Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Time: Nov 17 11:00:10 2014
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration

Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
Internal Standards					
1) 1,4-Dichlorobenzene-d4	5.081	152	429441	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1930251	20.00 ug/mL	0.00
5) Acenaphthene-d10	8.216	164	1053917	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.681	188	1614974	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	1022310	20.00 ug/mL	0.00
12) Perylene-d12	16.804	264	667430	20.00 ug/mL	0.01
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	574698	8.87 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery = ~~70.96%~~		
Target Compounds					Qvalue
2) MCHM	5.540	55	479363m	11.04 ug/mL	
4) PPH	6.857	94	166790	3.53 ug/mL	95
6) 1,4-CHDM	0.000		0	N.D. d	
8) DM-1,4-CHDC	0.000		0	N.D. d	
9) di-PPH	8.540	59	298561m	7.52 ug/mL	

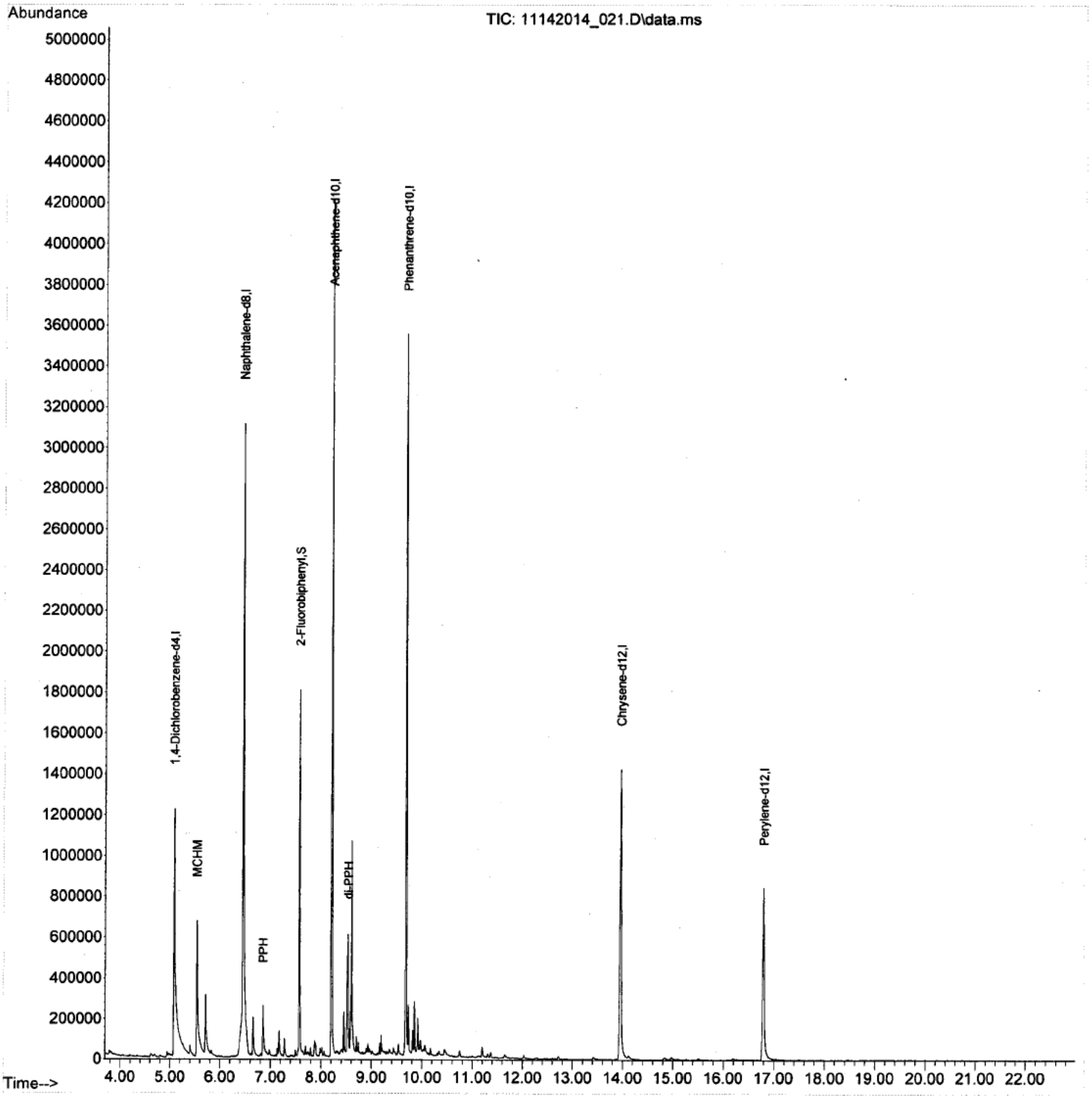
see Analyst Narrative, Surrogate Recovery [redacted] 1/7/15

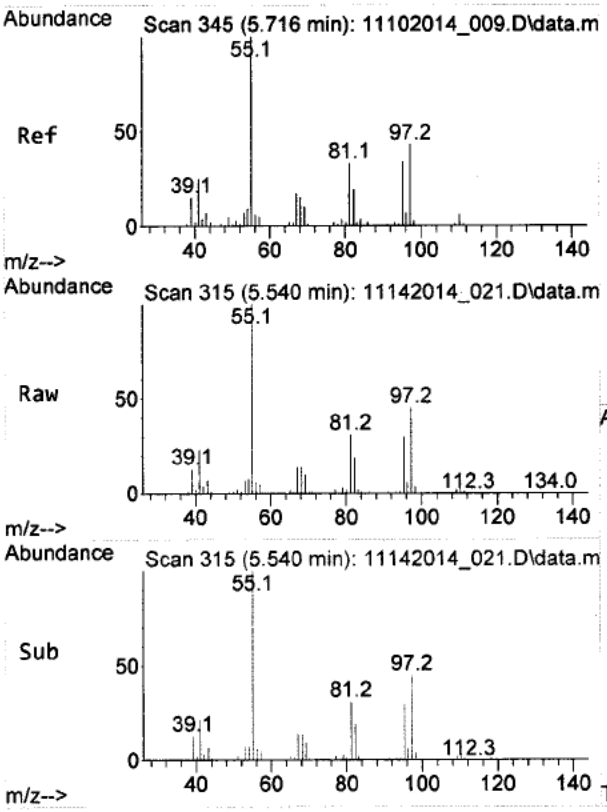
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Time: Nov 17 11:00:10 2014
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration

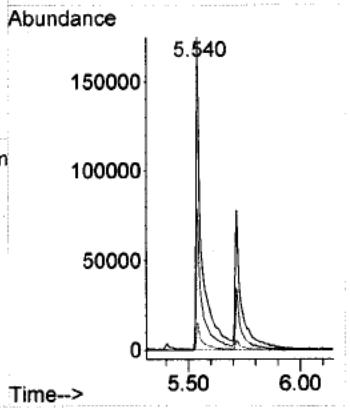


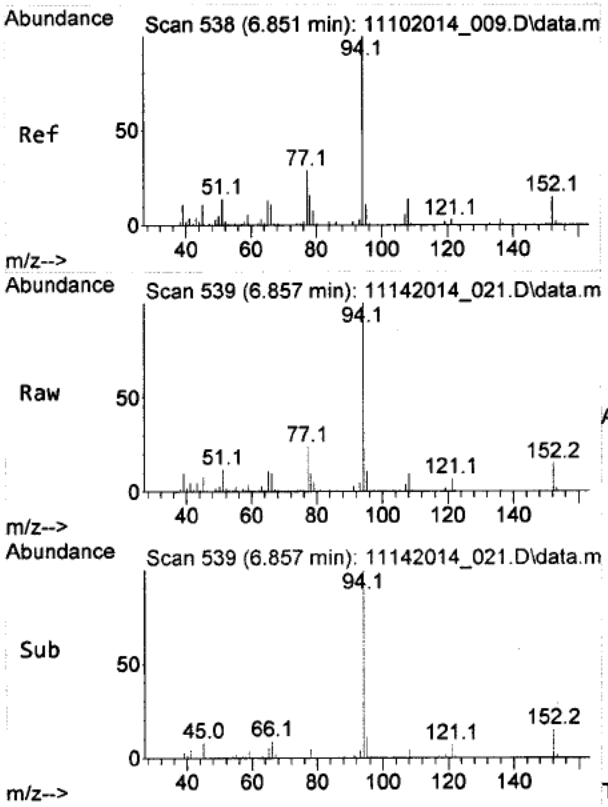


#2
MCHM
Concen: 11.04 ug/mL m
RT: 5.540 min Scan# 315
Delta R.T. -0.176 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 55 Resp: 479363

Ion	Ratio	Lower	Upper
55	100		
97	12.1	34.6	51.8#
110	1.8	4.8	7.2#

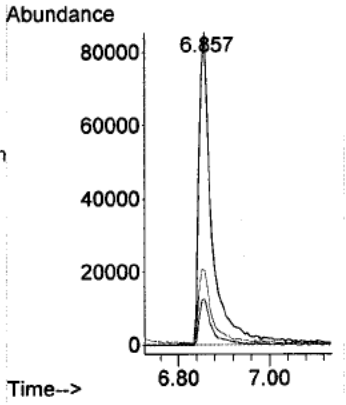


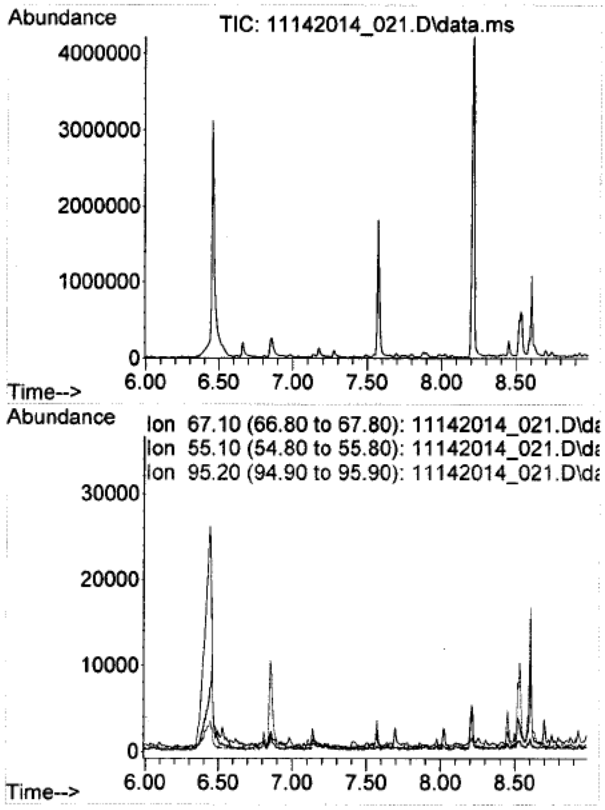


#4
PPH
Concen: 3.53 ug/mL
RT: 6.857 min Scan# 539
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 94 Resp: 166790

Ion	Ratio	Lower	Upper
94	100		
152	14.6	13.4	20.0
77	23.8	21.2	31.8



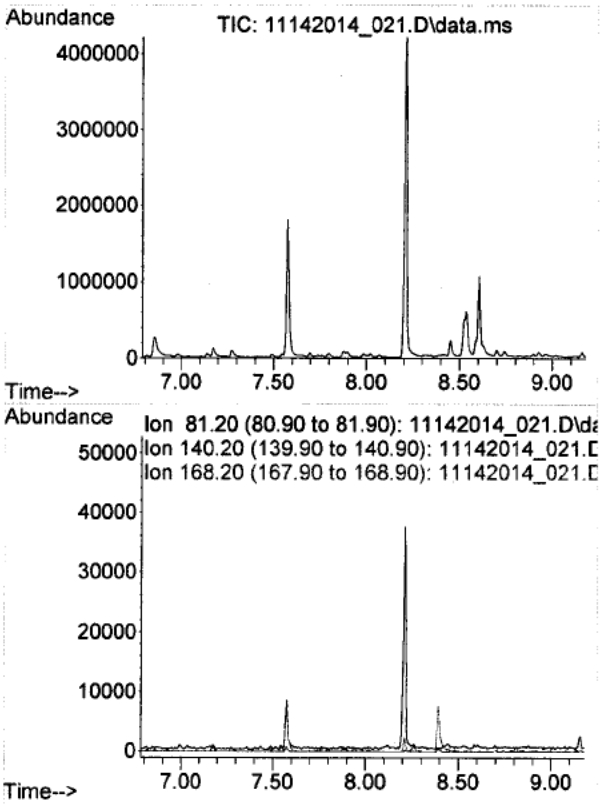


#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8

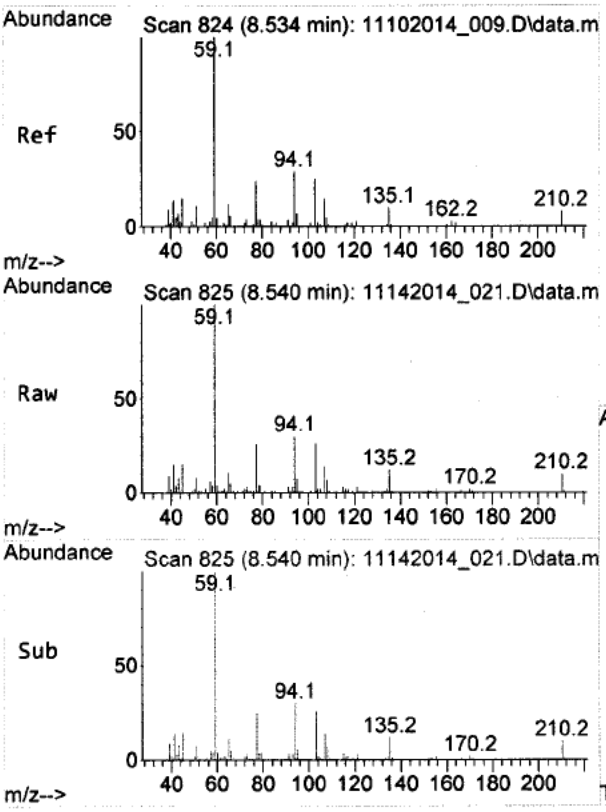


#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 81

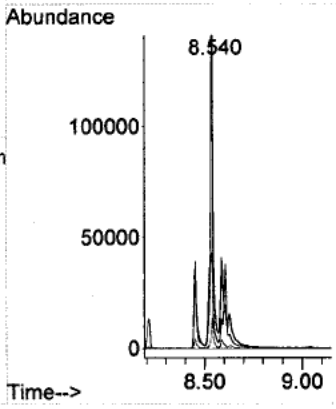
Sig	Exp Ratio
81	100
140	61.8
168	17.7



#9
di-PPH
Concen: 7.52 ug/mL m
RT: 8.540 min Scan# 825
Delta R.T. -0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 59 Resp: 298561

Ion	Ratio	Lower	Upper
59	100		
94	24.7	23.0	34.6
210	4.6	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Time: Dec 01 12:05:57 2014
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
Internal Standards					
1) 1,4-Dichlorobenzene-d4	5.081	150	745506	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1930251	20.00 ug/mL	0.00
24) Acenaphthene-d10	8.216	164	1053917	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.681	188	1614974	20.00 ug/mL	0.00
49) Chrysene-d12	13.963	240	1024320	20.00 ug/mL	-0.01
58) Perylene-d12	16.804	264	669761	20.00 ug/mL	0.00
Target Compounds					Qvalue
2) Bis(2-chloroethyl) ether	0.000		0	N.D. d	
3) n-Decane	4.975	57	4692	0.10 ug/mL#	51
4) 1,3-Dichlorobenzene	0.000		0	N.D.	
5) 1,4-Dichlorobenzene	0.000		0	N.D.	
6) 1,2-Dichlorobenzene	0.000		0	N.D.	
7) Benzyl Alcohol	0.000		0	N.D. d	
8) Bis(2-chloroisopropyl)...	0.000		0	N.D. d	
9) Hexachloroethane	0.000		0	N.D. d	
10) N-Nitrosodi-N-propylamine	0.000		0	N.D. d	
11) Nitrobenzene	0.000		0	N.D. d	
12) 4-Methylcyclohexanecar...	6.440	55	89531m	6.70 ug/mL	
14) n-Dodecane	6.528	57	8609	0.16 ug/mL#	91
15) Isophorone	0.000		0	N.D. d	
16) Bis(2-chloroethoxy) me...	0.000		0	N.D. d	
17) 1,2,4-Trichlorobenzene	0.000		0	N.D.	
18) Napthalene	6.475	128	62138	0.46 ug/mL	95
19) Hexachlorobutadiene	0.000		0	N.D.	
20) 2-Methylnapthalene	7.175	142	43194	0.50 ug/mL	99
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	0.000		0	N.D. d	
23) n-Tetradecane	7.698	57	9591	0.17 ug/mL	95
25) Dimethly Phthalate	0.000		0	N.D. d	
26) Acenaphthylene	0.000		0	N.D. d	
27) 2,6-Dinitrotoluene	0.000		0	N.D. d	
28) Acenaphthene	0.000		0	N.D. d	
29) Dibenzofuran	8.392	168	10159	0.09 ug/mL	92
30) 2,4-Dinitrotoluene	0.000		0	N.D. d	
31) n-Hexadecane	8.698	57	8884	0.15 ug/mL#	99
32) Fluorene	0.000		0	N.D. d	
33) Diethyl Phthalate	0.000		0	N.D. d	
34) 4-Chlorophenylphenyl E...	0.000		0	N.D. d	
35) N-Nitrosodiphenylamine	0.000		0	N.D. d	
36) Azobenzene	0.000		0	N.D. d	
38) 4-Bromophenylphenyl Ether	0.000		0	N.D.	
39) Hexachlorobenzene	0.000		0	N.D.	
40) n-Octadecane	9.645	57	7988	0.14 ug/mL#	97
41) Phenanthrene	9.698	178	26217	0.21 ug/mL	97
42) Anthracene	9.745	178	1911	0.02 ug/mL#	63
43) Carbazole	0.000		0	N.D. d	
44) Dibutyl Phthalate	0.000		0	N.D. d	
45) n-Eicosane	10.751	57	6718	0.12 ug/mL#	78

