**ENVIRONMENTALLY BENIGN MITIGATION OF MICROBIOLOGICALLY
INFLUENCED CORROSION (MIC)**

NINTH QUARTER REPORT

(October-December 2003)

Prepared by

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LIST OF ACRONYMS

Acronyms	Source Term
APB	Acid-Producing Bacteria
BAC	Biologically Active Compound
BCF	Billion Cubic Feet (of natural gas)
COS	Currently Off-the-Shelf (technology or products)
EETC	Emerging Energy Technology Campus
FERC	Federal Energy Regulatory Commission
GTI	Gas Technology Institute
GRI	Gas Research Institute
MCF	Million Cubic Feet (of natural gas)
MIC	Microbial Influenced Corrosion
MICC	Microbially Influenced Concrete Corrosion
MPN	Most Probable Number (statistical bacterial enumeration method)
PI	Principal Investigator
TCF	Trillion Cubic Feet (of natural gas)
SRB	Sulfate-Reducing Bacteria
HPLC	High Precision Liquid Chromatography
ESEM	Environmental Scanning Electron Microscopy

ABSTRACT

Title:	Environmentally Benign Mitigation of Microbiologically Influenced Corrosion (MIC)
Funding Sources:	U.S. Department of Energy and Gas Research Institute
Contract No:	DE-FC26-01NT41158
GTI Project Nos:	61138/30793-35
Principal Investigators:	John J. Kilbane II, Ph.D. and William Bogan Ph. D.
Report Period:	October 2003 through December 2003
Objective:	The overall program objective is to develop and evaluate environmentally benign agents or products that are effective in the prevention, inhibition, and mitigation of microbially influenced corrosion (MIC) in the internal surfaces of metallic natural gas pipelines. The goal is to develop one or more environmentally benign (a.k.a. “green”) products that can be applied to maintain the structure and dependability of the natural gas infrastructure.
Approach:	The technical approach for this quarter included the fractionation of extracts prepared from several varieties of pepper plants, and using several solvents, by high performance liquid chromatography (HPLC). A preliminary determination of antimicrobial activities of the new extracts and fractions using a growth inhibition assay, and evaluation of the extracts’ ability to inhibit biofilm formation was also performed.
Results:	The analysis of multiple extracts of pepper plants and fractions of extracts of pepper plants obtained by HPLC illustrated that these extracts and fractions are extremely complex mixtures of chemicals. Gas chromatography-mass spectrometry was used to identify the chemical constituents of these extracts and fractions to the greatest degree possible.
Conclusions:	Analysis of the chemical composition of various extracts of pepper plants has illustrated the complexity of the chemical mixtures present, and while additional work will be performed to further characterize the extracts to identify bioactive compounds the focus of efforts should now shift to an evaluation of the ability of extracts to inhibit corrosion in mixed culture biofilms, and in pure cultures of bacterial types which are known or believed to be important in corrosion.

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EXECUTIVE SUMMARY

The main goal of this project is to develop an environmentally benign compound that could prevent and/or control microbially influenced corrosion (MIC) in the interior of metal gas pipelines. The main activities for this quarter were focused on Objectives No. 4) to evaluate pepper oil components to inhibit and mitigate biofilm formation and MIC, and 5) identification and testing of biologically active compounds for biofilm inhibition or mitigation. Extracts from three varieties of *Capsicum sp.* (such as, Serrano, Habanero and Chile de Arbol) were obtained by Soxhlet extraction using hexane, methylene chloride, and an extract series using methanol and dimethyl sulfoxide (DMSO) solvent system was also obtained. These extracts were subjected to growth inhibition tests and subsequently to fractionation by HPLC. These extracts and fractions were subjected to Gas Chromatography with Mass Spectrometry (GC-MS) in order to identify chemical components. More fractions will have to be tested both for growth inhibition and biofilm formation while quantification of bioactive compounds is in progress. At this time the available data is not sufficient to allow correlations to be made between bioactivity in the inhibition of bacterial growth or biofilm formation and the presence/concentration of particular chemicals. Future tests will also include mixed cultures and obtaining metal corrosion data.

BACKGROUND

The overall objective of this project is to develop, test, and apply environmentally benign agent(s) to control microbial-caused corrosion on the internal surfaces of metal (iron or steel) pipes used for natural gas transmission. The overall hypothesis is that agents exist in nature that inhibit some or all of the steps executed by microorganisms in the formation of biofilm. As biofilm formation is an absolute prerequisite for the initiation and production of microbially influenced corrosion (MIC), blocking biofilm formation or propagation will block or mitigate MIC.

The general approach is to evaluate natural products isolated from plants, and, possibly, animals or microorganisms, for their abilities to block the attachment, physiology, or reproduction of microbial agents that are responsible for MIC. The first natural product to be tested is the oil that can be extracted from the seeds and pods of pepper plants. These plants are members of the Genus *Capsicum*. The effective components or constituents of this product will then be tested for its environmental impact and effects, effective concentrations, modes of application, and stability against isolated MIC microorganisms under simulated field conditions. A commercially viable agent that aids in MIC control and is environmentally friendly is the ultimate target, with preliminary data to determine commercialization potential and cost benefits.

Since the biocides have been identified, other chemicals that are used by the gas industry as biocides, anti-corrosion agents, drying agents, and coating are being evaluated for interactions. The suppliers have been identified, mainly through NACE, and they are being contacted to obtain samples (250 g to 500 g) of their chemicals.

The application of the pepper extract or its identified components using foams has initiated. This “foam pig” concept is accepted by the gas industry and some pipeline service companies are marketing this technology. GTI is looking at commercial foams and foams that are generated internally for a delivery system.

EXPERIMENTAL METHODS

Growth Inhibition (Antimicrobial) Screening

The microdilution assay method (Eloff, 1998) was used to determine the growth inhibition of the pepper components. They were subjected to antimicrobial screening against two sulfate reducing bacteria, *D. vulgaris* and *D. desulfuricans*. The test compounds were serially diluted 50% with sterile distilled water in 96-well microtiter plates. For the inoculum, an overnight bacterial culture was centrifuged at 4,000 rpm for five minutes, washed with a 50mM phosphate buffered saline, pH 6.8, and the optical density was adjusted at 600 nm to obtain a final cell concentration of 10^6 cfu/mL per well. ATCC # 1249 Modified Baar's Medium was used as a source of cell nutrients. The multi-well plates were then placed inside a modular anaerobic chamber, purged with nitrogen gas, and incubated at 30°C for *D. vulgaris* and 37°C for *D. desulfuricans*. Optical density at 600 nm was measured using the MRX II (Dynex Technologies) plate reader from 0 up to 168 hours. Growth inhibition was determined as the test compound limiting turbidity to <0.05 absorbance at 600nm (Cai *et al.*, 2000). The initially acquired 12 crude extracts were also tested against the denitrifier *Comamonas denitrificans* using this procedure.

High-Precision Liquid Chromatography for Fractionation of Pepper Extracts

Pepper extracts were analyzed with High Performance Liquid Chromatography (HPLC) with a Photo Diode Array lamp (PDA) at 285nm. Extracts were received at a 10% dilution; this was done because the initial extract was too thick to inject, making it impossible to inject 250ul. Using the Supleco Supelcosil LC-18 column (25cm x 4.5mm x 5um) the analysis of the extracts was done with a flow rate of 1.0 ml/min and an initial solvent ratio of 80% A (0.01M Phosphoric Acid) and 20% B (HPLC grade Methanol). The flow rate remained the same but the solvent ratio changed with time. The ratio changed gradually to equal 100% B by 57min of run time and then slowly went back to the original ratio by 66min. For each extract myristic, stearic, oleic, palmetic, caffeic, cinnamic, and coumaric acids were qualitatively analyzed along with capsaicin and dihydrocapsaicin. These final two compounds will act as an internal standard and concentration marker for future testing. In addition, this was done to determine how to initiate the next step of the process, which was to fractionate the extracts.

The Waters Fraction Collector III was used for the fractionating. It is a programmable stand-alone fraction collection module. When running a sample many choices can be made from a simple process of operation such as time, drop, volume, or signal per collection vessel or a more advanced mode can be used such as peak mode, manual, and sampling mode. The time mode was observed to be sufficient.

