100	253 23	126 23	250 21	125 19	113 7	112 6	248 5

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
252	C ₂₀ H ₁₂	*11,12-benzofluoranthene (benzo[K]fluoranthene)		252 100	126 27	253 21	250 19	125 14	113 7	112 7	248 6
254	C ₈ H ₅ O ₃ Cl ₃	*2,4,5-T (2,4,5-trichlorophenoxyacetic acid)		196 100	198 92	200 30	254 25	197 24	97 22	167 20	256 19
254	C ₁₈ H ₃₈	octadecane	1.7	57 100	43 94	71 60	41 45	85 39	55 23	42 12	69 10
254	C ₂ H ₂ Cl ₂ Br ₂	dibromodichloroethane 1,2-1,2 isomer assumed	0.7	177 100	175 62	179 45	100 23	96 22	61 19	129 18	26 15
256	C ₁₂ H ₇ Cl ₃	trichlorobiphenyl 2,2',4 assumed		256 100	258 98	186 37	260 32	259 15	257 15	188 11	150 9
256	C ₁₆ H ₃₂ O ₂	palmitic acid		73 100	71 34	83 25	129 23	256 22	98 21	85 20	97 17

MWt.	FORMULA	COMPCUND NAME	PARENT	MASS SPECTRA							
256	S ₈	octasulfur		64	256	160	128	192	258	96	32
				100	70	53	52	40	25	21	21
258	C ₄ Cl ₆	hexachloro-1,3-butadiene	19	225	227	223	190	260	188	118	141
				100	65	63	43	36	32	30	29
264	C ₆ HOC1 ₅	pentachlorophenol		266	268	264	165	167	95	130	60
				100	70	68	54	52	44	30	28

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
266	C ₁₂ H ₂₇ O ₄ P	tributylphosphate	0.0	99 100	155 22	57 16	41 13	211 12	29 11	125 6	55 5
268	C ₉ H ₇ O ₃ Cl ₃	*silvex (2,4,5-TP) (2,4,5-trichlorophenoxy- propionic acid)		196 100	198 89	200 25	270 18	268 17	97 17	45 15	27 14
268	C ₁₉ H ₄₀	nonadecane	1.2	57 100	71 65	43 58	85 47	113 29	99 16	41 15	55 13
269	C ₁₄ H ₂₀ Cl ₂ N	alachlor (Lasso) [2-chloro-2',6'-diethyl- N-(methoxymethyl)acetanilide]	1.8	45 100	160 29	188 25	146 12	132 10	91 10	77 10	118 9

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
270	C ₁₇ H ₃₄ O ₂	methyIpalmitate		74 100	87 62	43 27	75 21	41 20	270 18	55 18	57 16
276	C ₂₂ H ₁₂	*indeno(1,2,3-cd)pyrene									
276	C ₂₂ H ₁₂	*1,12-benzperylene		276 100	28 51	44 47	138 32	274 27	137 23	277 22	275 15
277	C ₉ H ₁₂ O ₅ NSP	*Fenitrothion [O,O-dimethyl-O-(3-methyl- 4-nitrophenyl)phosphoro- thioate]		125 100	109 96	277 82	79 46	260 44	47 41	63 33	93 32

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
278	C ₇ H ₃ OC1 ₅	pentachlorophenyl methylether		265 100	280 98	237 83	267 60	258 58	282 57	95 57	278 55
278	C ₁₆ H ₂₂ O ₄	diisobutylphthalate	0.1	149 100	57 23	150 10	29 8	41 8	223 7	56 5	104 5
278	C ₁₆ H ₂₂ O ₄	dibutylphthalate	0.8	149 100	150 9	223 6	41 5	29 5	57 5	205 5	56 4
278	C ₂₂ H ₁₄	*1,2,5,6-dibenzanthracene		278 100	139 24	279 24	276 16	138 13	125 6	137 6	140 6
280	C ₁₄ H ₁₆ O ₆	*ethylglycolylethyl- phthalate (ethylphthalylethylglycollate)	0.7	149 100	69 37	177 35	29 13	105 12	150 11	76 10	235 9