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Time: Dec 01 12:05:57 2014
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

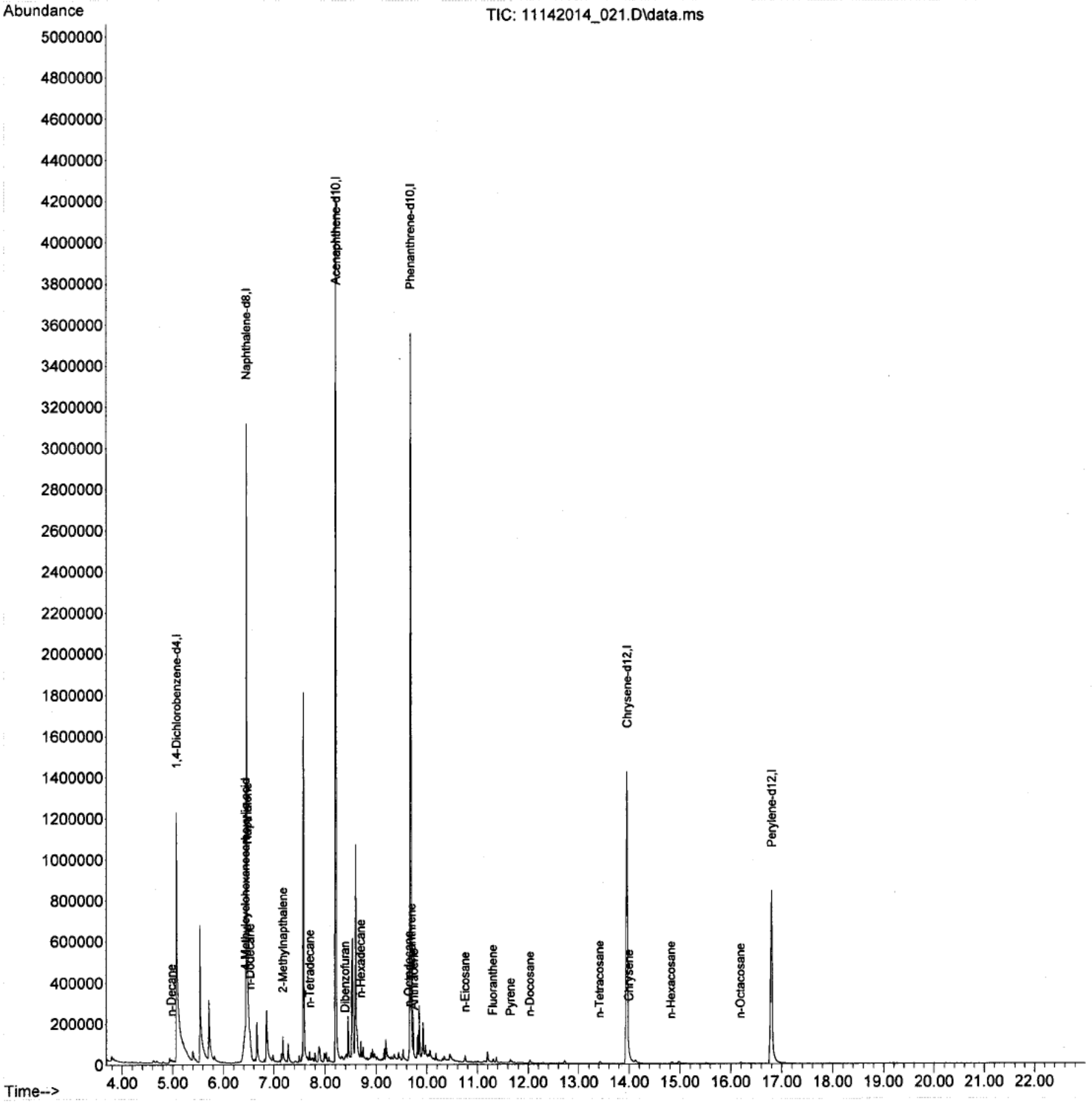
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	11.304	202	11904	0.09 ug/mL#	88
47) Pyrene	11.651	202	11417	0.09 ug/mL	98
48) n-Docosane	12.033	57	4986	0.10 ug/mL#	84
50) Benzyl Butyl Phthalate	0.000		0	N.D. d	
51) n-Tetracosane	13.416	57	5449	0.09 ug/mL#	95
52) n-Hexacosane	14.821	57	3920	0.08 ug/mL#	73
53) n-Octacosane	16.192	57	2103	0.05 ug/mL#	90
54) Benz[a]anthracene	0.000		0	N.D. d	
55) Chrysene	13.992	228	5895	0.07 ug/mL#	89
56) Bis(2-ethylhexyl) Phth...	0.000		0	N.D. d	
57) Di-n-octyl Phthalate	0.000		0	N.D.	
59) Benzo[b]fluoranthene	0.000		0	N.D. d	
60) Benzo(k)fluoranthene	0.000		0	N.D. d	
61) Benz[a]pyrene	0.000		0	N.D. d	
62) Indo[1,2,3-cd]pyrene	0.000		0	N.D.	
63) Dibenz[a,h]anthracene	0.000		0	N.D.	
64) Benzo[g,h,i]perylene	0.000		0	N.D. d	

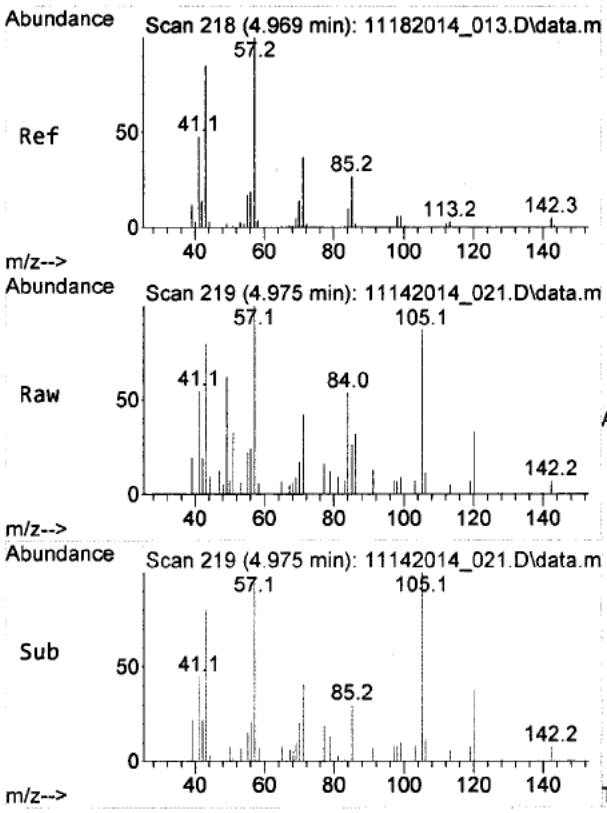
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Time: Dec 01 12:05:57 2014
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

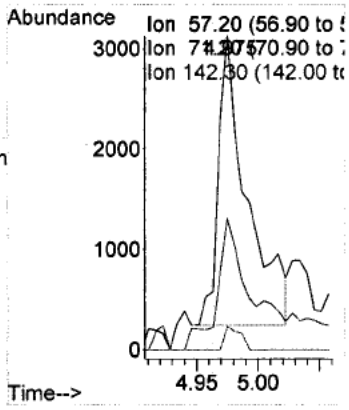


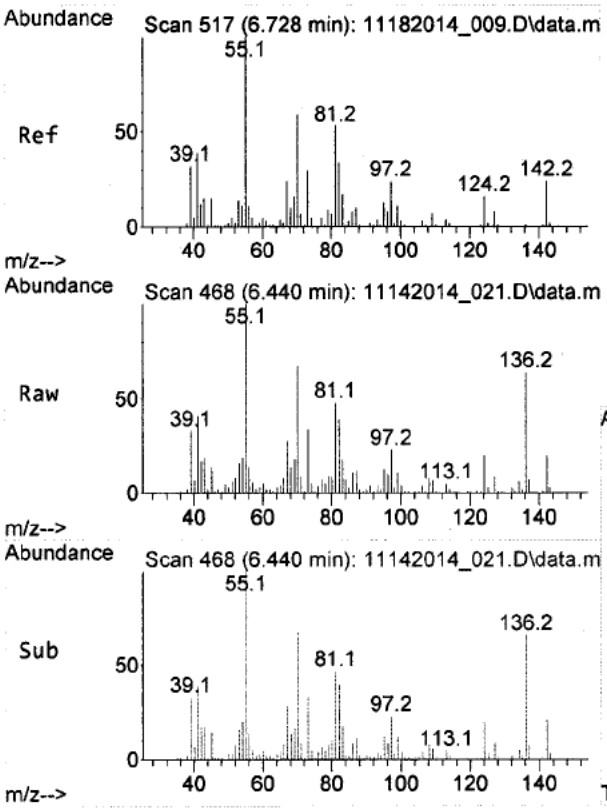


#3
n-Decane
Concen: 0.10 ug/mL
RT: 4.975 min Scan# 219
Delta R.T. 0.006 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 4692

Ion	Ratio	Lower	Upper
57	100		
71	69.2	29.4	44.2#
142	4.4	3.7	5.5

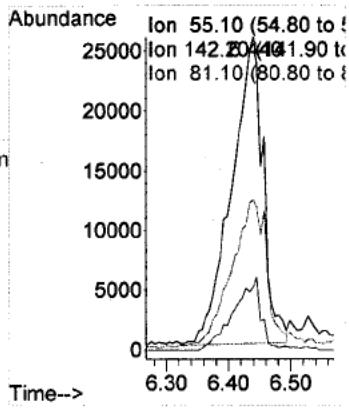


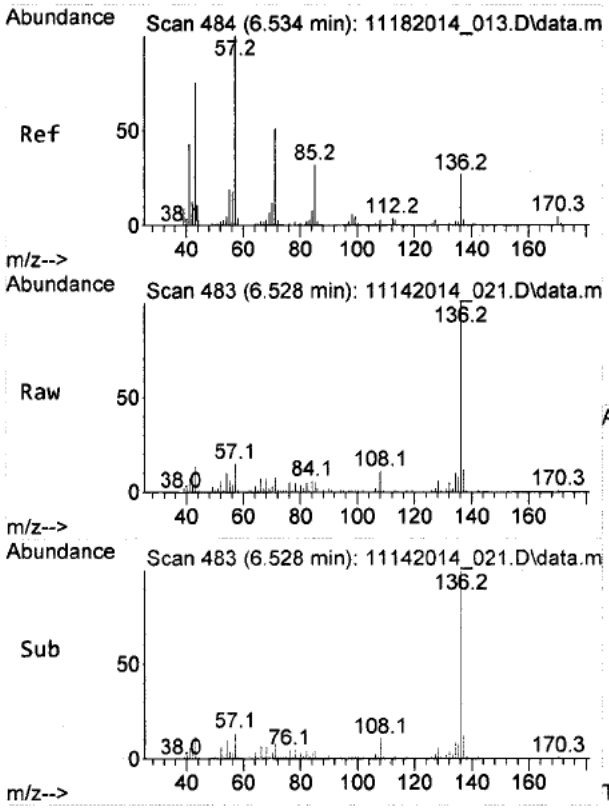


#12
4-Methylcyclohexanecarboxylic acid
Concen: 6.70 ug/mL m
RT: 6.440 min Scan# 468
Delta R.T. -0.288 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 55 Resp: 89531

Ion	Ratio	Lower	Upper
55	100		
142	0.4	19.1	28.7#
81	1.1	42.3	63.5#

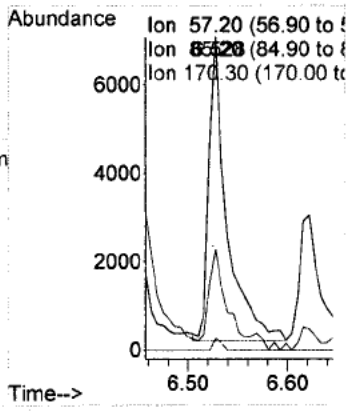


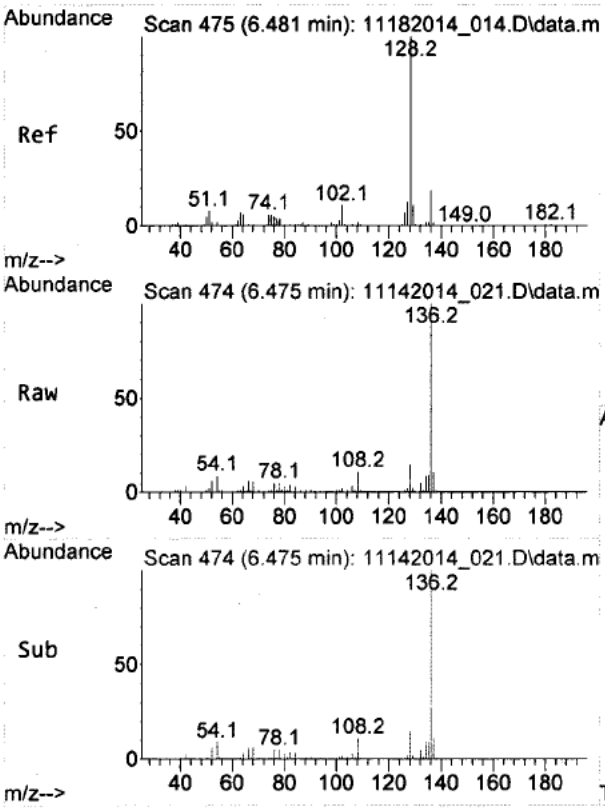


#14
n-Dodecane
Concen: 0.16 ug/mL
RT: 6.528 min Scan# 483
Delta R.T. -0.007 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 8609

Ion	Ratio	Lower	Upper
57	100		
85	36.3	25.3	37.9
170	1.8	4.2	6.2#

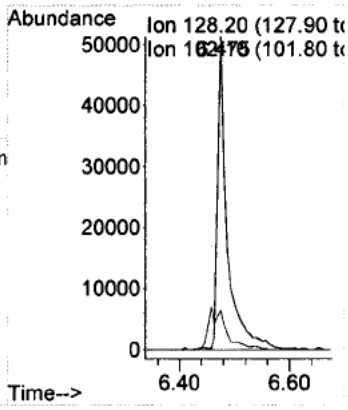


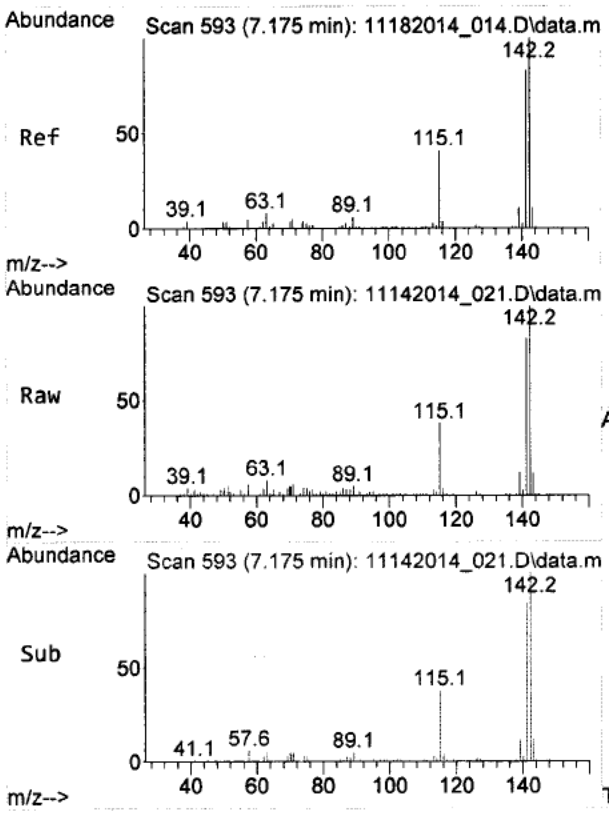


#18
Napthalene
Concen: 0.46 ug/mL
RT: 6.475 min Scan# 474
Delta R.T. -0.006 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:128 Resp: 62138