The collector was set up to collect samples in 13 vials at certain time frames. These samples were collected in test tubes every 5 min. After all extracts were fractionated, they were evaporated to dryness using a mini-evaporator. Upon dryness, the extracts were given to the microbiologist for further analysis.

Gas chromatography - mass spectrometry (GC/MS) was used to determine what compounds were present in pepper plant extracts and fractions.

Biofilm Formation

The crude extracts were tested against the two sulfate-reducing bacteria for their ability to inhibit biofilm formation. The methods used to look at the effects on biofilm formation and its measurements are discussed in detail by Djordjevic, *et al.* (2002), Fletcher (1999) and Horn and Jones (2002). The test compounds were incubated with bacterial cells at 10^8 cfu/mL (final concentration) and allowed to form biofilm up to 120 hrs. ATCC # 1249 Modified Baar's Medium was used as a source of cell nutrients. The biofilm assay was done by staining formed/residual biofilm with 1% crystal violet for 25 minutes, washing the wells with sterile distilled water and dissolving the cell-associated dye by adding 200 μ L of dimethyl sulfoxide (DMSO) per well (O'Tode and Kolter, 1998). Quantification of the formed biofilm was done by optical density measurement at 600 nm using the MRX II (Dynex Technologies) plate reader and comparing the results with the untreated biofilm.

Continuous Flow Cell System

Biofilm formation of *D. vulgaris* was studied using the continuous flow cell system (Stovall Life Science, Inc., Greensboro, NC). The sterile system consisted mainly of a 3-channel flow cell with individual channel dimensions of 1 mm D x 4 mm W x 40 mm L and the attached microscope coverslip #1 (0.13-0.16mm thick) that served as the substratum for biofilm growth. The TEST and CONTROL biofilms were grown in separate channels at 37°C supplied with Modified Baar's Medium that was prepared

under 97% N₂ and 3% H₂. Inocula used were from overnight cultures that were diluted to obtain a final cell concentration of 10⁸ cfu/mL as measured at OD₆₀₀. The medium was placed in a water bath and pumped into the system using the IsmaTec low flow peristaltic pump at a flow rate of 3mL/hr. The bubble trap near the influent side prevented the air bubbles from reaching the flow cell. After equilibrating the system with the culture media, the flow was stopped and the inoculum (0.5mL) was injected at the inlet of each channel. The inoculum for the TEST channel was mixed with crude pepper extract #5 while that of the CONTROL was suspended in the culture media only. The flow cell was turned upside down to allow the cells to establish on the glass surface (Christensen, et al, 1999; Ramos, et al, 2001). After 1 hr, it was inverted to the right-side up position and medium flow was re-started.

Biofilm development for the TEST channel was monitored every 4 hrs for 7 days using light microscopy (Carl Zeiss Axioskop 2 *plus*, Germany) equipped with time lapse program from Axiovision (Carl Zeiss, Inc.) as the software for image analysis. The Time Lapse software enables the camera to take photos at desired time intervals automatically for the whole duration of the experiment. For the CONTROL channel, photographs were taken manually at the beginning and the end of the run.

To check for cell viability, Live/Dead *BacLight* (Molecular Probes, Eugene, OR) was used. The biofilms were stained by injecting the dyes near the inlet of the flow cell. Prior to injection, the cells were rinsed with distilled water and both ends of the flow cells were clamped. With epifluorescent microscopy, dead cells appear fluorescent red while live ones are fluorescent green.

RESULTS AND DISCUSSION

Several different varieties of pepper plants were extracted several different solvents. The pepper plants tested included Chile de Arbol, Serrano, and Habanero. The extraction solvents tested included hexane, methylene chloride, and a mixture of dimethyl sulfoxide (DMSO) and methanol. As a general means of determining the composition and the “strength” of each extract the amount of capsaicin and dihydrocapsaicin was determined and the results are shown in Table 1.

TABLE 1. AMOUNTS OF CAPSAICIN AND DIHYDROCPSAICIN IN PEPPER PLANT EXTRACTS

Extract Type	Capsaicin mg/L	Dihydrocapsaicin mg/L
Arbol in Hexane	1071	525
Serrano in Hexane	642	288
Habanero in Hexane	1215	691
Arbol in Methylene Chloride	1536	432
Serrano in Methylene Chloride	1613	678
Habanero in Methylene Chloride	5360	3418
Arbol in DMSO/Methanol	322	103
Habanero in DMSO/Methanol	328	103

The results in Table 1 indicate that methylene chloride is the most effective solvent as regards the extraction of capsaicin and dihydrocapsaicin from these pepper plants. There is then a range of concentrations of the chemical compounds in these extracts (specifically capsaicin, dihydrocapsaicin and presumable other compounds as well) and directly comparing them with each other as regards bioactivity will make it difficult to interpret the results. To address this the quantity of each pepper extract that was used in microbial growth inhibition and biofilm formation assays was then adjusted, and normalized to the concentration of capsaicin and dihydrocapsaicin in each extract. In

this way it was hoped that valid comparisons of the bioactivities of each pepper extract could be obtained.

Microbial growth tests were performed with two species of sulfate reducing bacteria: *Desulfovibrio vulgaris*, and *Desulfovibrio desulfuricans*. The majority of extracts did not show growth inhibition, as reported last quarter and confirmed with further testing this quarter. However, several of the extracts and fractions derived from the extracts showed growth inhibition of these bacterial cultures. Unexpectedly the methylene chloride extracts did not exhibit the greatest degree of growth inhibition; rather, the hexane extracts yielded more growth inhibition of these two sulfate reducing bacterial cultures.

The extracts were further tested in biofilm formation assays and the results indicated that hexane extracts were more potent inhibitors of biofilm formation by both cultures of *Desulfovibrio vulgaris*, and *Desulfovibrio desulfuricans* than the methylene chloride extracts. However, the results of the biofilm formation assays were not as consistent as the results of the growth inhibition assays. Specifically, the hexane extracts from all three pepper species (Chile de Arbol, Serrano, and Habanero) exhibited growth inhibition of the bacterial cultures, but only the hexane extract of the Serrano peppers exhibited biofilm formation inhibition of the bacterial cultures. Since the approximate concentrations of capsaicin and dihydrocapsaicin in these experiments was equivalent, then these results must be due to some other compound(s) present in the pepper plant extracts. To identify what compounds were present in these pepper plant extracts an extensive amount of effort was expended this quarter in performing GC-MS analyses of these pepper plant extracts and fractions of these extracts prepared by HPLC. A large number of the pepper plant extracts and fractions were analyzed by GC-MS and data obtained from these analyses is included as an appendix to this report. The exhaustive analysis of all of the compounds present in these extracts is an enormous job. The computer databases for the analyses of GC-MS data did not allow the identification of all of the peaks/compounds present in these extracts, but a large amount of characterization data was obtained and the work is continuing.

CONCLUSIONS

Chemical characterization of the pepper plant extracts has yielded an enormous amount of information. However, in order to correlate the presence of any compounds present in pepper plant extracts with biological activity more data will be needed. Accordingly, activity planned for the next quarter will focus on obtaining data using mixed cultures and pepper plant extracts prepared using hexane. Data that includes actual metal corrosion rates will be crucial to determining the effectiveness of these pepper plant extracts.