MWt.	FORMULA	COMPOUND NAME	PARENT M	MASS SPECTRA							
282	C ₆ Cl ₆	hexachlorobenzene (HCB)(hexachlorane)		284 100	286 79	282 51	288 34	142 30	249 24	107 20	144 16
282	C ₂₀ F ₄₂	eicosane	5.1	57 100	43 91	71 67	85 48	41 42	29 28	55 27	56 15
284	C ₁₆ H ₂₈ O ₄	butyloctylmaleate									
284	C ₁₈ H ₃₆ O ₂	stearic acid	14	57 100	73 83	60 80	43 63	55 45	71 40	41 38	69 35
284	C ₆ H ₁₂ O ₄ Cl ₃ P	tris(chloroethyl)phosphate (trichloroethylphosphate)	0.0	63 100	28 67	49 34	62 28	27 28	65 26	124 24	107 21
284	C ₁₆ H ₂₈ O ₄	octylbutylfumarate (butyloctylfumarate)									

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
288	C ₆ H ₆ Cl ₆	*benzene hexachloride (hexachlorocyclohexane) (BHC)	0.6	181 100	183 96	109 95	217 68	77 59	78 58	219 58	112 58
288	C ₆ H ₆ Cl ₆	lindane (gamma-BHC)	0.6	181 100	183 96	109 95	217 68	77 59	78 58	219 58	112 58
290	C ₁₂ H ₆ Cl ₄	tetrachlorobiphenyl 2,2',5,5' assumed		292 100	290 75	230 68	294 46	232 41	293 15	255 12	84 12

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
296	C ₇ H ₂ Cl ₆	*1,2,3,4,6,6-hexachloronorbornadiene									
296	C ₂₁ H ₄₄	C ₂₁ -alkane n-isomer assumed	1.6	43 100	57 92	71 55	41 50	85 38	55 29	56 15	42 13
298	C ₁₉ H ₃₈ O ₂	methyl stearate		74 100	87 77	43 32	55 27	75 21	298 21	143 20	57 19

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
303 ^b	C ₁₄ H ₁₉ O ₂ NC1 ₂	alachlor(2Cl homolog) assumed	?	45 100	188 22	160 13	85 8	146 7	112 7	77 6	130 6
306	C ₁₈ H ₂₆ O ₄	*diaryl phthalate	0.3	149 100	42 16	41 15	43 14	55 13	70 11	150 10	29 7
310	C ₂₂ H ₄₆	docosane	1.5	43 100	57 91	71 54	41 48	85 39	55 29	56 15	69 13
310	C ₂₂ H ₄₆	C ₂₂ -alkane n-assumed	1.5	43 100	57 91	71 54	41 48	85 39	55 29	56 15	69 13

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
311	C ₁₇ H ₂₆ C ₂ NC1	butachlor [2-chloro-2',6'-diethyl-N-(butoxymethyl)-acetanilide]	1.9	57 100	176 68	160 59	188 29	41 27	146 18	162 16	132 15
312	C ₁₉ H ₂₀ C ₄	butylbenzylphthalate (benzylbutylphthalate)	3.0	149 100	91 50	206 18	104 12	150 12	41 11	105 11	132 11
314 ^a	C ₁₂ H ₂₇ CS ₃ P	*S,S,S-tributylphosphorotri- thioate	5.0	41 100	57 63	56 44	55 27	39 26	169 19	202 19	43 18

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA
316	C ₁₄ H ₈ Cl ₄	p,p'-DDE [1,1-dichloro-2,2-di(p-chlorophenyl)ethylene]		318 316 246 320 248 176 210 319 100 80 72 49 48 27 16 15
318	C ₁₄ H ₁₀ Cl ₄	*DDD (TDE) (tetrachlorodiphenylethane) o-p' assumed	2.0	235 237 165 199 200 236 176 178 100 65 57 22 18 18 17 13