Ion	Ratio	Lower	Upper
128	100		
102	9.3	9.0	13.4

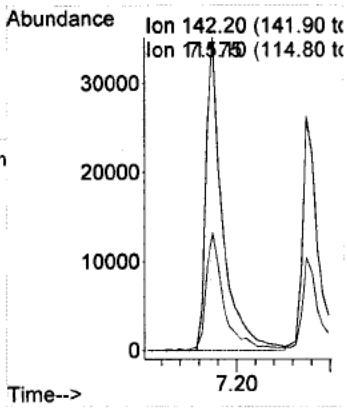


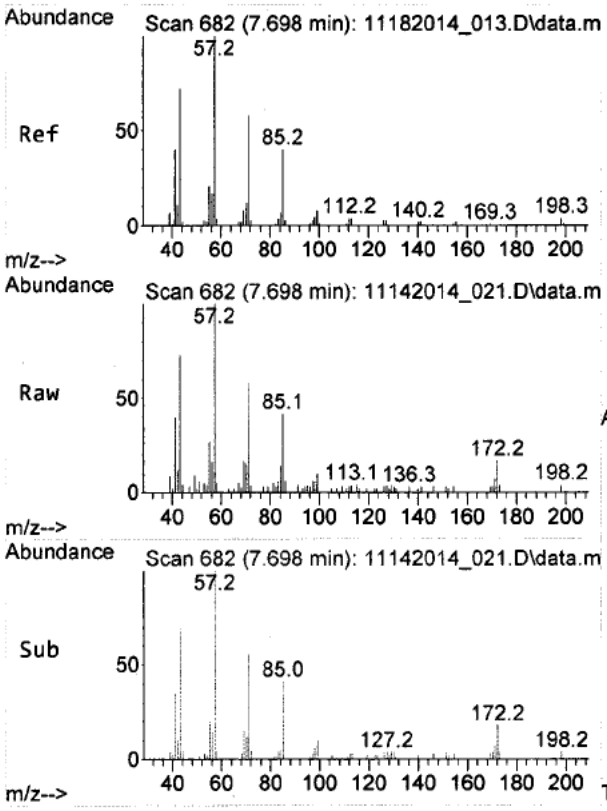


#20
2-Methylnapthalene
Concen: 0.50 ug/mL
RT: 7.175 min Scan# 593
Delta R.T. -0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:142 Resp: 43194

Ion	Ratio	Lower	Upper
142	100		
115	40.8	33.0	49.4

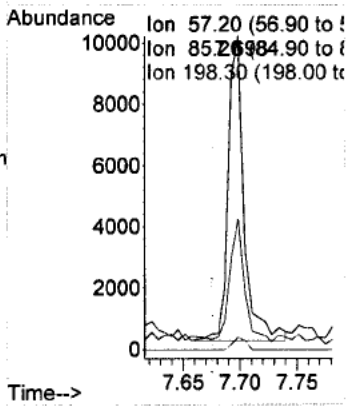


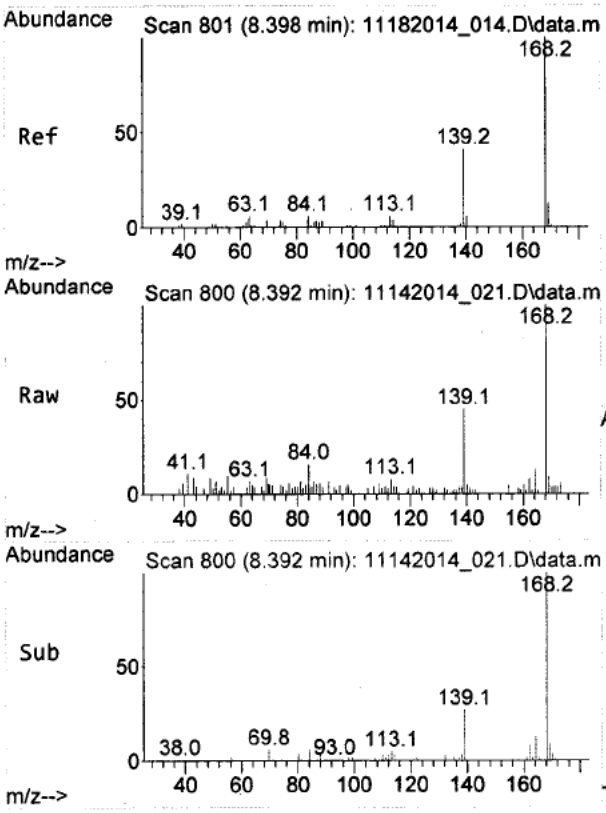


#23
n-Tetradecane
Concen: 0.17 ug/mL
RT: 7.698 min Scan# 682
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 9591

Ion	Ratio	Lower	Upper
57	100		
85	42.9	31.6	47.4
198	3.2	3.1	4.7

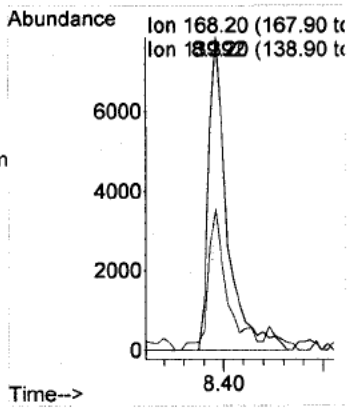


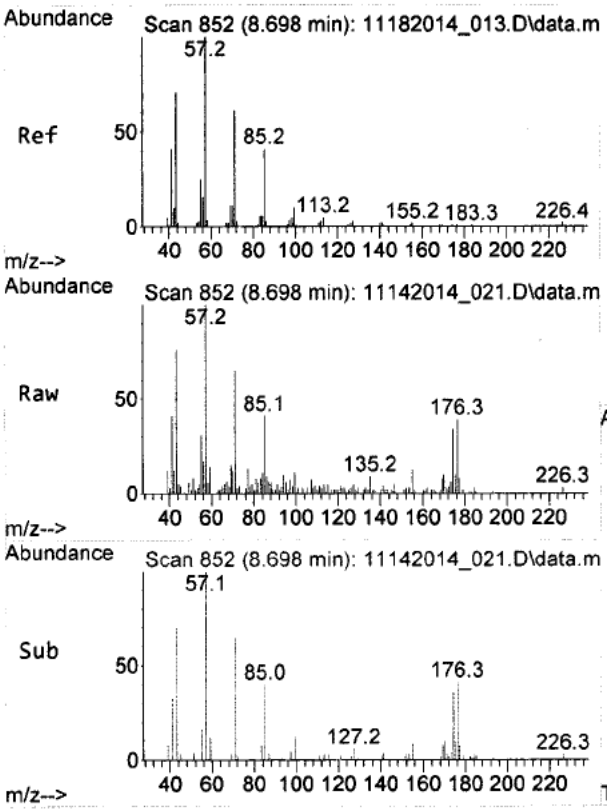


#29
Dibenzofuran
Concen: 0.09 ug/mL
RT: 8.392 min Scan# 800
Delta R.T. -0.006 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:168 Resp: 10159

Ion	Ratio	Lower	Upper
168	100		
139	45.9	32.9	49.3

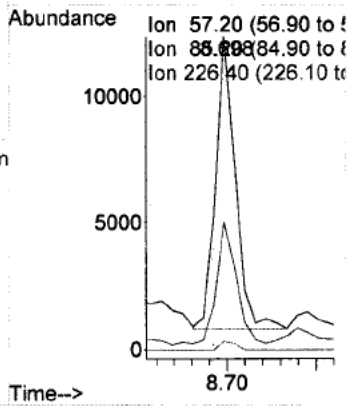


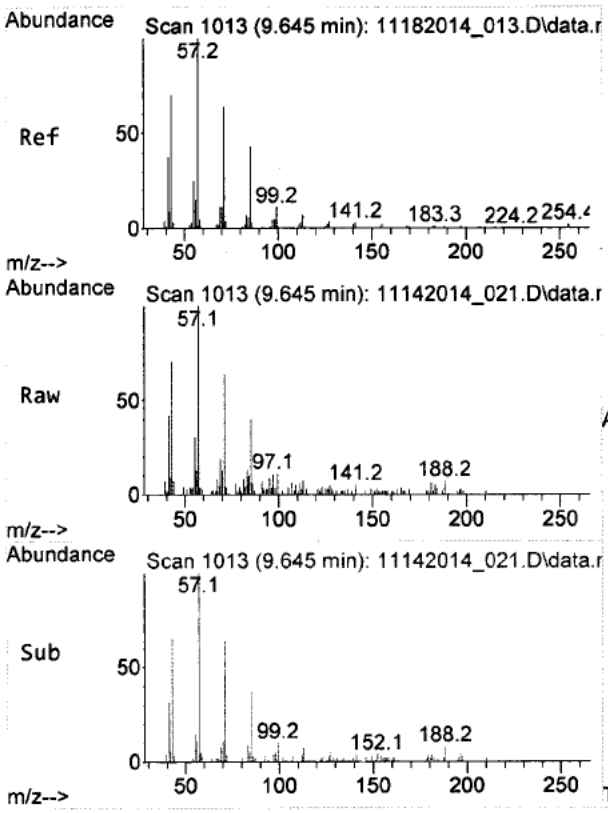


#31
n-Hexadecane
Concen: 0.15 ug/mL
RT: 8.698 min Scan# 852
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 8884

Ion	Ratio	Lower	Upper
57	100		
85	43.5	35.1	52.7
226	2.3	3.1	4.7#

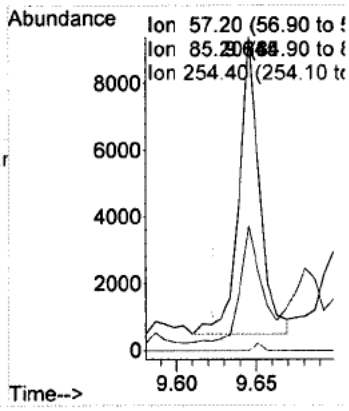


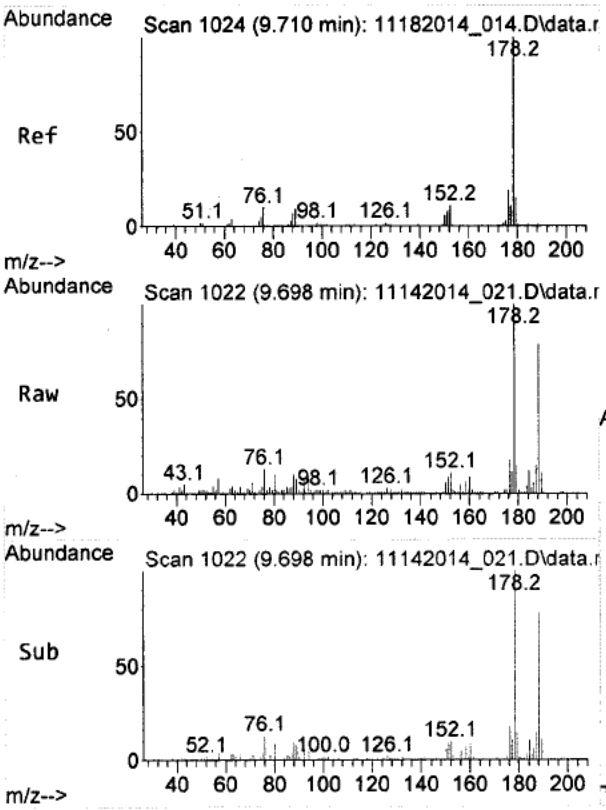


#40
n-Octadecane
Concen: 0.14 ug/mL
RT: 9.645 min Scan# 1013
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 7988

Ion	Ratio	Lower	Upper
57	100		
85	41.4	34.5	51.7
254	1.0	1.4	2.2#

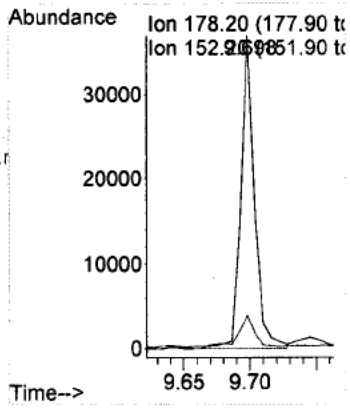


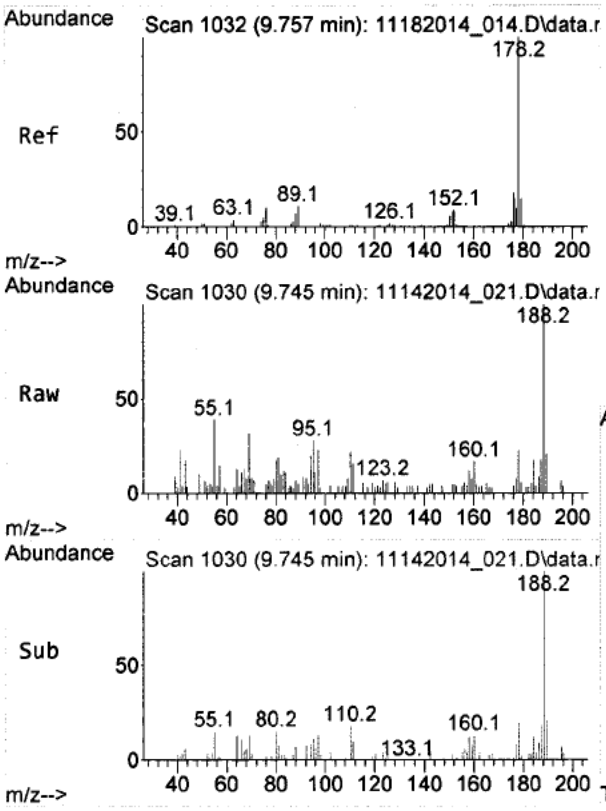


#41
Phenanthrene
Concen: 0.21 ug/mL
RT: 9.698 min Scan# 1022
Delta R.T. -0.012 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:178 Resp: 26217

Ion	Ratio	Lower	Upper
178	100		
152	11.8	8.5	12.7

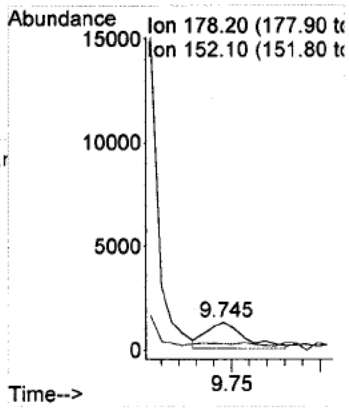


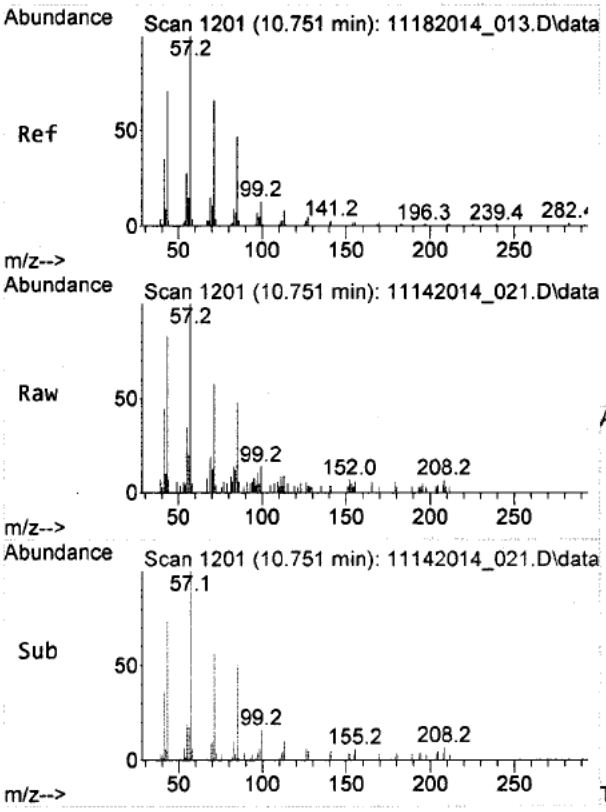


#42
Anthracene
Concen: 0.02 ug/mL
RT: 9.745 min Scan# 1030
Delta R.T. -0.012 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:178 Resp: 1911