CITATIONS

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APPENDIX A. GC-MS DATA FROM THE ANALYSIS OF PEPPER PLANT EXTRACTS

Data File: 1-1
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 17:32:34
 Run Time (min): 29.97
 Vial: 23
 Inj Vol (µL): 2.00
 Scans: 3064
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
5.07	5653	0.59
6.74	284537	29.62
8.47	184256	19.18
9.32	3728	0.39
9.59	35812	3.73
10.19	9520	0.99
10.74	48334	5.03
11.17	55050	5.73
11.63	872	0.09
12.02	16744	1.74
12.47	40018	4.17
13.08	13170	1.37
13.35	19271	2.01
13.51	37686	3.92
13.75	2189	0.23
13.91	16235	1.69
14.39	1388	0.14
14.56	6367	0.66
15.02	22611	2.35
15.36	9566	1.00
15.64	18611	1.94

16.23	11236	1.17
16.51	13816	1.44
17.96	4456	0.46
18.21	5830	0.61
19.30	7645	0.80
20.55	7821	0.81
20.68	4377	0.46
21.73	10669	1.11
22.09	1647	0.17
22.86	8091	0.84
23.01	1235	0.13
23.91	9105	0.95
24.77	13101	1.36
24.90	9177	0.96
25.46	3563	0.37
25.83	4811	0.50
26.70	1917	0.20
27.52	5476	0.57
27.77	4981	0.52

T	Name	I	rob.	F ormula	W	Ca s #
0.19	1H-Indene, 1-methylene-	15	3.32	C 10H8	28	24 71-84-3
0.19	Naphthalene	10	8.79	C 10H8	28	91- 20-3
0.19	NAPHTHALENE DB5-826	05	5.15			N A
0.19	4-Phenylbut-3-ene-1-yne	97	1.30	C 10H8	28	N A
0.19	AZULENE DB5-1140	96	0.86			N A

T	Name	I	rob.	For mula	W	Cas #
2.47	9H-Xanthen-9-one, 1,3,5,6-tetramethoxy-	88	4.46	C17 H16O6	16	3660- 86-4
2.47	3H-Xanthen-3-one, 10-deshydro-6-hydroxy-10-[2-carboxyphen-1-yl]-	83	1.66	C20 H12O5	32	518- 45-6
2.47	Silane, trimethyl([1,1':3',1''-terphenyl]-5'-yl)-	78	.39	C21 H22Si	02	12838 8-53-4
2.47	2,5-Dimethyl-4,6-dibenzyl-pyridine	77	.03	C21 H21N	87	36063 -39-5
2.47	Pyrazine, 2,5-diethyl-3,6-diphenyl-	67	.37	C20 H20N2	88	21798 -29-8

T	Name	I	rob.	Formula	W	Cas #
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5.36	Benzenesulfonamide, N-butyl-	51	5.28	C10H15 NO2S	13	362 2-84-2
5.36	1,3,5-Trisbenzene-sulphonyl- hexahydro-1,3,5-triazine	22	.59	C21H21 N3O6S3	07	NA
5.36	Benzenesulfonyl azide	21	.45	C6H5N3 O2S	83	938- 10-3
5.36	Diphenyl ether	03	.78	C12H10 O	70	101- 84-8
5.36	5-(Phenylsulphonyl)dihydro-1,3,5- dioxazine	98	.43	C9H11N O4S	29	562 21-07-9

T	Name	I	rob.	Formul a	W	Cas #
6.23	5 α -Cholan-24-oic acid, 12 α -hydroxy- 3,7-dioxo-, methyl ester	51	1.33	C25H3 8O5	18	1665 6-66-9
6.23	Octadecanoic acid, decyl ester	42	.22	C28H5 6O2	24	3250 9-55-0
6.23	Octadecanoic acid, eicosyl ester	40	.58	C38H7 6O2	64	2241 3-02-1
6.23	Ent-2b,3a-dihydroxy-13-iodomethyl- 16-oxo-8,13-epi-17,20-dinorgibberell-1(10)-en- 7,19-dioic acid,19,2-lactone,7-methyl ester	33	.81	C20H2 3IO6	86	1276 17-16-7
6.23	Benzene, 1-[2-[2-(2- chloroethoxy)ethoxy]ethoxy]-4-(1,1,3,3- tetramethylbutyl)-	26	.45	C20H3 3ClO3	56	6702 5-22-3

T	Name	I	rob.	Formula	W	Cas #
8.21	4a α ,4b α -Gibbane-1,1,10 α -tricarboxylic acid, 4a,7-dihydroxy-8-methylene-, 1 α ,4a-lactone, dimethyl ester	07	1.08	C21H26 O7	90	1845 0-95-8
8.21	9-Borabicyclo[3.3.1]nonane, 9-[[3-[2- (9-borabicyclo[3.3.1]non-9-yloxy)phenyl]-1- thioxopropyl]thio]-	95	.38	C25H36 B2OS2	38	1397 59-23-2
8.21	Ent-3a,10-dihydroxy-13-iodomethyl- 16-oxo-8,13-epi-17,20-dinorgibberell-1-en-7,19- dioic acid,19,10-lactone,7-methyl ester	94	.09	C20H23I O6	86	1164 28-84-3
8.21	Pregn-16-ene-11,14,18,20-tetrol, 3,9- epoxy-3-methoxy-, 11,20-diacetate, (3 α ,5 α ,11 α ,14 α ,20R)-	85	.15	C26H38 O8	78	3877 4-56-0
8.21	1,1'-Biphenyl, 4,2',3',4'-tetramethoxy-6- [N-methyl-N-acetylaminomethyl]	84	.95	C20H25 NO5	59	NA

Data File: 1-6
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 18:20:24
 Run Time (min): 29.98
 Vial: 24
 Inj Vol (µL): 2.00
 Scans: 3049
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.03 SM: 7G

RT	Peak Area	Area %
6.73	352609	24.80
8.46	264802	18.63
9.31	1615	0.11
9.58	56460	3.97
10.19	10897	0.77
10.73	56421	3.97
11.16	98980	6.96
12.02	21556	1.52
12.49	8547	0.60
12.78	1958	0.14
13.10	37165	2.61
13.34	69365	4.88
13.52	65975	4.64
13.74	7098	0.50
13.91	34951	2.46
14.38	9030	0.64
14.56	22063	1.55
15.00	24415	1.72
15.36	9213	0.65
15.64	131726	9.27
15.98	15211	1.07

16.23	38719	2.72
16.52	14714	1.04
17.96	2740	0.19
18.43	12743	0.90
19.29	3510	0.25
20.54	4367	0.31
21.74	6117	0.43
22.09	1356	0.10
22.86	2431	0.17
23.01	1797	0.13
23.92	3730	0.26
24.77	15658	1.10
25.12	2454	0.17
25.45	4526	0.32
25.84	657	0.05
27.78	6052	0.43

T	Name	I	rob.	Formula	W	Cas #
5.36	Benzenesulfonamide, N-butyl-	06	6.47	C10H15 NO2S	13	362 2-84-2
5.36	Benzene, [(trifluoromethyl)sulfonyl]-	51	.24	C7H5F3 O2S	10	426- 58-4
5.36	Diphenyl ether	47	.89	C12H10 O	70	101- 84-8
5.36	Benzene, (ethylsulfonyl)-	44	.67	C8H10 O2S	70	599- 70-2
5.36	5-(Phenylsulphonyl)dihydro-1,3,5-dioxazine	33	.15	C9H11 NO4S	29	562 21-07-9

T	Name	I	rob.	Formula	W	Cas #
5.98	3-[18-(3-Hydroxy-propyl)-3,3,7,12,17-pentamethyl-2,3,22,24-tetrahydro-porphin-2-yl]propan-1-ol	57	1.27	C31H38N4 O2	98	NA
5.98	Tungsten, pentacarbonyl(4,5-diethyl-2,2,3-trimethyl-1-phenyl-1-phospha-2-sila-5-boracyclohex-3-ene-P1)-, (oc-6-22)-	41	8.01	C21H26BO 5PSiW	12	1187 72-51-3
5.98	4'-Apo-á, .psi.-carotenoic acid	18	.57	C35H46O2	98	2468- 88-4
5.98	Hexadecanoic acid, N,N-bis[(methylcarboxy)ethyl-2-(2-butoxyethoxy)]-	12	.17	C36H69NO 9	59	NA
5.98	9,19-Cyclolanostane-6,7-dione, 3-acetoxy-	10	.76	C32H50O4	98	NA

T	Name	I	rob.	Formul a	W	Cas #
	3-[18-(3-Hydroxy-propyl)-3,3,7,12,17-			C31H3		NA