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA									
320	$C_8H_8O_3Cl_3SP$	*Ronnell (Trolene) [0,0-dimethyl-0-(2,4,5- tri-chlorophenyl)phosphoro- thionate	7.0	285 100	287 80	125 78	109 37	93 34	47 31	79 30	289 25		
324	$C_{12}H_5Cl_5$	pentachlorobiphenyl 2,2',4,5,5' assumed		326 100	328 66	324 63	354 43	184 41	356 38	127 31	128 30		
324	$C_{23}H_{48}$	C_{23} -alkane n-isomer assumed	1.3	57 100	43 91	71 61	85 40	41 36	55 25	29 24	56 14		
326	$C_{18}H_{15}O_4P$	triphenylphosphate		326 100	77 80	325 75	65 50	94 33	51 31	170 30	39 28		

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
330	$C_{10}H_6O_4Cl_4$	dacthal		301 100	299 77	303 50	59 24	332 23	142 21	221 18	330 18
332	$C_7H_3Cl_7$	1,2,3,4,5,7,7-heptachloronor- bornene	2.0	272 100	274 84	83 84	237 75	270 55	117 43	235 45	239 45
332	$C_7H_3Cl_7$	hepachloronorbornene isomer	0.4	43 100	85 73	55 60	237 45	272 43	83 43	73 38	274 32
334	$C_{20}H_{30}O_4$	dihexylphthalate 2-ethylbutyl isomer assumed	0.0	149 100	28 28	43 28	85 22	167 15	84 13	150 11	41 10

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
336	C ₁₈ H ₂₄ O ₆	*butylglycollylbutylphthalate (butylphthalylbutylglycollate)	0.0	149	263	57	77	41	133	104	56
				100	27	22	21	17	14	11	11
336	C ₁₀ H ₆ Cl ₆	chlordene	9.0	66	101	237	103	239	235	115	272
				100	80	39	33	27	27	26	26
338	C ₂₄ H ₅₀	C ₂₄ -alkane n-isomer assumed	4.4	57	43	71	85	41	55	29	69
				100	84	71	59	33	28	20	16

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
340	C ₂₂ H ₄₄ O ₂	behenic acid docosanoic acid	14	43 100	41 71	98 69	55 68	57 61	60 47	73 47	69 39
352	C ₂₅ H ₅₂	C ₂₅ -alkane n-assumed	1.7	43 100	57 93	71 55	41 43	85 39	55 29	69 15	56 14
352	C ₁₄ H ₉ Cl ₅	DDT [2,2-bis(p-chlorophenyl)- 1,1,1-trichloroethane]	0.0	235 100	165 33	212 31	282 17	176 15	236 13	88 12	36 12
354	C ₁₂ H ₆ O ₂ Cl ₄ S	*tedion (tetradifon) mass spectra of 3,4,3',4'		193 100	195 70	145 35	109 33	354 32	352 29	147 28	75 26

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
362	C ₁₂ H ₈ Cl ₆	aldrin	5.0	66 100	91 44	79 40	263 40	39 36	65 32	101 30	265 27
362	C ₁₂ H ₈ Cl ₆	*iscdrin (endo-endo isomer of aldrin)	12	193 100	66 80	195 80	263 37	197 33	147 33	40 32	44 32
366	C ₂₆ H ₅₄	C ₂₆ -alkane n-assumed	1.8	57 100	43 97	71 60	85 41	41 35	29 29	55 29	69 16

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
368	C ₂₄ H ₄₈ O ₂	lignoceric acid (tetracosanoic acid)		368 100	43 76	57 72	73 54	55 42	60 40	71 36	41 30
370	C ₂₂ H ₄₂ O ₄	dioctyladipate (DOF)	0.0	129 100	45 18	102 16	128 15	28 12	130 9	55 9	51 8
370	C ₂₂ H ₄₂ O ₄	*diethylhexyladipate MS cf (DOA)	0.0	129 100	45 18	102 16	128 15	28 12	130 9	55 9	51 8
370	C ₁₀ H ₅ Cl ₇	heptachlor	5.0	100 100	272 60	274 46	65 41	270 35	102 33	36 28	39 26