Ion	Ratio	Lower	Upper
178	100		
152	22.4	7.2	10.8#

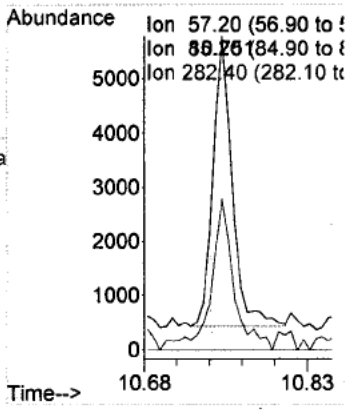


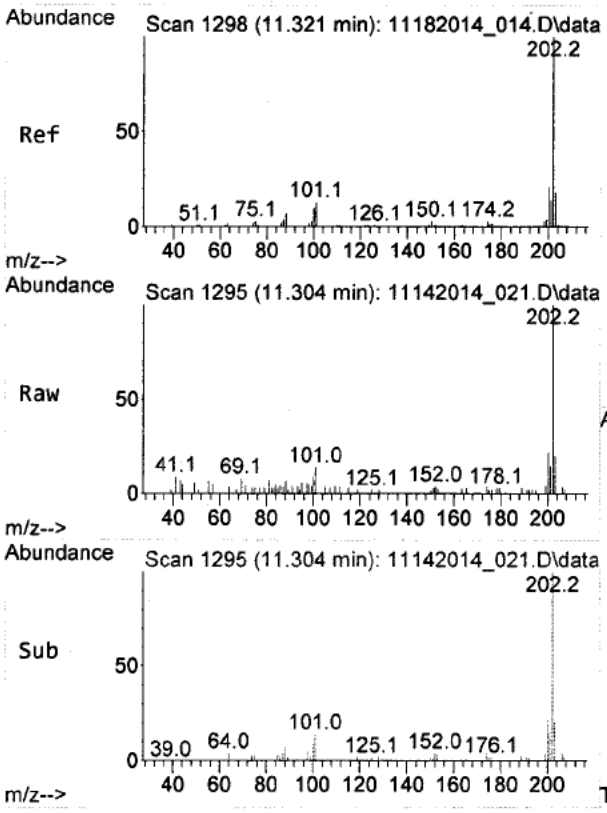


#45
n-Eicosane
Concen: 0.12 ug/mL
RT: 10.751 min Scan# 1201
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 6718

Ion	Ratio	Lower	Upper
57	100		
85	62.3	37.8	56.8#
282	0.0	1.4	2.2#

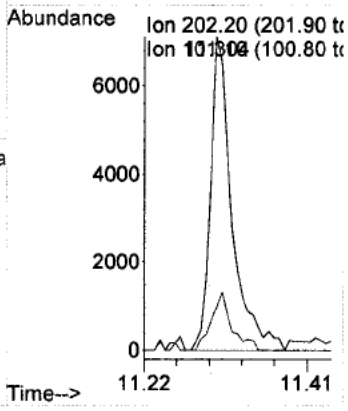


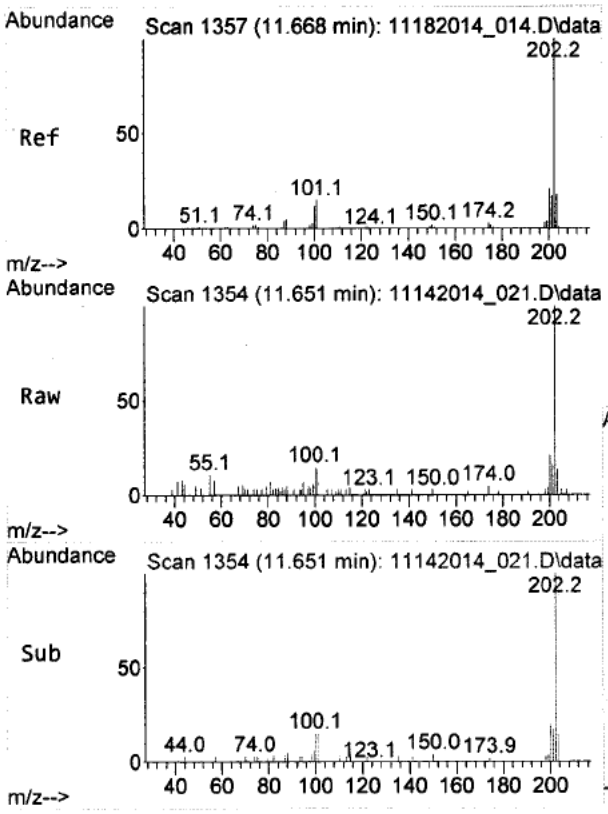


#46
Fluoranthene
Concen: 0.09 ug/mL
RT: 11.304 min Scan# 1295
Delta R.T. -0.017 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:202 Resp: 11904

Ion	Ratio	Lower	Upper
202	100		
101	17.4	10.1	15.1#

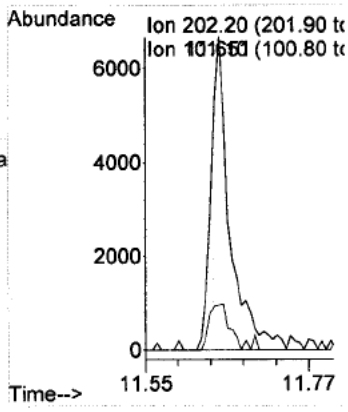


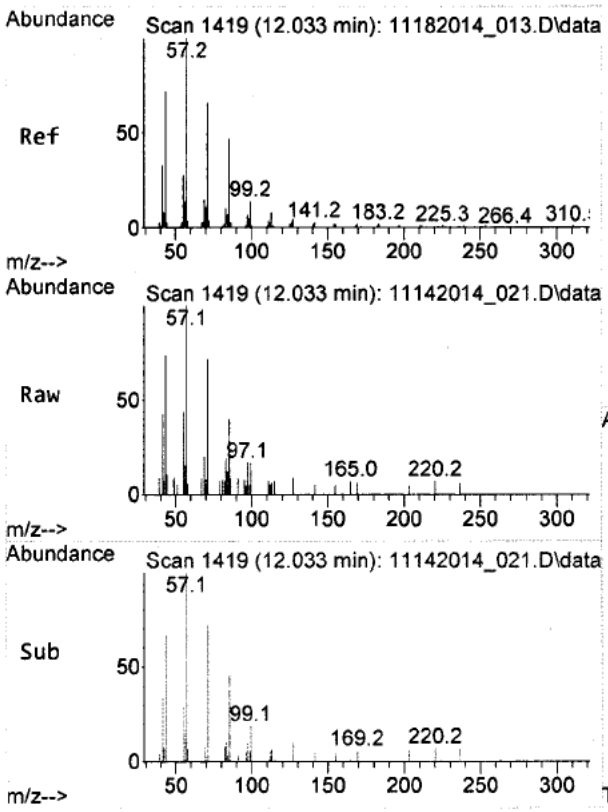


#47
Pyrene
Concen: 0.09 ug/mL
RT: 11.651 min Scan# 1354
Delta R.T. -0.017 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:202 Resp: 11417

Ion	Ratio	Lower	Upper
202	100		
101	15.6	11.7	17.5

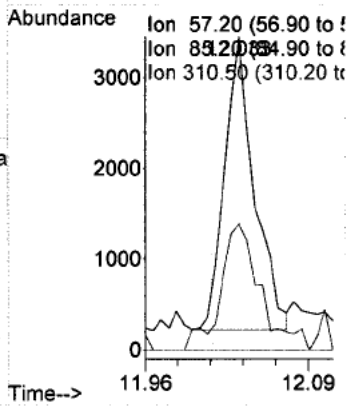


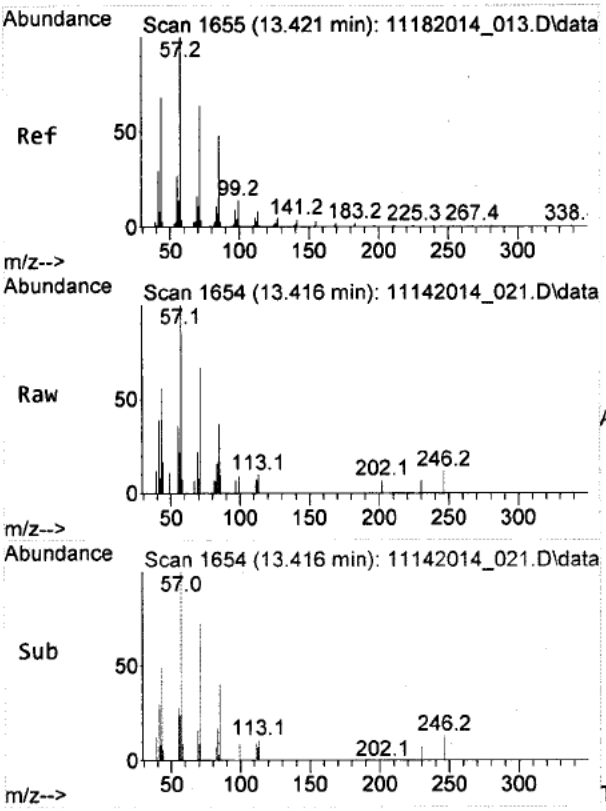


#48
n-Docosane
Concen: 0.10 ug/mL
RT: 12.033 min Scan# 1419
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 4986

Ion	Ratio	Lower	Upper
57	100		
85	57.5	37.5	56.3#
311	0.0	0.9	1.3#

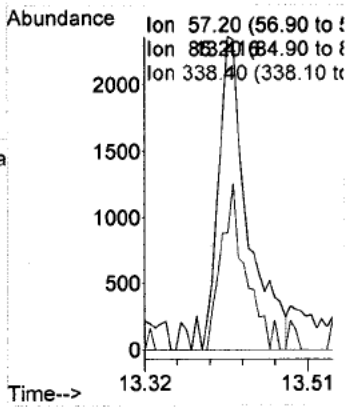


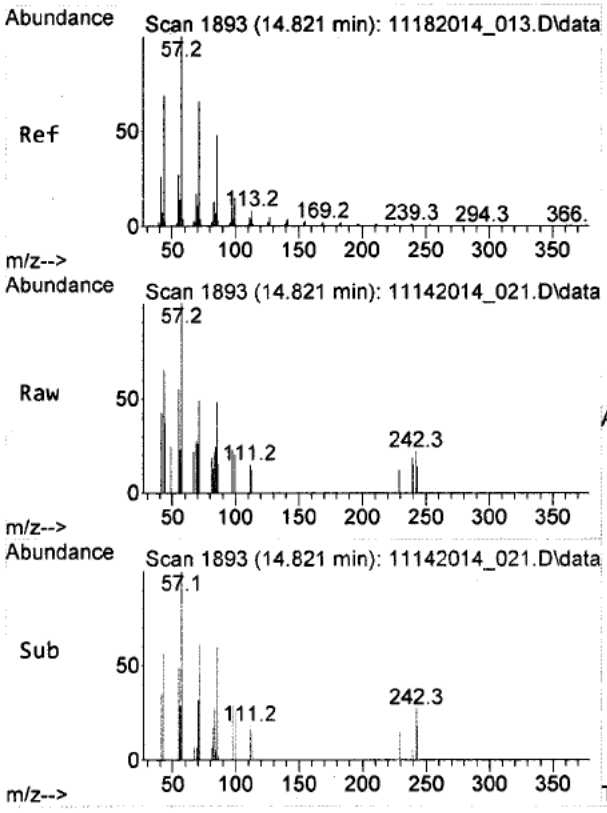


#51
n-Tetracosane
Concen: 0.09 ug/mL
RT: 13.416 min Scan# 1654
Delta R.T. -0.005 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 5449

Ion	Ratio	Lower	Upper
57	100		
85	44.4	38.5	57.7
338	0.0	0.8	1.2#

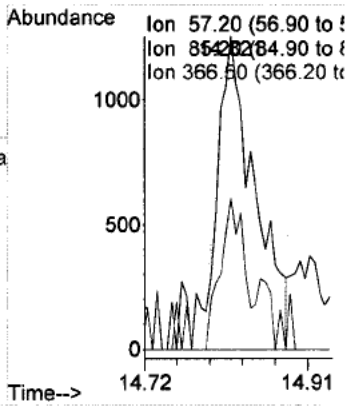


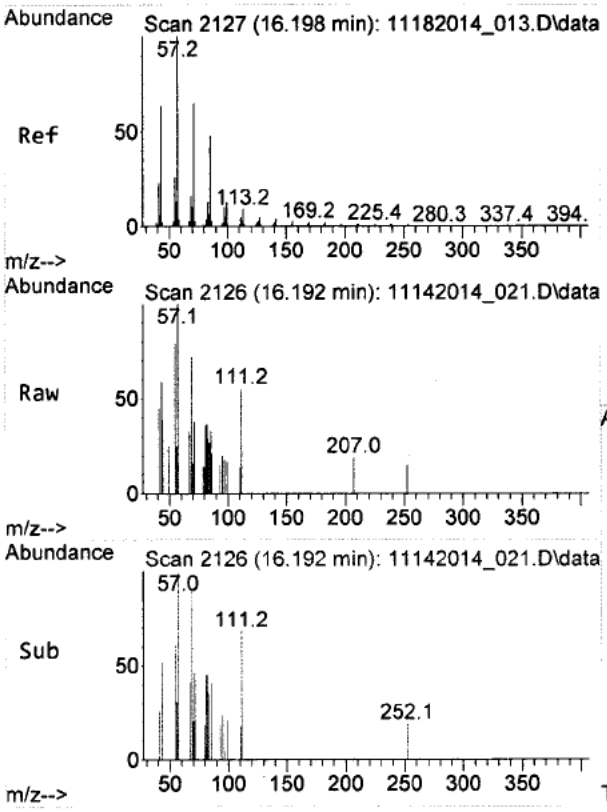


#52
n-Hexacosane
Concen: 0.08 ug/mL
RT: 14.821 min Scan# 1893
Delta R.T. 0.000 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 3920

Ion	Ratio	Lower	Upper
57	100		
85	29.8	38.6	58.0#
367	0.0	0.6	1.0#

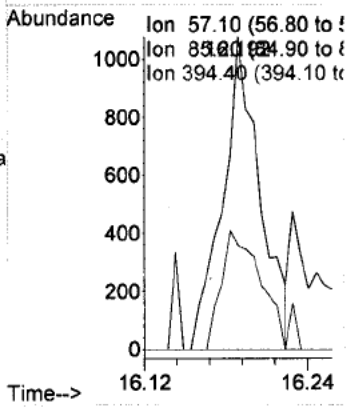


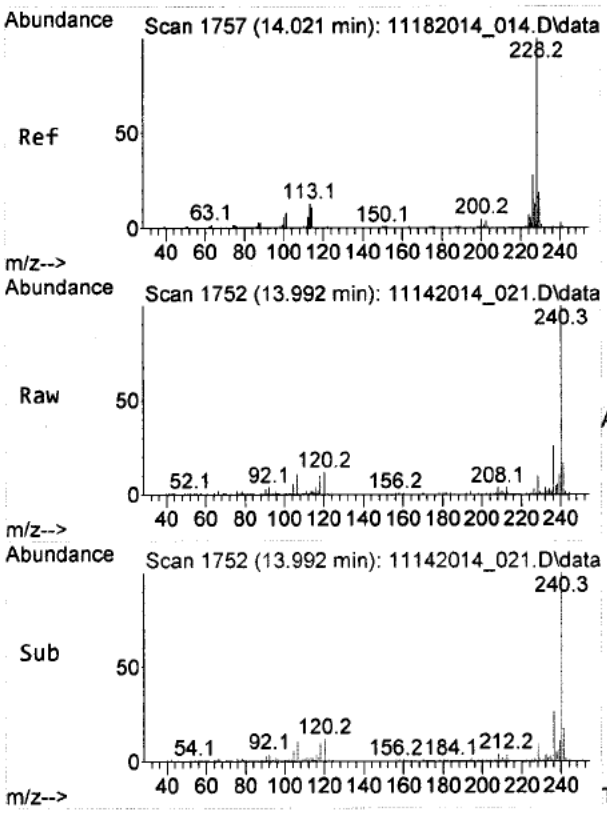


#53
n-Octacosane
Concen: 0.05 ug/mL
RT: 16.192 min Scan# 2126
Delta R.T. -0.006 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion: 57 Resp: 2103

Ion	Ratio	Lower	Upper
57	100		
85	42.5	39.5	59.3
394	0.0	0.3	0.5#

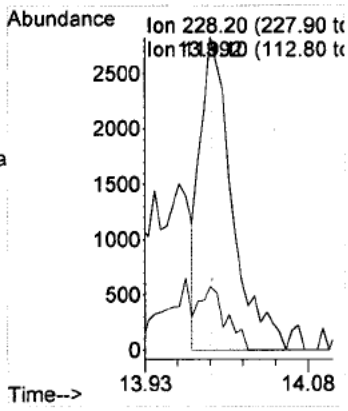




#55
Chrysene
Concen: 0.07 ug/mL
RT: 13.992 min Scan# 1752
Delta R.T. -0.029 min
Lab File: 11142014_021.D
Acq: 14 Nov 2014 07:39 pm

Tgt Ion:228 Resp: 5895

Ion	Ratio	Lower	Upper
228	100		
113	17.0	10.2	15.4#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.01 Max Peaks: 30
Stop Thrs : 0.02 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 0

Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Title : RP1616-MCHM Compounds