6.23	pentamethyl-2,3,22,24-tetrahydro-porphin-2-yl]propan-1-ol	28	9.55	8N4O2	98	
6.23	5 α -Cholan-24-oic acid, 12 α -hydroxy-3,7-dioxo-, methyl ester	26	8.03	C25H3 8O5	18	1665 6-66-9
6.23	Ent-2b,3a-dihydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1(10)-en-7,19-dioic acid,19,2-lactone,7-methyl ester	10	0.38	C20H2 3IO6	86	1276 17-16-7
6.23	(5 α ,13 α)3,19-Epoxyandrost-8-ene, 17-acetoxy-3-methoxy-4,4,13-trimethyl-	03	.95	C25H3 8O4	02	NA
6.23	Hexadecanoic acid, N,N-bis[(methylcarboxy)ethyl-2-(2-butoxyethoxy)]-	00	.03	C36H6 9NO9	59	NA

Data File: 1-13
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 19:11:20
 Run Time (min): 29.99
 Vial: 25
 Inj Vol (µL): 2.00
 Scans: 3058
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.03 SM: 7G

RT	Peak Area	Area %
6.35	2496	0.49
6.54	7934	1.57
6.73	98371	19.46
8.46	59647	11.80
8.64	18411	3.64
8.84	20349	4.03
9.18	9376	1.85
9.36	14293	2.83
9.58	46819	9.26
9.88	9406	1.86
10.18	6218	1.23
10.73	16732	3.31
11.15	1515	0.30
11.76	1627	0.32
12.02	18120	3.58
13.05	18656	3.69
13.34	1245	0.25
13.51	12056	2.38
13.73	4828	0.96
13.90	4683	0.93
14.39	2437	0.48

15.01	4575	0.90
15.64	12236	2.42
16.21	836	0.17
16.52	5398	1.07
16.71	1582	0.31
16.91	2791	0.55
17.10	1904	0.38
17.43	3707	0.73
17.96	1306	0.26
19.29	1983	0.39
20.01	334	0.07
20.54	3840	0.76
21.74	4860	0.96
22.10	822	0.16
22.86	7586	1.50
23.92	7151	1.41
24.77	18955	3.75
24.89	10634	2.10
25.45	7093	1.40
25.58	6555	1.30
25.83	4082	0.81
26.25	1827	0.36
26.70	7046	1.39
26.89	2891	0.57
27.53	3499	0.69
27.77	6840	1.35

T	Name	I	rob.	Form ula	W	Cas #
.88	(22S)-21-Acetoxy-6a,11a-dihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	18	1.63	C27H 36O8	88	937 89-66-3
.88	(22S)-6a,11a,21-Trihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	97	.20	C25H 34O7	46	938 61-53-1
.88	17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one	96	.84	C35H 52O	88	NA
.88	(22S)-6a,11a,21-Trihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	93	.81	C25H 34O7	46	NA
.88	5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 2,4a,9,9a-tetrakis(acetyloxy)-3,[(acetyloxy)methyl]-1,1a,1b,2,3,4,4a,7a,7b,8,9,9a-dodecahydro-2,7b-dihydroxy-1,1,6,8-tetramethyl-, [1aR-(1aà,1bà,2à,3à,4aà,7aà,7bà,8à,9a,9aà)]-	88	.29	C30H 40O13	08	775 73-25-2

T	Name	I	rob.	Formul a	W	C as #
0.18	AZULENE DB5-1140	29	5.29			N A
0.18	Naphthalene	26	3.51	C10H8	28	9 1-20-3
0.18	1H-Indene, 1-methylene-	16	.53	C10H8	28	2 471-84-3
0.18	NAPHTHALENE DB5-826	11	.68			N A
0.18	2á,4a-Epoxymethylphenanthrene-7-methanol, 1,1-dimethyl-2-methoxy-8-(1,3-dithiin-2-ylidene)methyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-, acetate	06	.19	C27H3 8O4S2	90	N A

T	Name	I	rob.	Form ula	W	Cas #
1.76	Pregn-16-ene-11,14,18,20-tetrol, 3,9-epoxy-3-methoxy-, 11,20-diacetate, (3á,5á,11á,14á,20R)-	23	0.65	C26H 38O8	78	387 74-56-0
1.76	9-Desoxo-9x-hydroxy-7-ketoingol 3,8,9,12-tetraacetate	19	.00	C28H 38O10	34	NA
1.76	4a,7a-Epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-4(1H)-one, 2,7,10,11-tetrakis(acetyloxy)-1a,2,3,6,7,10,11,11a-octahydro-1,1,3,6,9-pentamethyl-, [1ar-(1ar*,2R*,3S*,4ar*,6S*,7S*,7as*,8E,10R*,11R*,11as*)]-	10	.53	C28H 38O10	34	519 06-02-6
1.76	9-Desoxo-9-x-acetoxy-3-desoxy-7.8.12-tri-O-acetylingol-3-one	09	.28	C28H 38O10	34	NA
1.76	Pregn-16-en-20-one, 11,18-bis(acetyloxy)-3,9-epoxy-3-methoxy-, (3á,5á,11á)-	05	.30	C26H 36O7	60	303 84-39-5

T	Name	I	rob.	Formu la	W	Cas #
0.01	.psi.,.psi.-Carotene, 3,3',4,4'-tetrahydro-1,1',2,2'-tetrahydro-1-hydroxy-1'-methoxy-	71	.96	C41H 58O2	82	161 76-79-7
0.01	2,4a-Oxymethano-1,2,3,4,4a,5,6,7,8,8a,9-dodecahydrophenanthren-9-one, 8-cyanomethyl-2-methoxy-7-methoxycarbonyl-1,1,7-trimethyl-	69	.26	C23H 31NO5	01	NA
0.01	.psi.,.psi.-Carotene, 3,4-didehydro-1,2,7',8'-tetrahydro-1-methoxy-2-oxo-	66	.30	C41H 58O2	82	138 36-70-9
0.01	9-Desoxo-9-x-acetoxy-3,8,12-tri-O-acetylingol	58	.44	C28H 40O10	36	NA
0.01	17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-	56	.02	C35H 52O	88	NA

	styrylhexadecahydrocyclopenta[a]phenanthren-2-one					
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Data File:	2-1
Curr Data Path:	D:\Xcalibur\Data\GemmaH\peppers100703\
Acquisition Date:	10/07/03 20:02:38
Run Time (min):	29.96
Vial:	26
Inj Vol (μL):	2.00
Scans:	3039
Low Mass (m/z):	35.00
High Mass (m/z):	550.00
Inst Method:	D:\Xcalibur\methods\pepper_PTV.meth
Proc Method:	D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.00 SM: 7G

RT	Peak Area	Area %
6.73	401534	24.09
7.33	72661	4.36
8.46	311460	18.69
9.32	1634	0.10
9.59	65545	3.93
10.19	3475	0.21
10.72	42135	2.53
11.16	19509	1.17
11.40	5237	0.31
11.57	12648	0.76
11.74	11092	0.67
12.02	26299	1.58
12.51	1902	0.11
13.11	32731	1.96
13.35	95343	5.72
13.52	88223	5.29
13.74	5195	0.31
13.90	52142	3.13
14.12	2487	0.15
14.39	10265	0.62
14.56	27085	1.63

15.01	32223	1.93
15.36	11203	0.67
15.65	168871	10.13
15.97	30934	1.86
16.23	79134	4.75
16.51	21353	1.28
17.95	2720	0.16
19.29	2915	0.17
20.54	1251	0.08
21.75	831	0.05
22.10	1388	0.08
22.86	679	0.04
24.77	11771	0.71
25.45	4519	0.27
27.79	8287	0.50

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
6.73	302004	18.78
7.22	72522	4.51
8.46	298467	18.56
9.32	1888	0.12
9.58	75871	4.72
10.19	1406	0.09
10.73	49595	3.08
11.16	36887	2.29
11.53	19393	1.21
11.75	19524	1.21
12.03	36871	2.29
12.29	1643	0.10
13.10	25625	1.59
13.35	91997	5.72
13.53	78974	4.91
13.74	4753	0.30
13.91	46985	2.92
14.39	9582	0.60
14.56	25891	1.61
15.00	29041	1.81
15.66	214740	13.36

16.25	106713	6.64
16.51	30976	1.93
17.95	1943	0.12
19.30	2882	0.18
20.55	1511	0.09
21.74	1916	0.12
22.09	1702	0.11
24.77	5956	0.37
25.45	5103	0.32
27.77	5556	0.35