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
378	C ₁₂ H ₈ OC ₁₆	dieldrin	27	79 100	345 73	347 52	343 50	380 47	349 40	382 38	82 35
378	C ₁₂ H ₈ OC ₁₆	endrin (exo-exo isomer of dieldrin)	11	81 100	82 60	263 60	39 55	78 54	67 51	27 49	265 48
380	C ₂₇ H ₅₆	C ₂₇ alkane n-assumed	1.2	43 100	57 97	71 56	41 40	85 39	55 30	69 16	56 15
382	C ₂₅ H ₅₀ O ₂	methyltetracosanoate (methyllignocerate)		74 100	87 80	382 38	75 34	55 30	57 29	43 26	69 23

Mwt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
386	C ₁₀ H ₅ OC ₁₅	heptachlorepoxyde (HCE)	5.0	81 100	353 82	355 68	27 54	351 46	29 41	53 34	39 34
390	C ₂₄ H ₃₈ O ₄	di-2-ethylhexylphthalate (DEHP)	0.0	149 100	57 72	43 48	41 42	54 39	167 38	70 30	55 28
390	C ₂₄ H ₃₈ O ₄	dioctylphthalate (DOP)	0.0	149 100	67 41	57 40	43 34	31 33	70 33	71 29	41 23

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA							
404	$C_{13}H_6O_2Cl_6$	hexachlorophene	19	196	198	209	211	208	210	406	200
				100	95	61	50	44	39	36	30
404	$C_9H_6O_3Cl_6S$	*endosulfan (thiodan)	6	201	203	243	273	214	271	245	283
				100	85	55	53	53	52	47	46
406	$C_{10}H_6Cl_8$	chlordan	7.0	100	45	39	135	27	65	43	66
				100	61	57	55	47	47	39	36
410?	$C_{10}H_{10}Cl_8$	*toxaphene (mixture) (octachlorocamphene)									

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA
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446	$C_{28}H_{46}O_4$	*diisodecylphthalate (DIDP)		
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900- 20,000	unknown	*fulvic acid		
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unk.	C_2H_x	C_2 -hydrocarbon		
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unk.	C_3H_x	C_3 -hydrocarbon		
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unk.	C_4H_x	C_4 -hydrocarbon		
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MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA
unk.	C_7H_x	> C_7 -hydrocarbons		
unk.	$C_{10}H_x$	> C_{10} -hydrocarbons		
unk.	$C_{15}H_x$	* C_{15} -hydrocarbons		
unk.	$C_{15}H_x$ to $C_{29}H_x$	* C_{15-29} -hydrocarbons		
unk.	C_xH_y	*hydrocarbons (kerosene)		
unk.	C_xH_y	alkylnaphthalenes		
unk.	C_xH_y	alkylindan (alkyl-2,3-dihydroindene)		
unk.	C_xH_y	alkylbenzenes		
unk.	$C_xH_y(X)$	substituted benzenes		
unk.	C_xH_y	polynuclear aromatics (PNA) polyaromatic hydrocarbons (PAH)		
unk.	$C_xH_ySO_3$	alkylbenzenesulfonates (ABS)		
unk.	C_xH_yO	*aldehydes		
unk.	C_xH_yO	*ketones		
unk.	C_xH_yO	alcohols		
unk.	C_xH_yO	*alkylphenols		

MWt.	FORMULA	COMPOUND NAME	PARENT	MASS SPECTRA
unk.	C_xH_yOX	phenolic compounds		
unk.	$C_xH_yO_2$	*phthalate		
unk.	$C_xH_yO_2$	dialkylphthalate		
unk.	$C_xH_yO_3$	alkylphthalates		
unk.	$C_xH_yO_2$	*esters		
unk.	$C_xH_yO_2$	*organic acid		
unk.	$C_xH_yCl_z$	polychlorinated biphenyl (PCB)		
unk.	$C_xH_yP_z$	organophosphorus pesticides		
unk.	C_xH_yS	alkylbenzothiophene		

*These organics have not been identified in drinking water but are potential contaminants since they have been found in other waters.

†When the parent ion is not one of the eight most intense peaks, the relative intensity of the parent ion is listed in this column.

^aNo std. sample M.S. available.

^bNo std. sample M.S. available. Compound may be an alachlor isomer with 269 molecular weight.