Signal : TIC: 11142014_021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.793	13	18	55	rVB3	28714	128354	2.52%	0.389%
2	5.081	227	237	287	rVV	1217563	3191721	62.58%	9.683%
3	5.404	287	292	309	rVV4	53906	131421	2.58%	0.399%
4	5.540	309	315	341	rVV	667780	1261323	24.73%	3.827%
5	5.716	341	345	361	rVV	303449	530409	10.40%	1.609%
6	6.457	445	471	495	rBV	3108899	5100040	100.00%	15.473%
7	6.663	495	506	525	rVV	194414	326547	6.40%	0.991%
8	6.857	525	539	557	rVV	252763	536230	10.51%	1.627%
9	7.175	575	593	603	rVV2	127747	234025	4.59%	0.710%
10	7.275	603	610	627	rVV	91999	130875	2.57%	0.397%
11	7.575	653	661	679	rVV	1802980	1833810	35.96%	5.564%
12	7.881	707	713	725	rVV2	77688	170210	3.34%	0.516%
13	8.216	761	770	783	rVV	4205319	4641177	91.00%	14.081%
14	8.451	795	810	815	rVV2	225214	371151	7.28%	1.126%
15	8.534	815	824	831	rVV2	604546	1088222	21.34%	3.302%
16	8.604	831	836	849	rVV2	1063502	1302889	25.55%	3.953%
17	8.739	855	859	869	rVV	76052	158737	3.11%	0.482%
18	8.928	877	891	895	rVV4	66577	186723	3.66%	0.566%
19	9.192	933	936	953	rVV2	110985	257964	5.06%	0.783%
20	9.534	987	994	1007	rVV	65626	157222	3.08%	0.477%
21	9.681	1007	1019	1025	rVV2	3549544	4472967	87.70%	13.571%
22	9.728	1025	1027	1037	rVV2	259355	321943	6.31%	0.977%
23	9.851	1037	1048	1053	rVV	278119	485055	9.51%	1.472%
24	9.922	1053	1060	1065	rVV2	195208	333765	6.54%	1.013%
25	9.975	1065	1069	1075	rVV	83908	176257	3.46%	0.535%
26	10.057	1075	1083	1099	rVV4	61143	249613	4.89%	0.757%
27	10.175	1099	1103	1121	rVV	46575	124659	2.44%	0.378%
28	10.451	1141	1150	1171	rVV7	40230	181711	3.56%	0.551%
29	13.963	1725	1747	1767	rBV	1424271	2949618	57.84%	8.949%
30	16.804	2215	2230	2263	rBV	843057	1926294	37.77%	5.844%

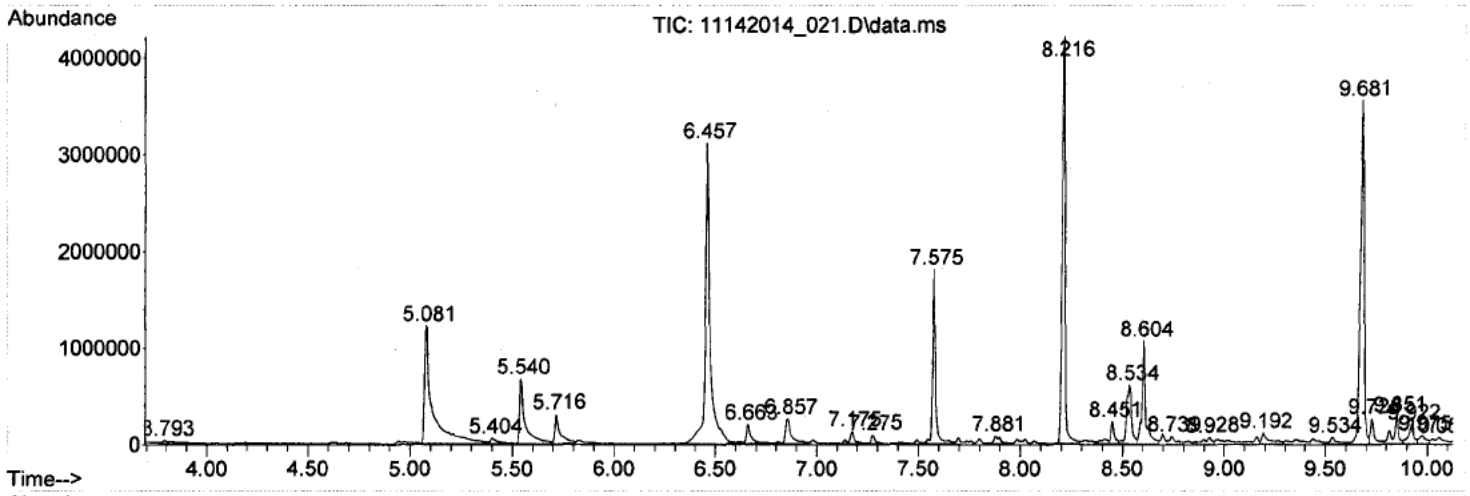
Sum of corrected areas: 32960932

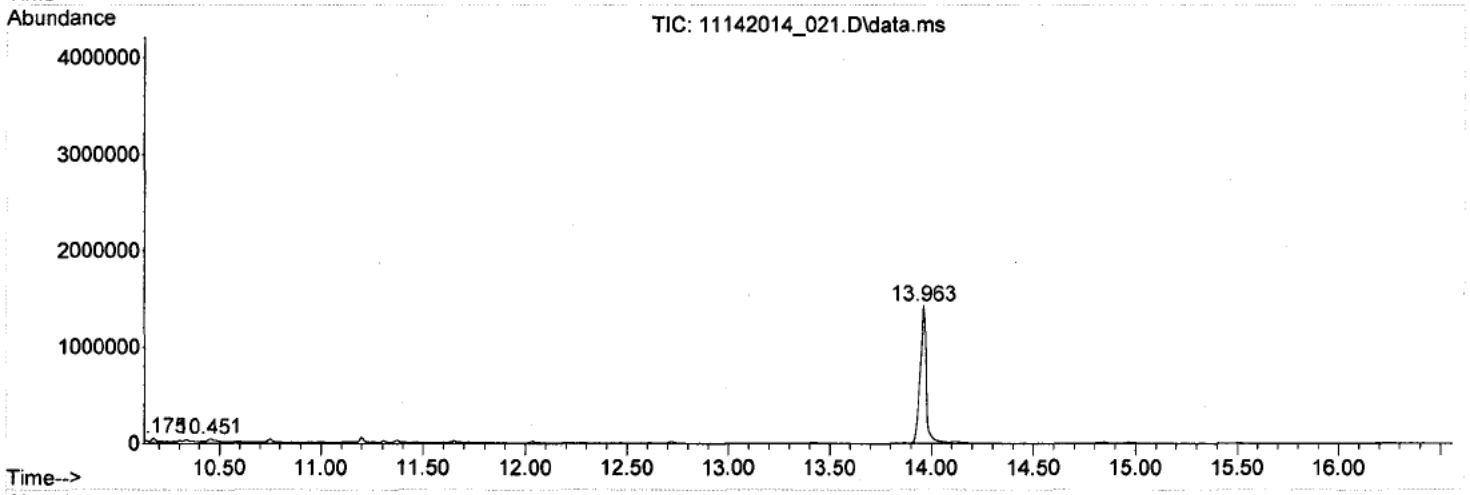
LSC Report - Integrated Chromatogram

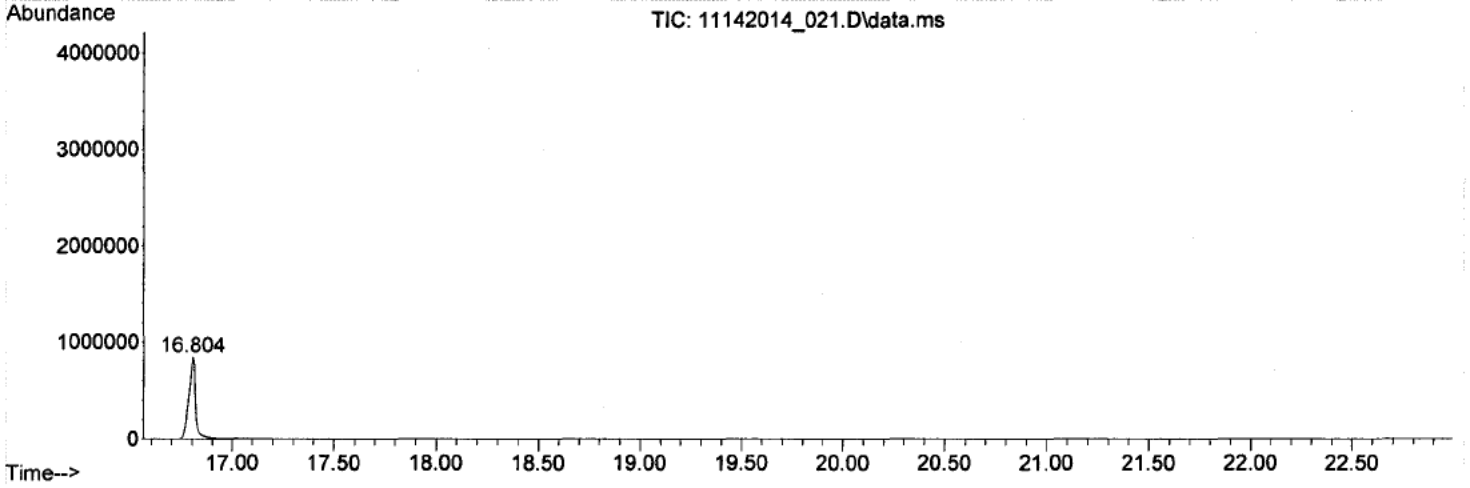
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P







Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

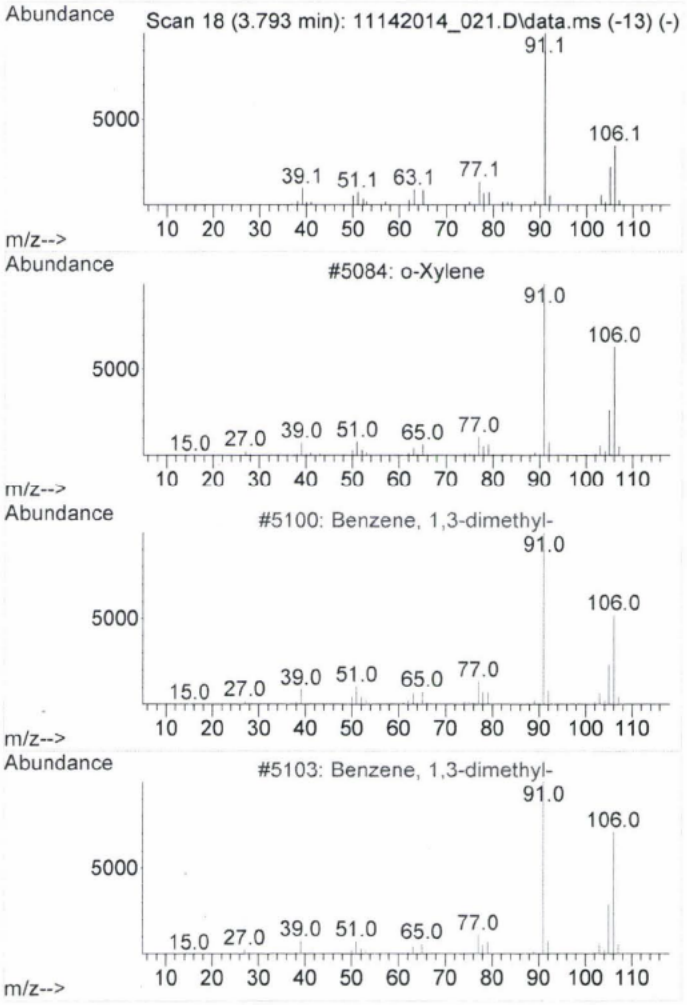
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

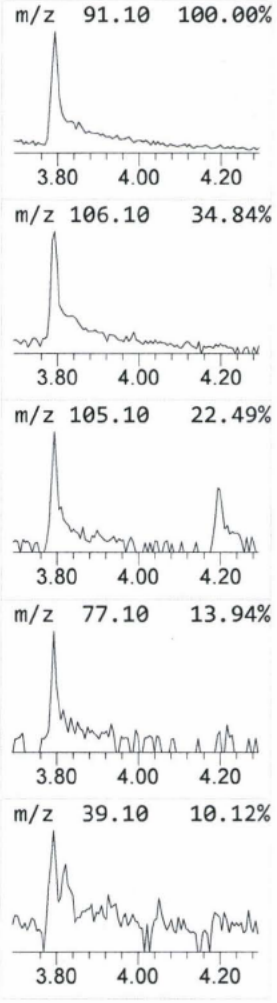
****

Peak Number 1 o-Xylene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.793	0.80 ug/mL	128354	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Xylene	106	C8H10	000095-47-6	90
2	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
4	p-Xylene	106	C8H10	000106-42-3	87
5	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87





Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

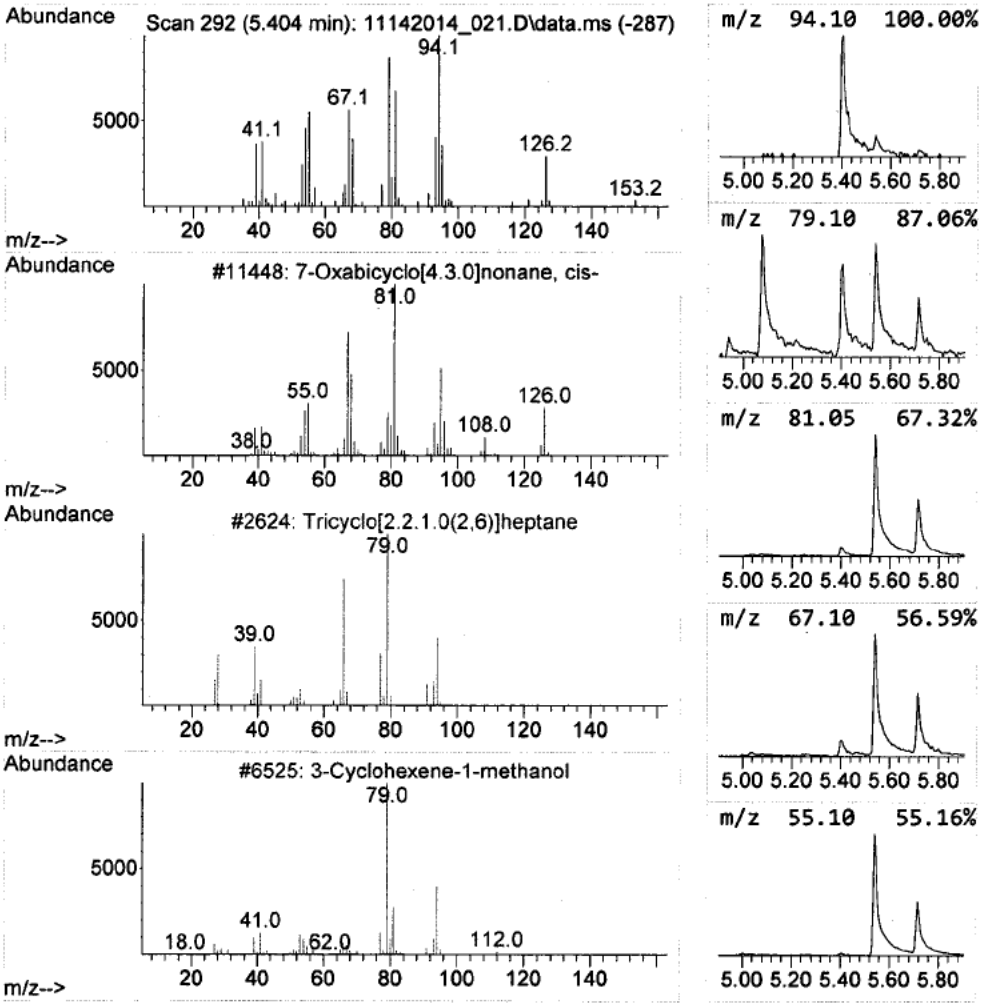
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 2 7-Oxabicyclo[4.3.0]nonane, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.404	0.82 ug/mL	131421	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[4.3.0]nonane, cis-	126	C8H14O	013149-01-4	46
2	Tricyclo[2.2.1.0(2,6)]heptane	94	C7H10	000279-19-6	43
3	3-Cyclohexene-1-methanol	112	C7H12O	001679-51-2	38
4	6-Nonynoic acid, methyl ester	168	C10H16O2	020731-17-3	38
5	5-Vinyl-pyrazole	94	C5H6N2	1000288-36-8	38