T	Name	I	rob.	F ormula	W	C as #
5.45	Benzo[k]fluoranthene	74	6.53	C 20H12	52	2 07-08-9
5.45	Perylene	51	0.64	C 20H12	52	1 98-55-0
5.45	Benzo[j]fluoranthene	27	.91	C 20H12	52	2 05-82-3
5.45	Benz[e]acephenanthrylene	24	.11	C 20H12	52	2 05-99-2
5.45	Benzo[e]pyrene	21	.40	C 20H12	52	1 92-97-2

Data File: 2-13
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 21:46:05
 Run Time (min): 29.98
 Vial: 28
 Inj Vol (µL): 2.00
 Scans: 3044
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.02 SM: 7G

RT	Peak Area	Area %
5.78	339	0.04
6.73	161692	18.89
7.33	1449	0.17
7.67	2495	0.29
8.46	151082	17.65
9.30	5226	0.61
9.58	53555	6.25
10.73	33938	3.96
12.02	23054	2.69
13.07	11387	1.33
13.51	50208	5.86
13.73	2857	0.33
13.90	15376	1.80
14.38	1884	0.22
14.56	3887	0.45
15.02	16343	1.91
15.66	65229	7.62
16.09	29838	3.48
16.28	31230	3.65
16.52	55859	6.52
16.89	38573	4.51

17.33	7072	0.83
17.96	5288	0.62
18.70	9196	1.07
18.90	2864	0.33
19.30	5307	0.62
20.54	7509	0.88
21.74	6652	0.78
22.86	7535	0.88
23.92	9414	1.10
24.90	8594	1.00
25.44	4347	0.51
25.83	5192	0.61
26.26	1055	0.12
26.70	3054	0.36
26.89	6191	0.72
27.53	5061	0.59
27.77	6359	0.74

T	Name	I	rob.	For mula	W	Cas #
6.89	Hexadecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-(1aà,2à,5á,5aá,6á,8aà,9à,10aà)]-	74	0.05	C36 H58O6	86	525 57-26-3
6.89	9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol, (3á,5Z,7E)-	41	.25	C27 H44O3	16	400 13-87-4
6.89	4a-Phorbol 12,13-didecanoate	36	.23	C40 H64O8	72	NA
6.89	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	32	.57	C35 H68O5	68	761- 35-3
6.89	Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester	32	.57	C39 H76O5	24	504- 40-5

Data File: 3-1
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 22:39:02
 Run Time (min): 29.96
 Vial: 29
 Inj Vol (µL): 2.00
 Scans: 3040
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.00 SM: 7G

RT	Peak Area	Area %
5.09	5429	0.32
6.74	327311	19.27
7.14	46885	2.76
7.43	87232	5.14
8.47	475319	27.99
9.31	3469	0.20
9.59	103286	6.08
10.19	2326	0.14
10.73	69963	4.12
11.00	1242	0.07
11.17	19646	1.16
11.76	4156	0.24
12.02	27609	1.63
13.11	15077	0.89
13.35	82022	4.83
13.53	57075	3.36
13.91	29026	1.71
14.11	1686	0.10
14.39	8320	0.49
14.56	18951	1.12
15.00	21167	1.25

15.36	1450	0.09
15.67	186522	10.98
16.18	57070	3.36
16.52	18945	1.12
17.95	442	0.03
19.30	1672	0.10
20.54	1802	0.11
21.74	1028	0.06
22.09	291	0.02
22.87	1774	0.10
23.91	272	0.02
24.77	8767	0.52
25.45	3440	0.20
27.53	2239	0.13
27.77	5407	0.32

T	Name	I	rob.	Formula	W	Cas #
4.39	Acetic acid, 3-acetoxy-5-pentyl-2-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)phenyl ester	02	.80	C25H34O4	98	NA
4.39	2á,4a-Epoxymethylphenanthrene-7-methanol, 1,1-dimethyl-2-methoxy-8-(1,3-dithiin-2-ylidene)methyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-, acetate	97	.48	C27H38O4S2	90	NA
4.39	4H-Cyclopropa[5',6']benz[1',2':7,8]azuleno[5,6-b]oxiren-4-one, 8,8a-bis(acetyloxy)-2a-[(acetyloxy)methyl]-1,1a,1b,1c,2a,3,3a,6a,6b,7,8,8a-dodecahydro-6b-hydroxy-3a-methoxy-1,1,5,7-tetramethyl-, [1aR-(1aà,1bà,1cà,2aà,3aà,6aà,6bà,7à,8à,8aà)]-	97	.48	C27H36O10	20	648 07-01-8
4.39	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1-methyl-5-[1-methyl-3-[(trimethylsilyl)oxy]butyl]-3-(trimethylsilyl)-	97	.48	C18H36N2O4Si2	00	573 97-42-9
4.39	9-Desoxy-9x-chloroingol 3,7,8,12-tetraacetate	96	.26	C28H39ClO9	54	NA

T	Name	I	rob.	For mula	W	Cas #
2.09	Chrysene-d12	39	4.65	C18D12	40	171 9-03-5
2.09	1',1'-Dicarboethoxy-1á,2á-dihydro-3'H-cycloprop[1,2]cholesta-1,4,6-trien-3-one	84	.78	C34H50O5	38	758 57-74-8
2.09	Ferrocene, 1-ethenyl-1'-ethyl-	78	.75	C14H16Fe	40	710 35-62-6
2.09	Ferrocene, 1,1'-(1,4-butanediyl)-	70	.80	C14H16Fe	40	330 39-65-5
2.09	12,13-Di-O-acetyl-20-desoxytigla-(1,6(20),7)-trien-3-one	69	.69	C24H30O7	30	NA

Data File: 3-6
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/07/03 23:30:53
 Run Time (min): 29.97
 Vial: 30
 Inj Vol (µL): 2.00
 Scans: 3034
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
6.73	365979	17.85
7.12	80723	3.94
7.43	56404	2.75
8.46	401758	19.60
9.31	2295	0.11
9.59	99874	4.87
10.19	5559	0.27
10.73	61608	3.01
11.17	21609	1.05
11.49	5529	0.27
11.74	8106	0.40
12.03	29582	1.44
13.11	23917	1.17
13.36	112932	5.51
13.53	98725	4.82
13.90	54014	2.63
14.11	1256	0.06
14.38	19011	0.93
14.56	31123	1.52
15.01	38668	1.89
15.67	197585	9.64

15.96	56096	2.74
16.24	258318	12.60
17.95	1123	0.05
19.29	1539	0.08
21.73	2865	0.14
24.78	4820	0.24
25.46	3958	0.19
26.71	2965	0.14
27.76	2224	0.11

T	Name	I	rob.	Formula	W	Cas #
4.38	Acetic acid, 3-acetoxy-5-pentyl-2-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)phenyl ester	46	9.80	C25H34O4	98	NA
4.38	3-Methoxydizepam	42	6.73	C17H15ClN2O2	14	171-91-70
4.38	Pregnan-11-one, 17-hydroxy-3,20-bis[(trimethylsilyl)oxy]-, (3R,5R,20S)-	04	.00	C27H50O4Si2	94	511-66-36-0
4.38	1-Pentanol, 1-[2(diphenylhydroxymethyl)phenyl]-	02	.69	C24H26O2	46	NA
4.38	Cholan-6-ol-3-one-24-acid, ethyl ester	96	.90	C26H42O4	18	NA

Data File: 3-13
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 01:13:21
 Run Time (min): 29.99
 Vial: 51
 Inj Vol (µL): 2.00
 Scans: 3035
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.04 SM: 7G

RT	Peak Area	Area %
6.74	342528	16.14
7.18	99528	4.69
8.46	386301	18.21
9.59	105172	4.96
10.20	1683	0.08
10.72	64953	3.06
11.18	2884	0.14
11.76	4946	0.23
12.02	33491	1.58
13.11	16751	0.79
13.36	96445	4.55
13.53	89238	4.21
13.74	3019	0.14
13.91	49590	2.34
14.38	14625	0.69
14.57	27384	1.29
15.01	35461	1.67
15.69	82756	3.90
16.33	244312	11.52
16.52	175138	8.25
16.89	167100	7.88

17.96	5201	0.25
18.67	3492	0.16
19.29	6001	0.28
20.55	5926	0.28
21.74	4996	0.24
22.86	4522	0.21
23.91	5252	0.25
24.77	4297	0.20
24.90	4239	0.20
25.45	2037	0.10
25.83	3479	0.16
26.24	4266	0.20
26.69	2261	0.11
26.89	10955	0.52
27.05	4491	0.21
27.52	5228	0.25
27.78	1684	0.08

T	Name	I	rob.	Formula	W	Cas #
1.76	(5á)Pregnane-3,20á-diol, 14á,18á-[4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-, diacetate	36	2.97	C28H43NO6	89	NA
1.76	17á-Acetoxy-1',1'-dicarboethoxy-1á,2á-dihydro-17á-methyl-3'H-cycloprop[1,2]-5á-androst-1-en-3-one	26	.15	C29H42O7	02	800 97-22-9
1.76	Pregnane-15,20-dione, 3,12,14-tris(acetyloxy)-, (3á,5á,12á,14á)-	22	.73	C27H38O8	90	554 93-82-8
1.76	2á,4a-Epoxymethylphenanthrene-7-methanol, 1,1-dimethyl-2-methoxy-8-(1,3-dithiin-2-ylidene)methyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-, acetate	16	.08	C27H38O4S2	90	NA
1.76	5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 2,4a,9,9a-tetrakis(acetyloxy)-3,[(acetyloxy)methyl]-1,1a,1b,2,3,4,4a,7a,7b,8,9,9a-dodecahydro-2,7b-dihydroxy-1,1,6,8-tetramethyl-, [1aR-(1aá,1bá,2á,3á,4aá,7aá,7bá,8á,9á,9aá)]-	15	.84	C30H40O13	08	775 73-25-2

T	Name	I	rob.	Formula	W	Cas #
6.33	4'-Apo-á,á,psi.-carotenoic acid	88	9.26	C35H46O2	98	2468- 88-4
6.33	Ent-3a,10-dihydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1-en-7,19-dioic acid,19,10-lactone,7-methyl ester	52	.23	C20H23IO6	86	1164 28-84-3
	D-Homo-24-nor-17-oxachola-20,22-diene-			C28		5565

6.33	3,16-dione, 7-(acetyloxy)-1,2:14,15:21,23-triepoxy-4,4,8-trimethyl-, (5à,7à,13à,14à,15à,17aà)-	47	.83	H34O8	98	8-66-7
6.33	9,19-Cyclolanostane-6,7-dione, 3-acetoxy-	43	.92	C32 H50O4	98	NA
6.33	10'-Apo-à,psi.-carotenoic acid, 5,6-dihydro-5,6-dihydroxy-, methyl ester, (5R,6R)-	37	.87	C28 H40O4	40	1256- 21-9

T	Name	I	rob.	Formula	W	Cas #
6.89	4'-Apo-à,psi.-carotenoic acid	92	7.96	C35H46 O2	98	2468- 88-4
6.89	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester, [1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	77	0.88	C32H39 NO10	97	5190 6-00-4
6.89	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	64	.03	C16H50 O7Si8	78	1909 5-24-0
6.89	D-Homo-24-nor-17-oxachola-20,22-diene-3,16-dione, 7-(acetyloxy)-1,2:14,15:21,23-triepoxy-4,4,8-trimethyl-, (5à,7à,13à,14à,15à,17aà)-	60	.94	C28H34 O8	98	5565 8-66-7
6.89	Ent-3a,10-dihydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1-en-7,19-dioic acid,19,10-lactone,7-methyl ester	60	.94	C20H23 IO6	86	1164 28-84-3

Data File:	4-1
Curr Data Path:	D:\Xcalibur\Data\GemmaH\peppers100703\
Acquisition Date:	10/08/03 02:05:24
Run Time (min):	29.96
Vial:	52
Inj Vol (μL):	2.00
Scans:	3032
Low Mass (m/z):	35.00
High Mass (m/z):	550.00
Inst Method:	D:\Xcalibur\methods\pepper_PTV.meth
Proc Method:	D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
6.73	435435	16.53
7.45	186247	7.07
8.46	552347	20.97
9.31	3272	0.12
9.59	136652	5.19
10.72	77951	2.96
11.77	5271	0.20
12.02	40707	1.55
12.22	1791	0.07
12.54	148	0.01
13.12	16874	0.64
13.36	113965	4.33
13.53	100603	3.82
13.91	53385	2.03
14.38	15688	0.60
14.57	30937	1.17
15.01	37802	1.44
15.36	7645	0.29
15.70	85235	3.24
16.33	296976	11.28
16.51	394413	14.98

17.95	7072	0.27
19.29	1878	0.07
20.54	2701	0.10
21.73	2671	0.10
22.86	836	0.03
23.92	2656	0.10
24.77	5380	0.20
24.89	5090	0.19
25.44	4095	0.16
25.82	1961	0.07
26.70	2271	0.09
27.77	3466	0.13

T	Name	I	rob.	Formul a	W	Cas #
1.77	2á,4a-Epoxymethylphenanthrene-7-methanol, 1,1-dimethyl-2-methoxy-8-(1,3-dithiin-2-ylidene)methyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-, acetate	39	5.72	C27H3 8O4S2	90	NA
1.77	Pregn-9(11)-en-3-one, 18,20-dihydroxy-, cyclic 1,2-ethanediyl acetal, (5á,20R)-	12	.56	C23H3 6O4	76	397 66-63-7
1.77	D-Homo-24-nor-17-oxachola-20,22-dien-16-one, 1,3,7-tris(acetyloxy)-14,15:21,23-diepoxy-4,4,8-trimethyl-, (1á,3á,5á,7á,13á,14á,15á,17áá)-	12	.56	C32H4 2O10	86	252 4-38-1
1.77	3'H-Cycloprop(1,2)cholesta-1,4,6-trien-3-one, 1'-carboethoxy-1'-cyano-1á,2á-dihydro-	06	.94	C32H4 5NO3	91	758 57-78-2
1.77	1H-Cyclopropa[3,4]benz[1,2-e]azulene-3-carboxaldehyde, 9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5,9-dioxo-, [1aR-(1aá,1bá,4aá,7aá,7bá,8á,9aá)]-	00	.67	C22H2 6O7	02	775 73-49-0

T	Name	I	rob.	Formula	W	Cas #
5.70	4'-Apo-á,psi.-carotenoic acid	68	8.04	C35H46 O2	98	2468- 88-4
5.70	Ent-3a,10-dihydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1-en-7,19-dioic acid,19,10-lactone,7-methyl ester	47	.67	C20H23 IO6	86	1164 28-84-3
5.70	D-Homo-24-nor-17-oxachola-20,22-diene-3,16-dione, 7-(acetyloxy)-1,2:14,15:21,23-triepoxy-4,4,8-trimethyl-, (5á,7á,13á,14á,15á,17áá)-	45	.08	C28H34 O8	98	5565 8-66-7
5.70	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester, [1aR-	45	.08	C32H39 NO10	97	5190 6-00-4

	(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-						
5.70	9,19-Cyclolanostane-6,7-dione, 3-acetoxy-	37	.28	O4	C32H50	98	NA

T	Name	I	rob.	Formula	W	Cas #
6.33	4'-Apo-á,psi.-carotenoic acid	85	7.98	C35H46 O2	98	2468-88-4
6.33	Ent-3a,10-dihydroxy-13-iodomethyl-16-oxo-8,13-epi-17,20-dinorgibberell-1-en-7,19-dioic acid,19,10-lactone,7-methyl ester	51	.17	C20H23 IO6	86	1164-28-84-3
6.33	D-Homo-24-nor-17-oxachola-20,22-diene-3,16-dione, 7-(acetyloxy)-1,2:14,15:21,23-triepoxy-4,4,8-trimethyl-, (5à,7à,13à,14à,15á,17aà)-	46	.78	C28H34 O8	98	5565-8-66-7
6.33	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester, [1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	45	.55	C32H39 NO10	97	5190-6-00-4
6.33	9,19-Cyclolanostane-6,7-dione, 3-acetoxy-	41	.69	C32H50 O4	98	NA