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

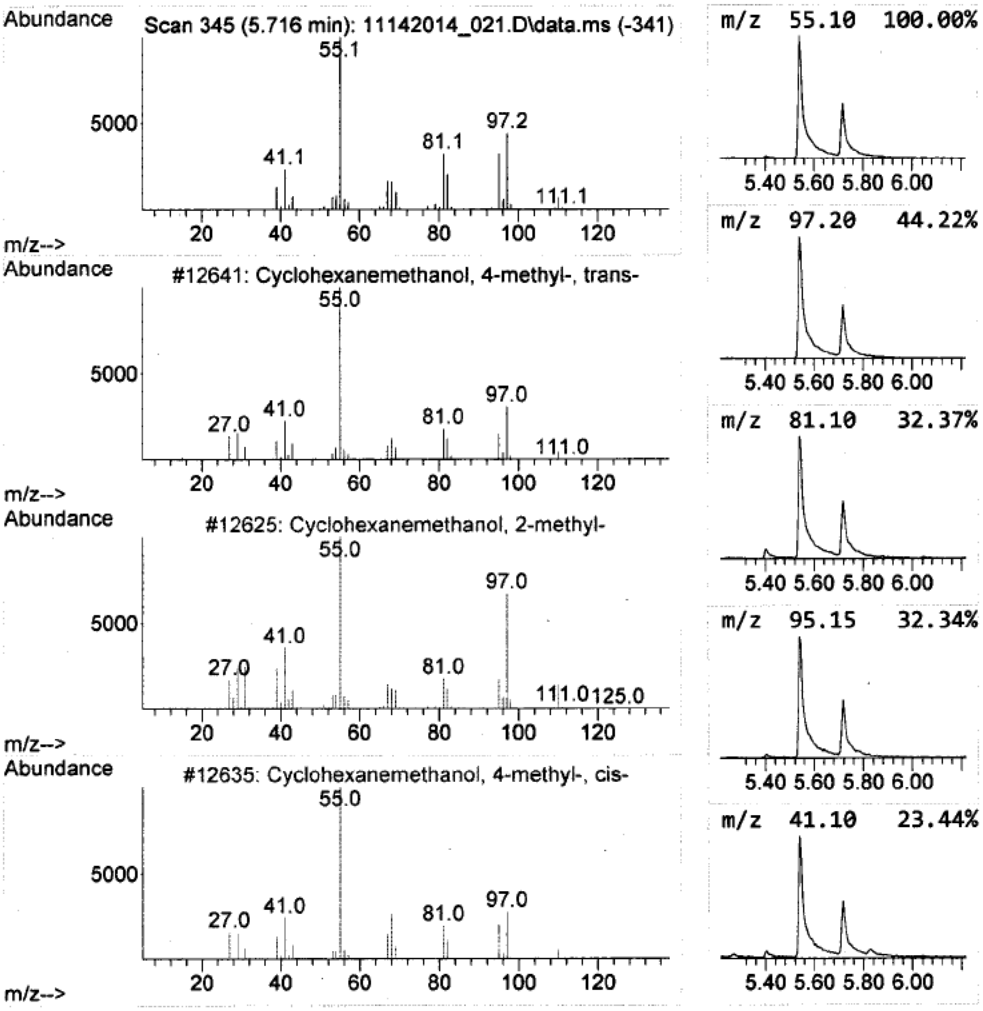
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 3 Cyclohexanemethanol, 4-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	3.32 ug/mL	530409	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	83
2	Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	72
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	56
4	Oxalic acid, di(cyclohexylmethyl...	282	C16H26O4	1000309-68-5	50
5	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	50



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

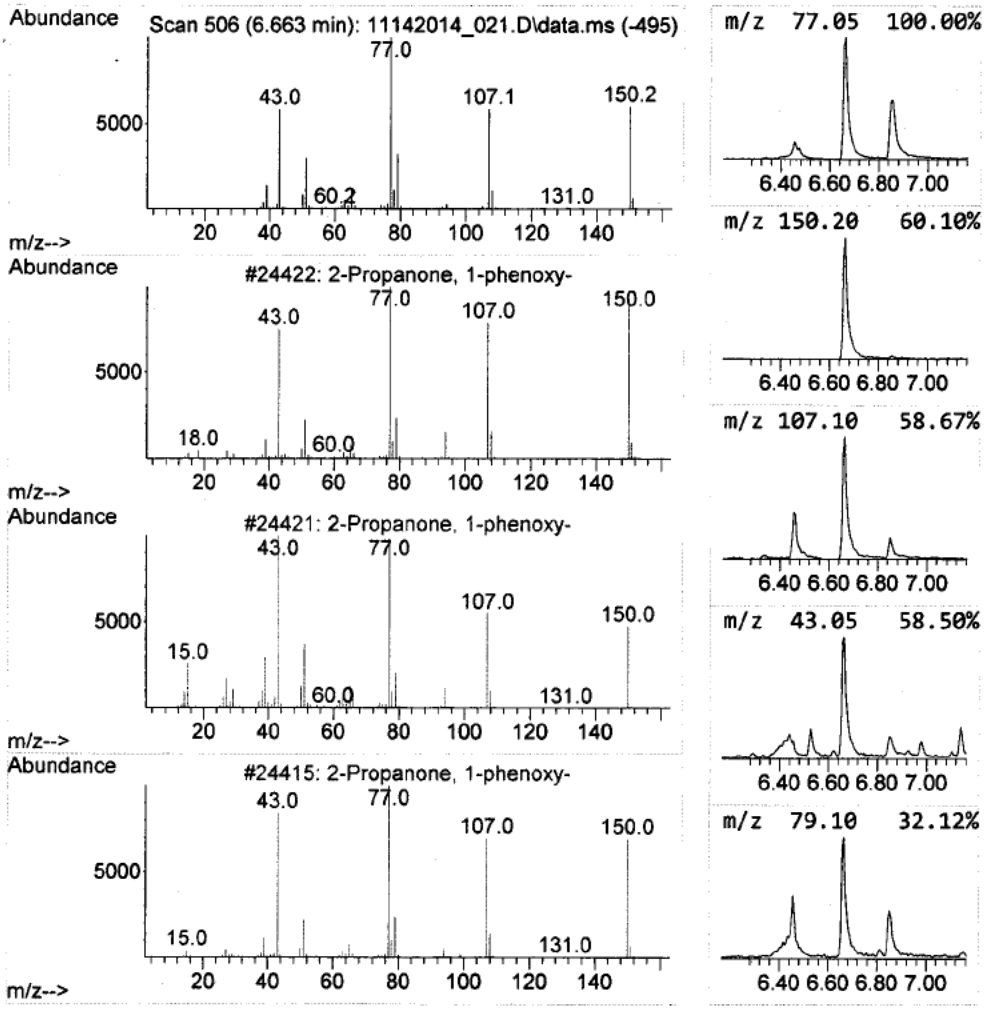
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 4 2-Propanone, 1-phenoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.663	1.28 ug/mL	326547	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-phenoxy-	150	C9H10O2	000621-87-4	87
2	2-Propanone, 1-phenoxy-	150	C9H10O2	000621-87-4	72
3	2-Propanone, 1-phenoxy-	150	C9H10O2	000621-87-4	53
4	Benzene, nitroso-	107	C6H5NO	000586-96-9	50
5	Benzene, nitroso-	107	C6H5NO	000586-96-9	47



Library Search Compound Report

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Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

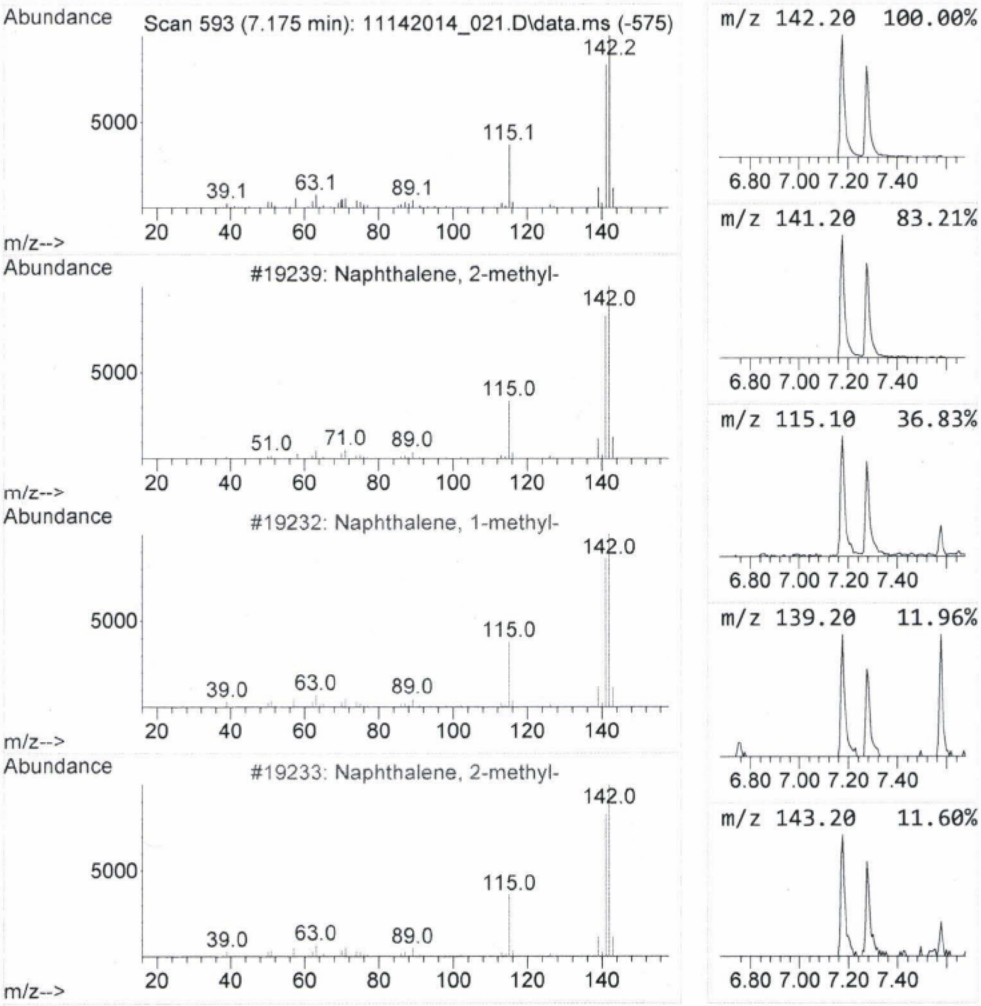
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.175	0.92 ug/mL	234025	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90



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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

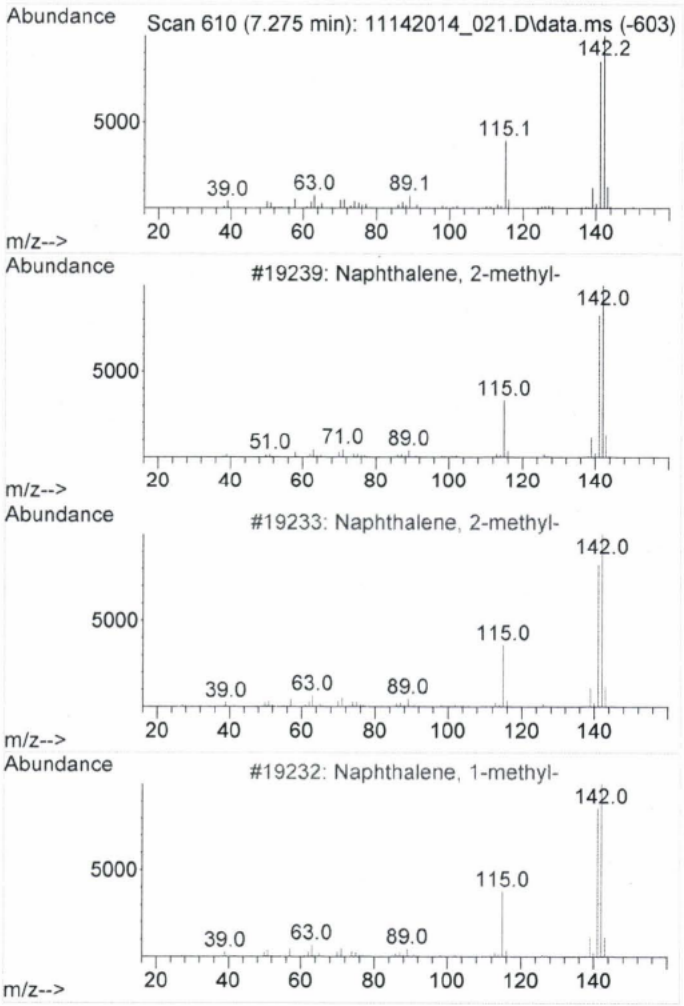
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

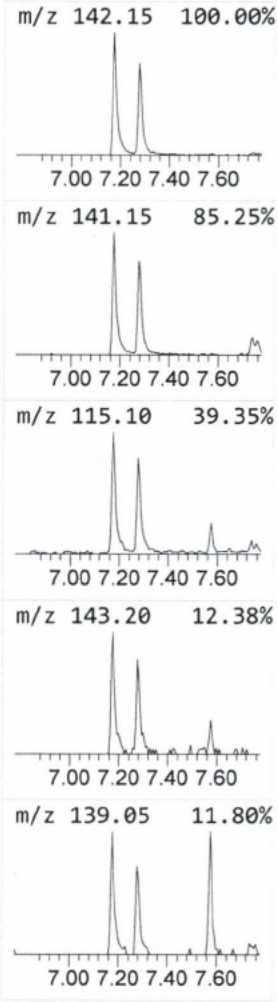
****

Peak Number 6 Naphthalene, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.275	0.51 ug/mL	130875	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5	Benzocycloheptatriene	142	C11H10	000264-09-5	91





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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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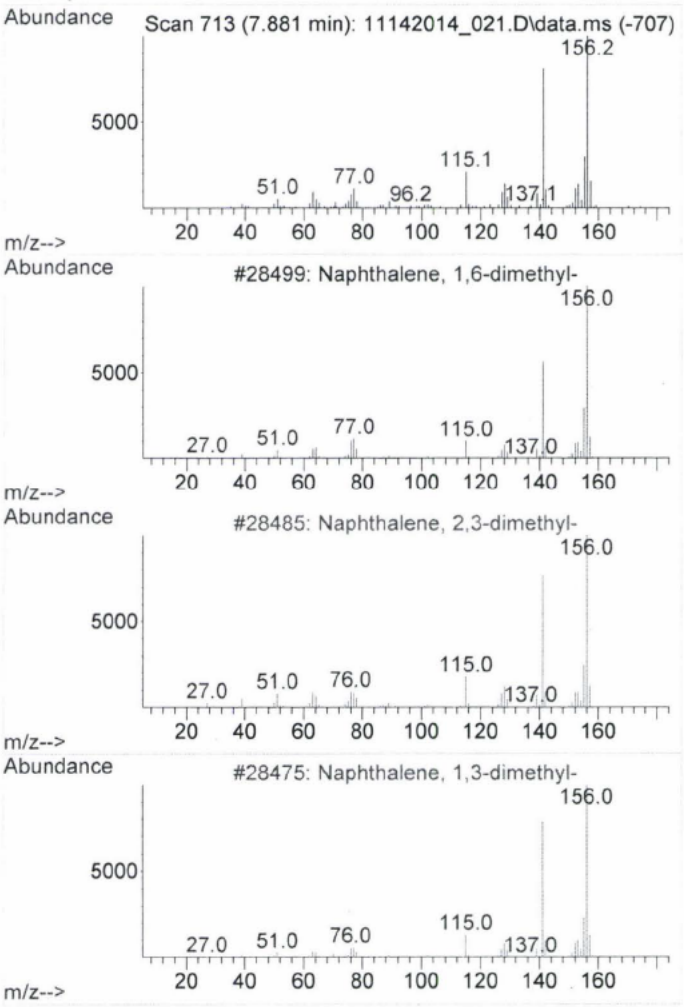
Quant Title : RP1616-MCHM Compounds

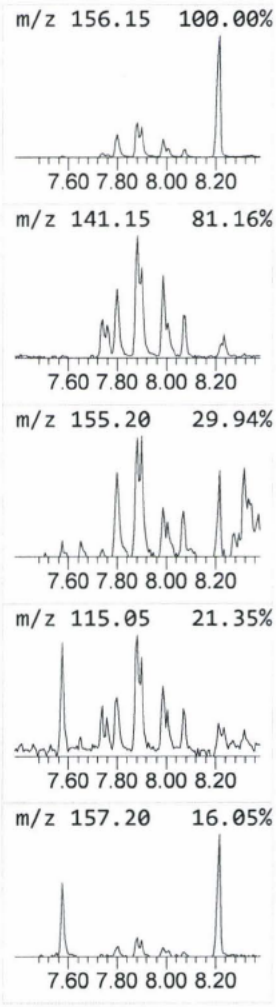
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 7 Naphthalene, 1,6-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.881	0.73 ug/mL	170210	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96