Data File: 4-6
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 02:56:46
 Run Time (min): 29.99
 Vial: 53
 Inj Vol (µL): 2.00
 Scans: 3031
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.03 SM: 7G

RT	Peak Area	Area %
6.73	433819	17.98
7.13	36185	1.50
7.43	124320	5.15
8.46	499933	20.73
9.31	1537	0.06
9.58	140021	5.80
10.21	945	0.04
10.73	83312	3.45
11.76	1918	0.08
12.02	38250	1.59
12.29	2486	0.10
12.55	844	0.04
13.12	16806	0.70
13.35	100623	4.17
13.52	98451	4.08
13.92	73567	3.05
14.38	15120	0.63
14.56	29370	1.22
15.00	35845	1.49
15.35	8660	0.36
15.68	18117	0.75

16.50	616282	25.55
17.95	3818	0.16
19.29	2878	0.12
20.54	2755	0.11
21.74	3502	0.15
22.87	3107	0.13
23.91	1873	0.08
24.77	4247	0.18
24.90	2984	0.12
25.45	1294	0.05
25.82	1234	0.05
26.69	1503	0.06
27.52	897	0.04
27.77	5717	0.24

T	Name	I	rob.	Formula	W	Cas #
3.35	21H-Biline-8,12-dipropanoic acid, 3,17-diethyl-1,2,3,4,5,19,23,24-octahydro-2,7,13,18-tetramethyl-1,19-dioxo-, dimethyl ester, (2R,3R,4R)-	48	6.00	C35H46 N4O6	18	318 62-23-4
3.35	21H-Biline-8,12-dipropanoic acid, 2,17-diethyl-1,2,3,4,5,19,23,24-octahydro-3,7,13,18-tetramethyl-1,19-dioxo-, dimethyl ester, (2R,3R,4R)-	20	6.17	C35H46 N4O6	18	297 89-77-3
3.35	1'H-Cholest-2-eno[3,2-b]indole, 5'-chloro-, (5à)-	03	.82	C33H48 ClN	93	345 35-54-1
3.35	Silane, [(dichlorostannylene)dimethylidyne]tetrakis(trimethyl-	98	.11	C14H38 Cl2Si4Sn	08	627 89-73-5
3.35	21H-Biline-8,12-dipropanoic acid, 2,18-diethyl-1,4,5,19,23,24-hexahydro-3,7,13,17-tetramethyl-1,19-dioxo-, dimethyl ester, (4R)-	42	.35	C35H44 N4O6	16	297 89-75-1

Data File: 4-13
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 03:47:33
 Run Time (min): 29.96
 Vial: 54
 Inj Vol (µL): 2.00
 Scans: 3033
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
6.74	247541	23.99
7.70	2720	0.26
8.46	269868	26.16
9.32	2745	0.27
9.58	105355	10.21
10.72	49817	4.83
12.02	32746	3.17
13.07	6424	0.62
13.51	47817	4.64
13.73	2899	0.28
13.90	14332	1.39
14.56	2178	0.21
15.02	20584	2.00
15.36	1103	0.11
16.52	10803	1.05
16.90	11747	1.14
17.26	26199	2.54
17.45	35654	3.46
17.95	22349	2.17
18.17	2902	0.28
18.68	24370	2.36

18.90	2706	0.26
19.29	8188	0.79
20.54	8645	0.84
21.74	8256	0.80
22.86	8363	0.81
23.91	6551	0.63
24.90	6585	0.64
25.44	1953	0.19
25.83	5068	0.49
26.25	5195	0.50
26.71	4977	0.48
26.89	18668	1.81
27.51	2002	0.19
27.77	4328	0.42

RT	Name	I	rob.	Formula	W	Cas #
6.90	Pregnane-3,11,20,21-tetrol, cyclic 20,21-(butyl boronate), (3 α ,5 α ,11 α ,20R)-	57	0.98	C25H43BO4	18	555 56-74-6
6.90	Spirost-8-en-11-one, 3-hydroxy-, (3 α ,5 α ,14 α ,20 α ,22 α ,25R)-	47	.75	C27H40O4	28	580 72-54-1
6.90	Tetradecanoic acid, 12-methyl-, methyl ester	44	.85	C16H32O2	56	512 9-66-8
6.90	17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one	43	.58	C35H52O	88	NA
6.90	2,7-Diphenyl-1,6-dioxypyridazino[4,5-2',3']pyrrolo[4',5'-D]pyridazine	40	.82	C20H13N5O2	55	917 57-06-1
T	Name	I	rob.	Formula	W	Cas #
8.68	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	14	0.59	C21H36O4	52	184 65-99-1
8.68	Cyclooctenone, dimer	11	.35	C16H24O2	48	612 19-51-0
8.68	Pseudosolasodine diacetate	05	.35	C31H49NO4	99	NA
8.68	9,12-Octadecadienoic acid, methyl ester, (E,E)-	98	.63	C19H34O2	94	256 6-97-4
8.68	Acetic acid, 17-acetoxy-3-hydroxyimino-4,4,13-trimethyl-hexadecahydrocyclopenta[a]phenanthren-10-ylmethyl ester	90	.20	C25H39NO5	33	NA

T	Name	I	rob.	Formula	W	Cas #
8.90	Spirosolan-3-ol, 28-acetyl-, acetate (ester), (3 α ,5 α ,22 α ,25S)-	11	.11	C31H49NO4	99	118 1-86-8
	Butanoic acid, 1 α ,2,5,5 α ,6,9,10,10 α -			C24H		775

8.90	octahydro-5a-hydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-6,11-dioxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1aR-(1aà,2à,5à,5aà,8aà,9à,10aà)]-	04	.97	32O6	16	08-70-4
8.90	(5à,13à) Androst-8-en-3-one, 17-19-diacetoxy-4,4-dimethyl-	96	.20	C25H36O5	16	NA
8.90	Hexadecanoic acid, 2-(hexadecyloxy)ethyl ester	91	.19	C34H68O3	24	288 43-32-5
8.90	6-(1,5-Dimethyl-hex-4-enyl)-1,6-dihydroxy-1,8a-dimethyl-3-oxo-1,2,3,3a,5a,6,7,8,8a,9,10,10a-dodecahydrodicyclopenta[a,E]cyclooctene	91	.19	C25H38O4	02	NA

T	Name	I	rob.	Formula	W	Cas #
6.89	Stigmastan-3-ol, 5-chloro-, acetate, (3à,5à)-	36	1.19	C31H53ClO2	92	557 24-19-1
6.89	Stigmastan-3,5-dien	23	3.69	C29H48	96	NA
6.89	Stigmast-5-en-3-ol, oleate	21	2.62	C47H82O2	78	NA
6.89	à-Sitosterol acetate	15	.92	C31H52O2	56	915- 05-9
6.89	Sitosterol acetate	02	.41	C31H52O2	56	NA

Data File: 5-1
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 06:18:17
 Run Time (min): 29.95
 Vial: 57
 Inj Vol (µL): 2.00
 Scans: 3037
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.00 SM: 7G

RT	Peak Area	Area %
6.73	570024	19.29
7.18	56481	1.91
7.39	138209	4.68
8.47	652059	22.07
9.58	192279	6.51
10.73	102313	3.46
11.11	1827	0.06
12.02	43760	1.48
13.36	118029	3.99
13.52	126853	4.29
13.91	83966	2.84
14.11	6038	0.20
14.38	15289	0.52
14.56	29181	0.99
15.01	52553	1.78
15.36	21608	0.73
15.52	5191	0.18
15.69	2456	0.08
15.95	7874	0.27
16.51	77810	2.63
17.00	289649	9.80

17.25	281766	9.54
17.95	35271	1.19
19.29	3056	0.10
20.54	4500	0.15
21.73	3482	0.12
22.86	3778	0.13
23.92	4445	0.15
24.90	7286	0.25
25.44	2300	0.08
25.83	4522	0.15
26.69	4081	0.14
27.52	2304	0.08
27.77	4230	0.14

T	Name	I	rob.	Formula	W	Cas #
4.56	21H-Biline-8,12-dipropanoic acid, 3,17-diethyl-1,2,3,4,5,19,23,24-octahydro-2,7,13,18-tetramethyl-1,19-dioxo-, dimethyl ester, (2R,3R,4R)-	89	3.16	C35H46N4O6	18	318 62-23-4
4.56	1'H-Cholest-2-eno[3,2-b]indole, 5'-chloro-, (5à)-	84	8.66	C33H48ClN	93	345 35-54-1
4.56	21H-Biline-8,12-dipropanoic acid, 2,17-diethyl-1,2,3,4,5,19,23,24-octahydro-3,7,13,18-tetramethyl-1,19-dioxo-, dimethyl ester, (2R,3R,4R)-	81	6.49	C35H46N4O6	18	297 89-77-3
4.56	Silane, [(dichlorostannylene)dimethylidyne]tetrakis(trimethyl-	79	5.21	C14H38Cl2Si4Sn	08	627 89-73-5
4.56	Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2'-[1,3-dihydro-1-(4-methoxyphenyl)-3-oxo-1-isobenzofuranyl]-	21	.80	C35H22O6	38	555 17-71-0

Data File: 5-6
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 05:27:56
 Run Time (min): 29.97
 Vial: 56
 Inj Vol (µL): 2.00
 Scans: 3024
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.02 SM: 7G

RT	Peak Area	Area %
6.73	419161	21.36
7.14	33061	1.69
7.36	71658	3.65
8.46	499370	25.45
9.31	818	0.04
9.58	146813	7.48
10.21	1476	0.08
10.73	85025	4.33
12.03	36556	1.86
13.11	12552	0.64
13.35	82530	4.21
13.52	102853	5.24
13.90	51714	2.64
14.38	10629	0.54
14.56	23750	1.21
15.01	44436	2.26
15.35	5441	0.28
15.51	4641	0.24
15.69	1750	0.09
15.96	2214	0.11
16.52	56429	2.88

16.90	233271	11.89
17.95	4638	0.24
19.30	5125	0.26
20.54	3436	0.18
21.74	3267	0.17
22.86	4473	0.23
23.91	485	0.02
24.78	2912	0.15
25.45	2101	0.11
25.82	2661	0.14
26.69	3680	0.19
27.78	3155	0.16

T	Name	I	rob.	Formula	W	Cas #
0.21	Dihydrofuro[2,3-e]phenalene, 6-methoxy-8-oxo-2,3,3,10-tetramethyl-4,5,7-trihydroxy-	17	3.02	O6 C20H20	56	NA
0.21	Stearic acid, 3-(octadecyloxy)propyl ester	02	.89	O3 C39H78	94	173 67-40-7
0.21	Formyl colchicine	95	.04	NO7 C23H25	27	NA
0.21	Acetic acid, [bis[(trimethylsilyl)oxy]phosphinyl]-, trimethylsilyl ester	92	.34	O5PSi3 C11H29	56	530 44-27-2
0.21	Fluoren-9-ol, 3,6-dimethoxy-9-(2-phenylethynyl)-	91	.13	O3 C23H18	42	NA

Data File: 5-13
 Curr Data Path: D:\Xcalibur\Data\GemmaH\peppers100703\
 Acquisition Date: 10/08/03 04:37:58
 Run Time (min): 29.97
 Vial: 55
 Inj Vol (µL): 2.00
 Scans: 3035
 Low Mass (m/z): 35.00
 High Mass (m/z): 550.00
 Inst Method: D:\Xcalibur\methods\pepper_PTV.meth
 Proc Method: D:\Xcalibur\methods\qualitativeID

RT: 0.00 - 35.01 SM: 7G

RT	Peak Area	Area %
6.74	246064	28.07
7.48	964	0.11
7.70	4195	0.48
8.46	247064	28.19
9.32	2964	0.34
9.58	95242	10.87
10.73	48097	5.49
12.02	32848	3.75
13.07	1918	0.22
13.35	4386	0.50
13.51	23540	2.69
13.90	11480	1.31
15.02	13358	1.52
15.19	661	0.08
15.94	1223	0.14
16.52	9106	1.04
16.89	11972	1.37
17.24	5921	0.68
17.40	1926	0.22
17.95	5584	0.64
18.66	20098	2.29

18.91	1578	0.18
19.29	3566	0.41
20.55	3525	0.40
21.73	6996	0.80
22.87	5629	0.64
23.92	6678	0.76
24.90	7876	0.90
25.45	1361	0.16
25.83	3253	0.37
26.25	11461	1.31
26.70	4427	0.51
26.88	24464	2.79
27.52	2921	0.33
27.77	4214	0.48

RT	Name	I	rob.	Formula	W	Cas #
6.89	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester, [1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	69	2.52	C32H39NO10	97	519 06-00-4
6.89	Hexadecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-(1a,2a,5a,5a,6a,8a,9a,10a)]-	64	0.09	C36H58O6	86	525 57-26-3
6.89	Tetradecanoic acid, 12-methyl-, methyl ester	46	.20	C16H32O2	56	512 9-66-8
6.89	2-Hexyldecanoic acid	40	.09	C16H32O2	56	253 54-97-6
6.89	Pregnan-20-one, 3-(acetyloxy)-5,6-epoxy-6-methyl-, cyclic 20-(1,2-ethanediy l acetal), (3a,5a,6a)-	39	.93	C26H40O5	32	567 84-25-9

T	Name	I	rob.	Formula	W	Cas #
7.40	(22R)-6a,11a,21-Trihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	93	.93	C25H34O7	46	NA
7.40	(22S)-6a,11a,21-Trihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	88	.20	C25H34O7	46	NA
7.40	3,9-Epoxypregn-16-ene-14-18-diol-20-one, 7,11-diacetoxy-3-methoxy-	79	.22	C26H36O9	92	NA
7.40	(22S)-6a,11a,21-Trihydroxy-16a,17a-propylmethylenedioxypregna-1,4-diene-3,20-dione	78	.02	C25H34O7	46	938 61-53-1
7.40	Demecolcine	74	.24	C21H25NO5	71	477- 30-5

	Name			For		Cas
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T		I	rob.	mula	W	#
8.66	9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)-	08	.42	C21 H36O4	52	184 65-99-1
8.66	Nonanoic acid, 9-(3-hexenylidenecyclopropylidene)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester, (Z,Z,Z)-	03	.18	C21 H36O4	52	552 68-58-1
8.66	9,12-Octadecadienoic acid, methyl ester, (E,E)-	02	.98	C19 H34O2	94	256 6-97-4
8.66	Cyclooctenone, dimer	98	.20	C16 H24O2	48	612 19-51-0
8.66	9,11-Octadecadienoic acid, methyl ester, (E,E)-	96	.88	C19 H34O2	94	130 38-47-6

T	Name	I	rob.	Formula	W	Cas #
8.91	Dodecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-6,11-dioxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1aR-(1aà,2à,5á,5aá,8aà,9à,10aà)]-	44	5.68	C32H 48O6	28	775 08-68-0
8.91	Hexadecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-(1aà,2à,5á,5aá,6á,8aà,9à,10aà)]-	43	5.07	C36H 58O6	86	525 57-26-3
8.91	4'-Apo-á,psi.-carotenoic acid	43	5.07	C35H 46O2	98	246 8-88-4
8.91	Hexadecanoic acid, N,N-bis[(methylcarboxy)ethyl-2-(2-butoxyethoxy)]-	18	.59	C36H 69NO9	59	NA
8.91	Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester	13	.70	C39H 76O5	24	504- 40-5

T	Name	I	rob.	Formul a	W	Cas #
6.88	Stigmast-5-en-3-ol, oleate	30	3.79	$C_{47}H_{78}O_2$	78	NA
6.88	Stigmastan-3,5-dien	21	7.27	$C_{29}H_{48}$	96	NA
6.88	Stigmastan-3-ol, 5-chloro-, acetate, (3 β ,5 α)-	16	3.92	$C_{31}H_{53}ClO_2$	92	557 24-19-1
6.88	Sitosterol acetate	13	2.30	$C_{31}H_{52}O_2$	56	NA
6.88	α -Sitosterol acetate	02	.43	$C_{31}H_{52}O_2$	56	915- 05-9