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Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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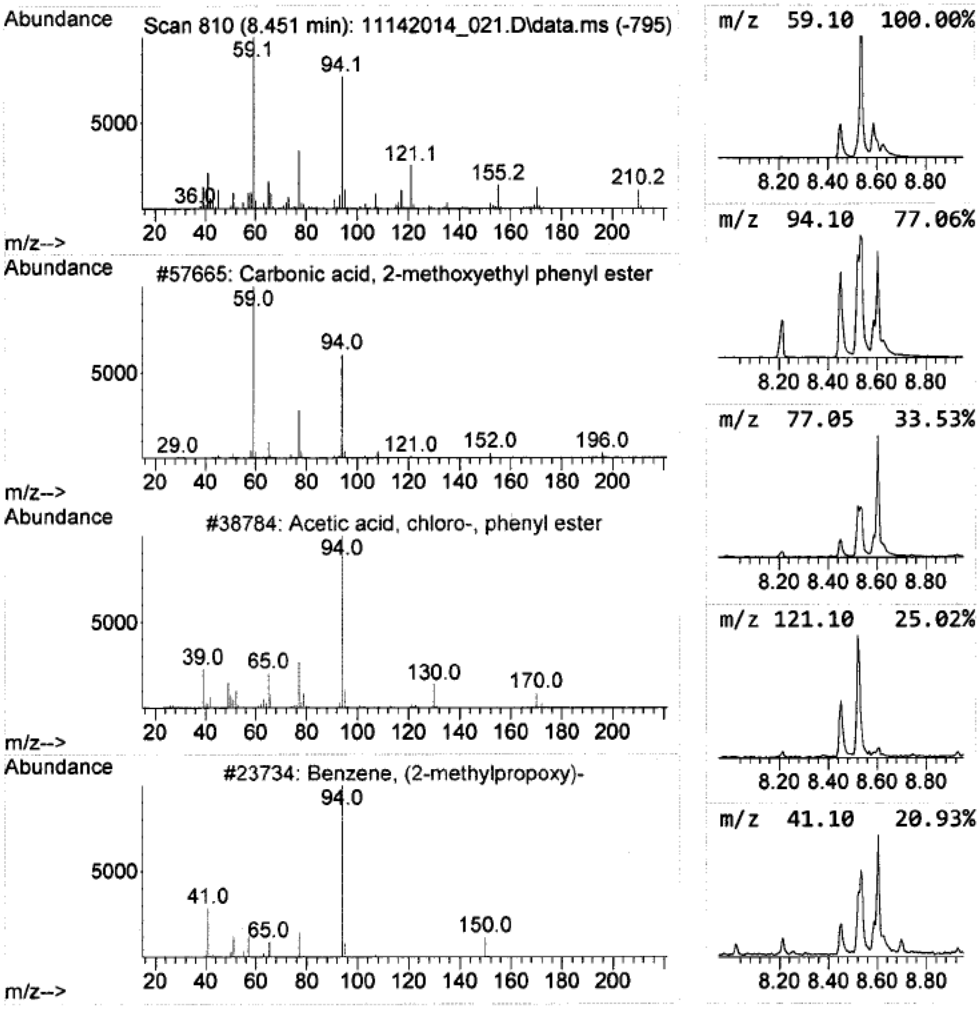
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 8 Carbonic acid, 2-methoxyeth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	1.60 ug/mL	371151	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	45
2	Acetic acid, chloro-, phenyl ester	170	C8H7ClO2	000620-73-5	38
3	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	35
4	2-Phenoxybutyric acid	180	C10H12O3	013794-14-4	35
5	1-Phenoxy-2-chloropropane	170	C9H11ClO	053491-30-8	35



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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

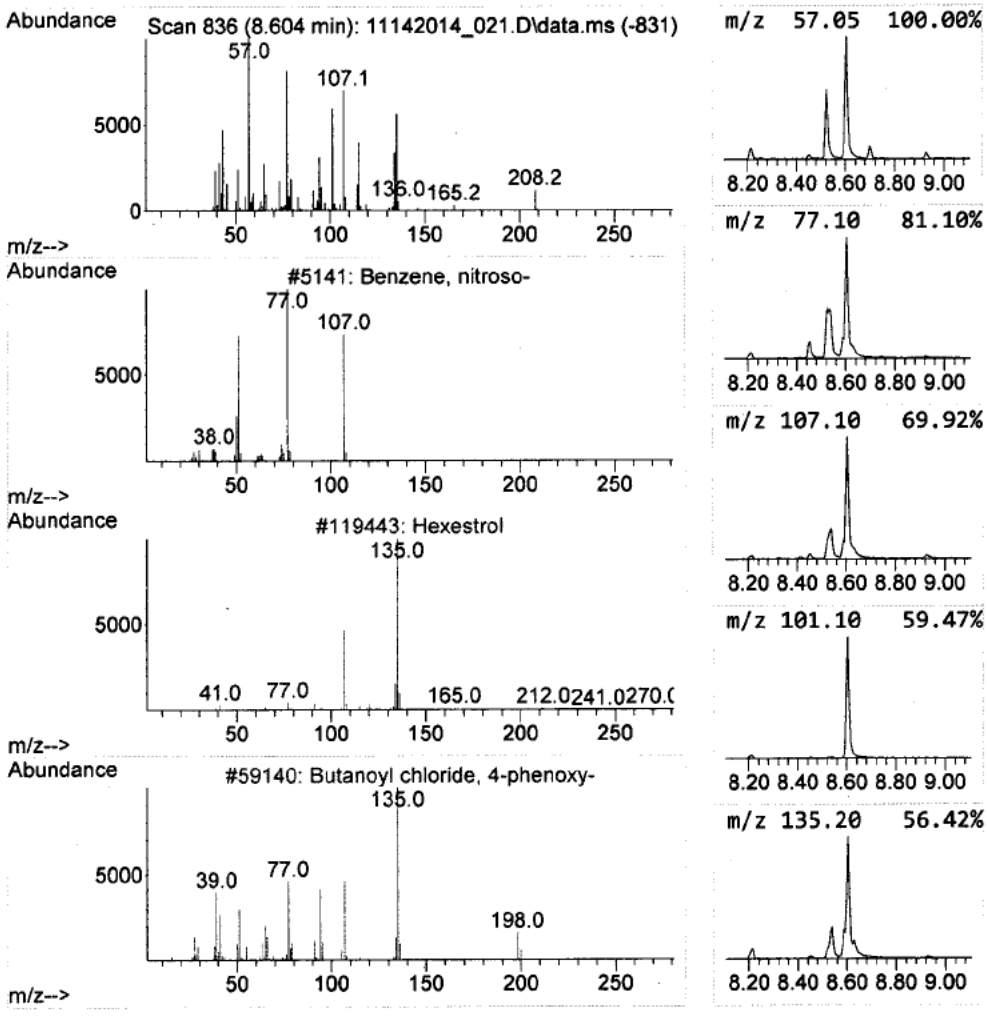
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 9 Benzene, nitroso- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	5.61 ug/mL	1302890	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, nitroso-	107	C6H5NO	000586-96-9	22
2	Hexestrol	270	C18H22O2	000084-16-2	22
3	Butanoyl chloride, 4-phenoxy-	198	C10H11ClO2	005139-89-9	22
4	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	14
5	Benzeneacetonitrile, 2-fluoro-	135	C8H6FN	000326-62-5	14



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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 10 Naphthalene, 1,6,7-trimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.739	0.68 ug/mL	158737	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	94
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
3	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
4	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
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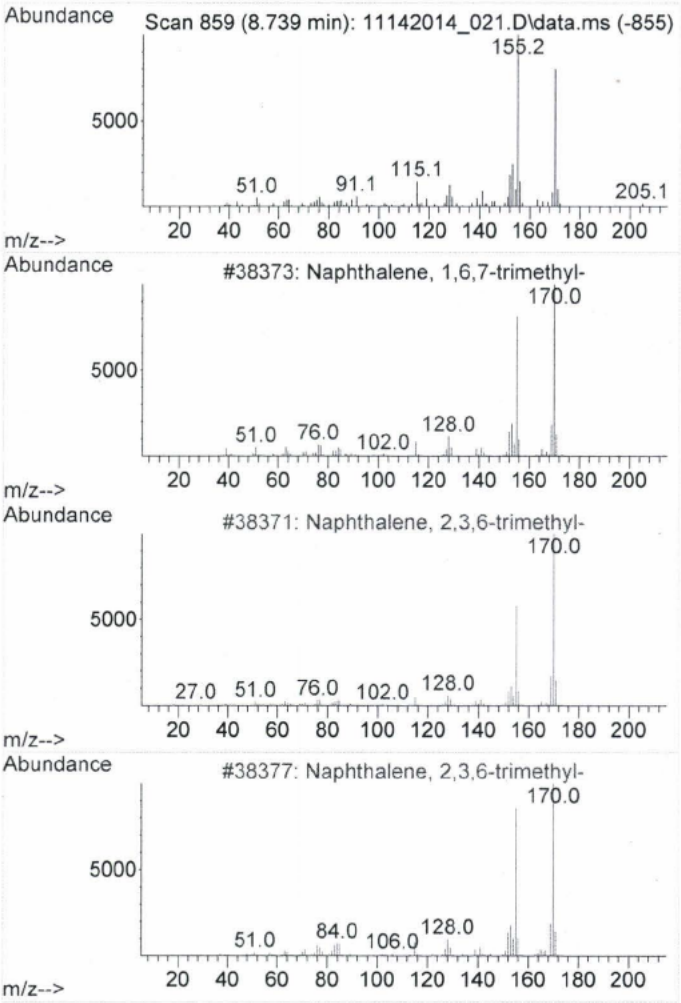

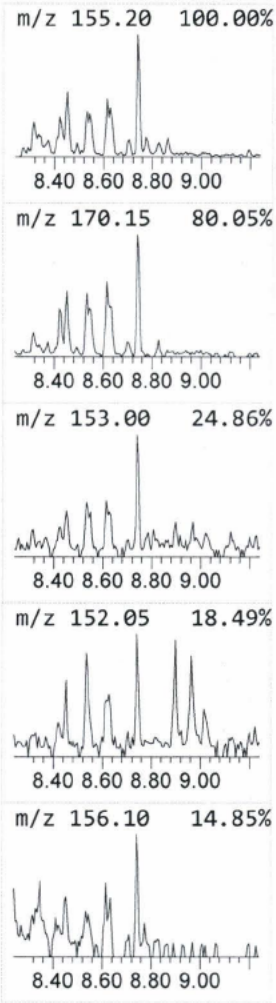

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Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

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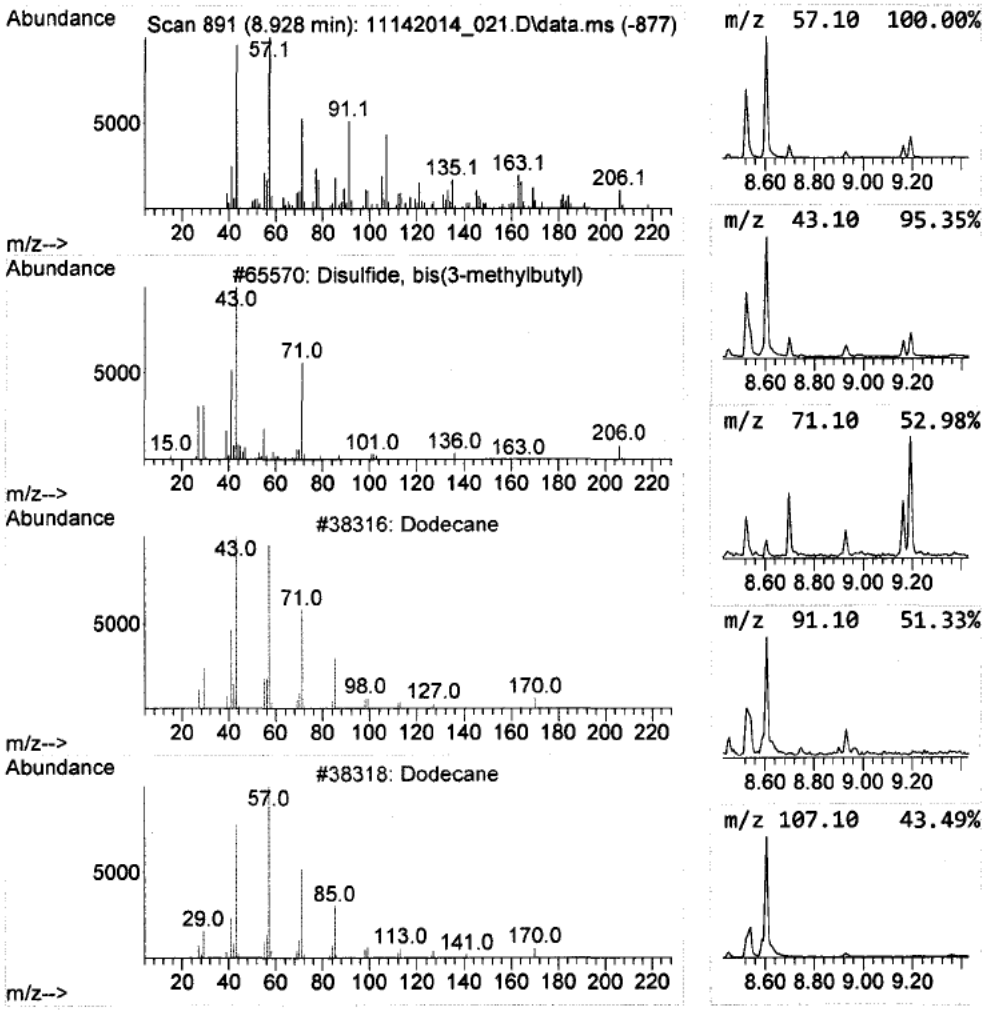
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 11 Disulfide, bis(3-methylbutyl) Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.928	0.80 ug/mL	186723	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, bis(3-methylbutyl)	206	C10H22S2	002051-04-9	18
2	Dodecane	170	C12H26	000112-40-3	15
3	Dodecane	170	C12H26	000112-40-3	15
4	Tridecane	184	C13H28	000629-50-5	15
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	14



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Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

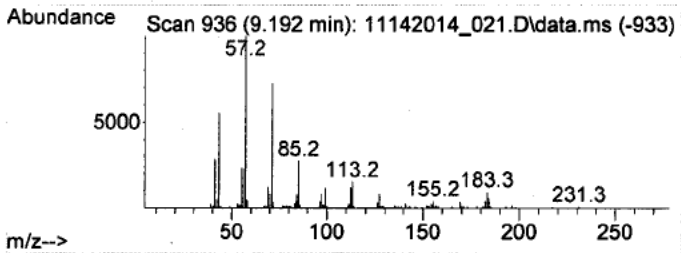
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

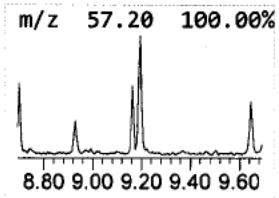
****

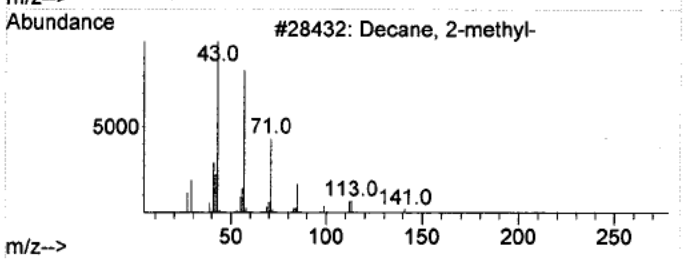
Peak Number 12 Decane, 2-methyl- Concentration Rank 7

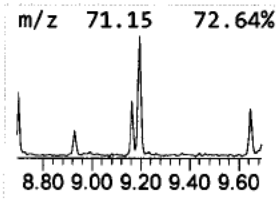
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.192	1.15 ug/mL	257964	Phenanthrene-d10	9.681

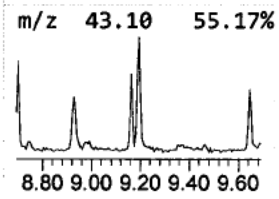
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	87
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	86
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	86
4	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83
5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83

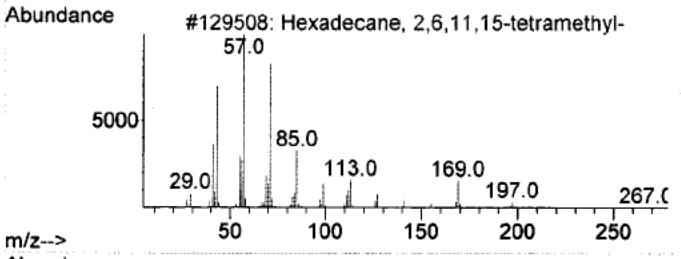


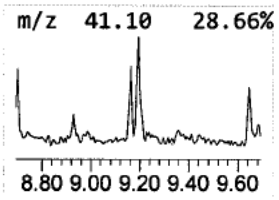


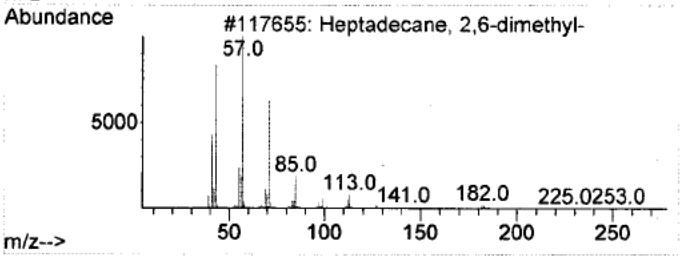


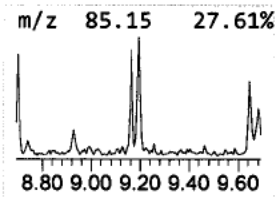












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Sample : NE36694
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Quant Title : RP1616-MCHM Compounds

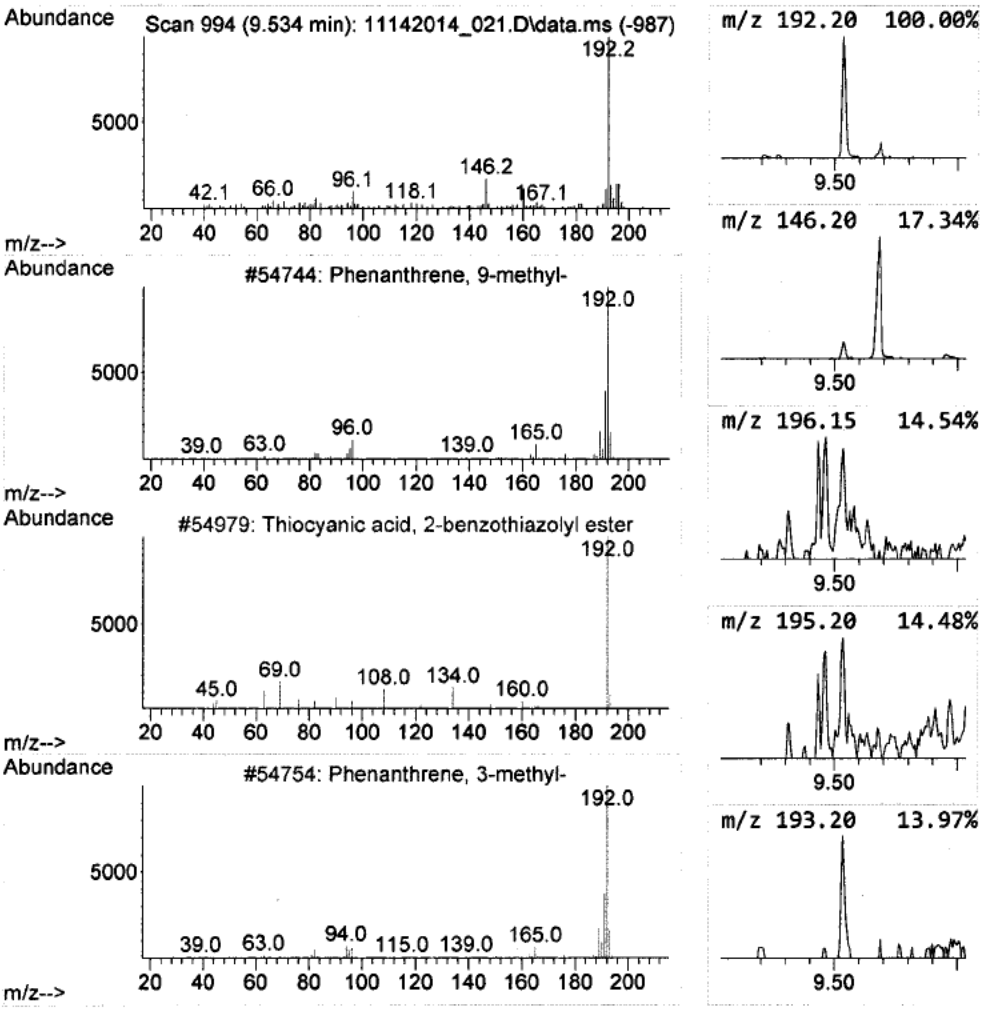
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 13 Phenanthrene, 9-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.534	0.70 ug/mL	157222	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	53
2	Thiocyanic acid, 2-benzothiazoly...	192	C8H4N2S2	006011-99-0	53
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	52
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	52
5	1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	50



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ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

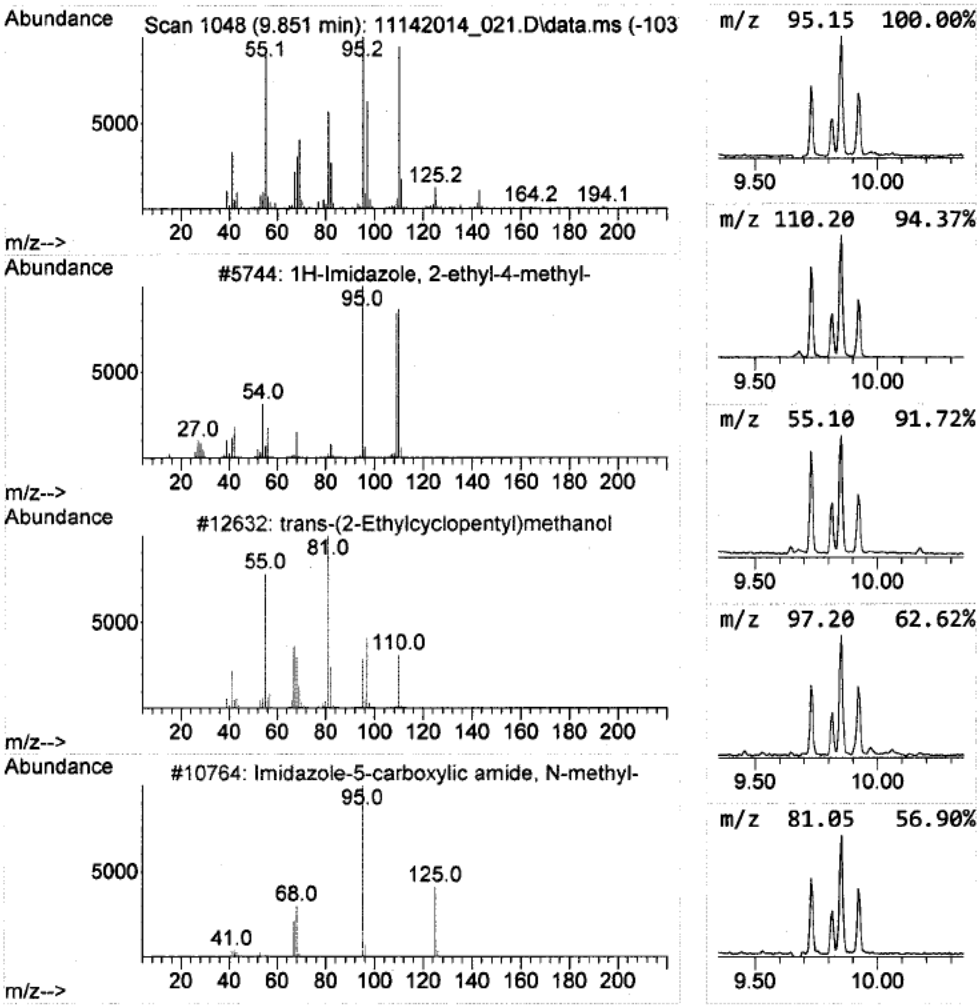
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 14 1H-Imidazole, 2-ethyl-4-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	2.17 ug/mL	485055	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	47
2	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	40
3	Imidazole-5-carboxylic amide, N-...	125	C5H7N3O	053525-55-6	38
4	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	37
5	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	37



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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

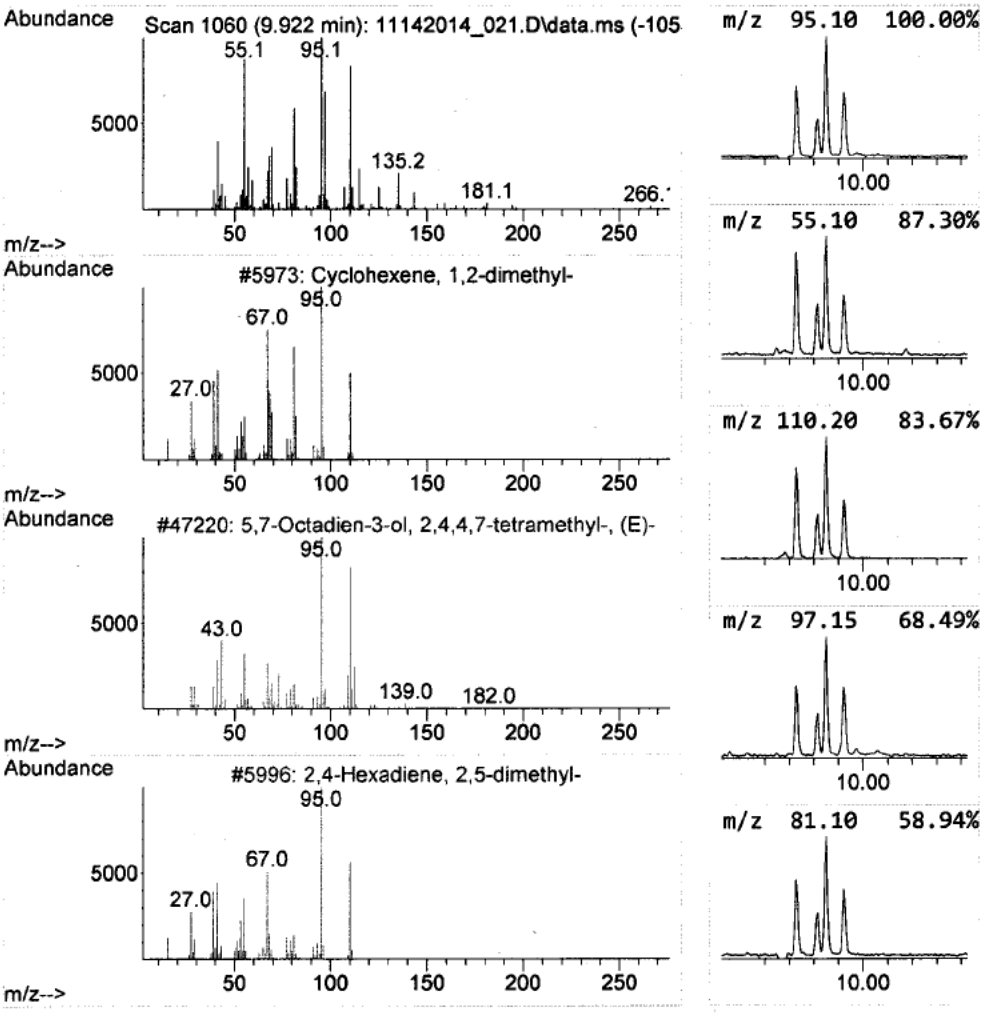
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 15 Cyclohexene, 1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	1.49 ug/mL	333765	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	49
2	5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	47
3	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	43
4	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	43
5	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	43



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Operator : [redacted]
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Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

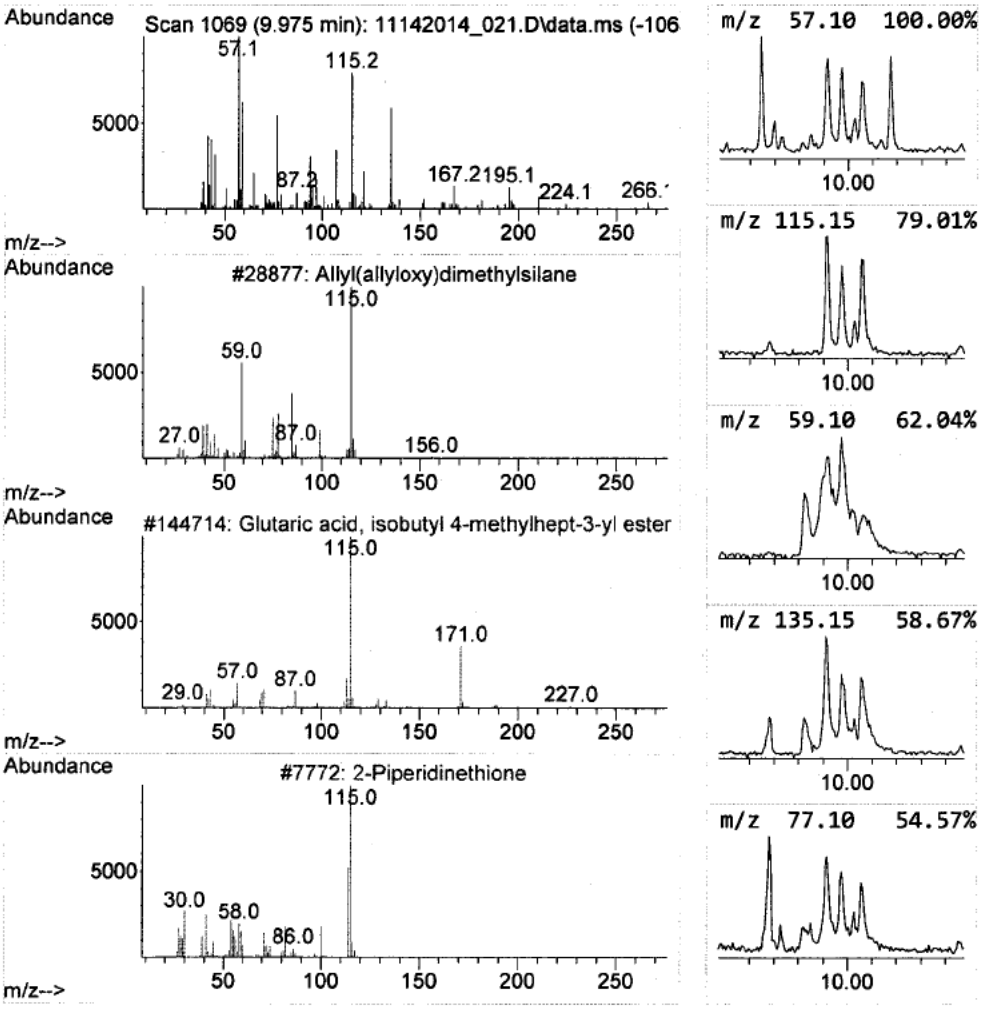
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 16 Allyl(allyloxy)dimethylsilane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	0.79 ug/mL	176257	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl(allyloxy)dimethylsilane	156	C8H16OSi	124659-59-2	25
2	Glutaric acid, isobutyl 4-methyl...	300	C17H32O4	1000377-15-1	14
3	2-Piperidinethione	115	C5H9NS	013070-01-4	14
4	Glutaric acid, but-3-yn-2-yl non...	310	C18H30O4	1000359-88-0	14
5	Benzene, isothiocyanato-	135	C7H5NS	000103-72-0	14



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Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

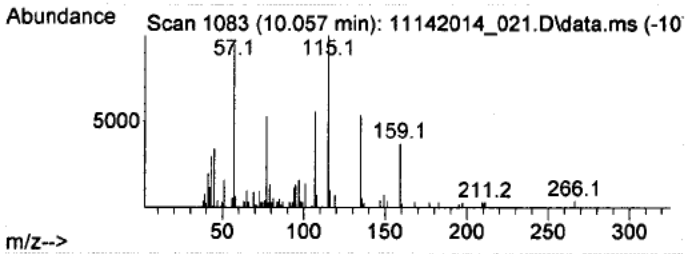
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

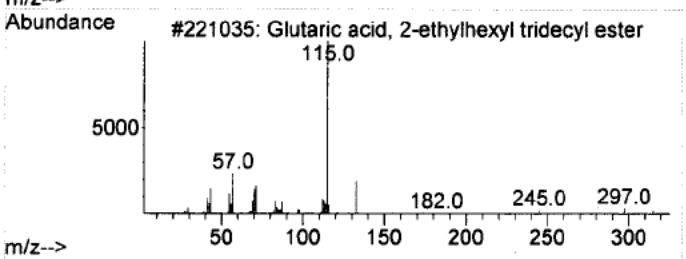
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

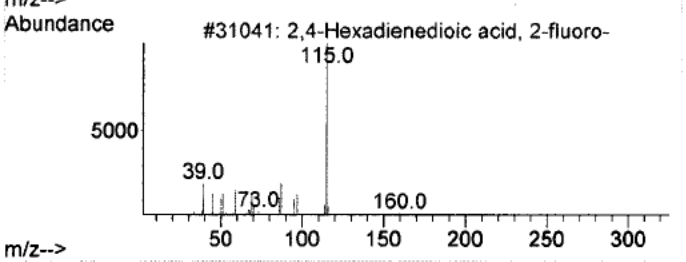
****
Peak Number 17 Glutaric acid, 2-ethylhexyl... Concentration Rank 8

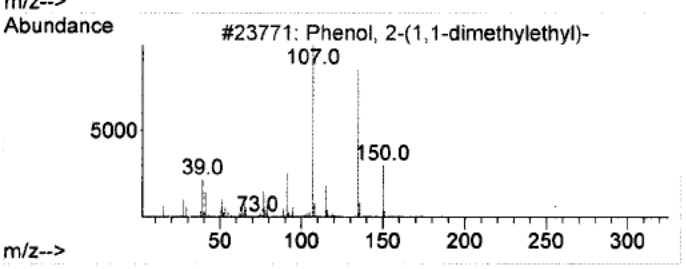
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.057	1.12 ug/mL	249613	Phenanthrene-d10	9.681

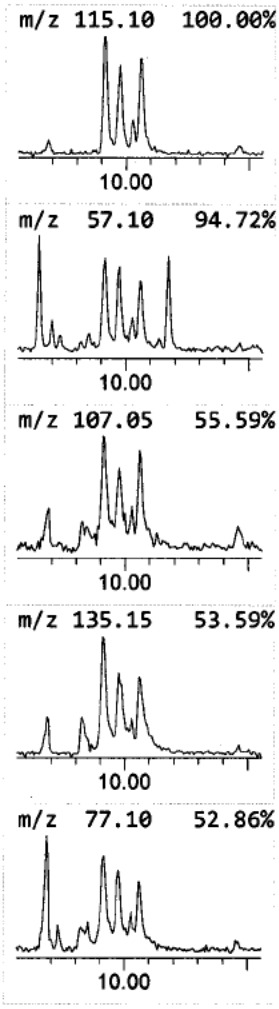
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, 2-ethylhexyl trid...	426	C26H50O4	1000358-24-5	22
2	2,4-Hexadienedioic acid, 2-fluoro-	160	C6H5FO4	010318-01-1	16
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	14
4	Benzene, isothiocyanato-	135	C7H5NS	000103-72-0	14
5	4-Hydroxy-2-methylbenzaldehyde	136	C8H8O2	041438-18-0	14











Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

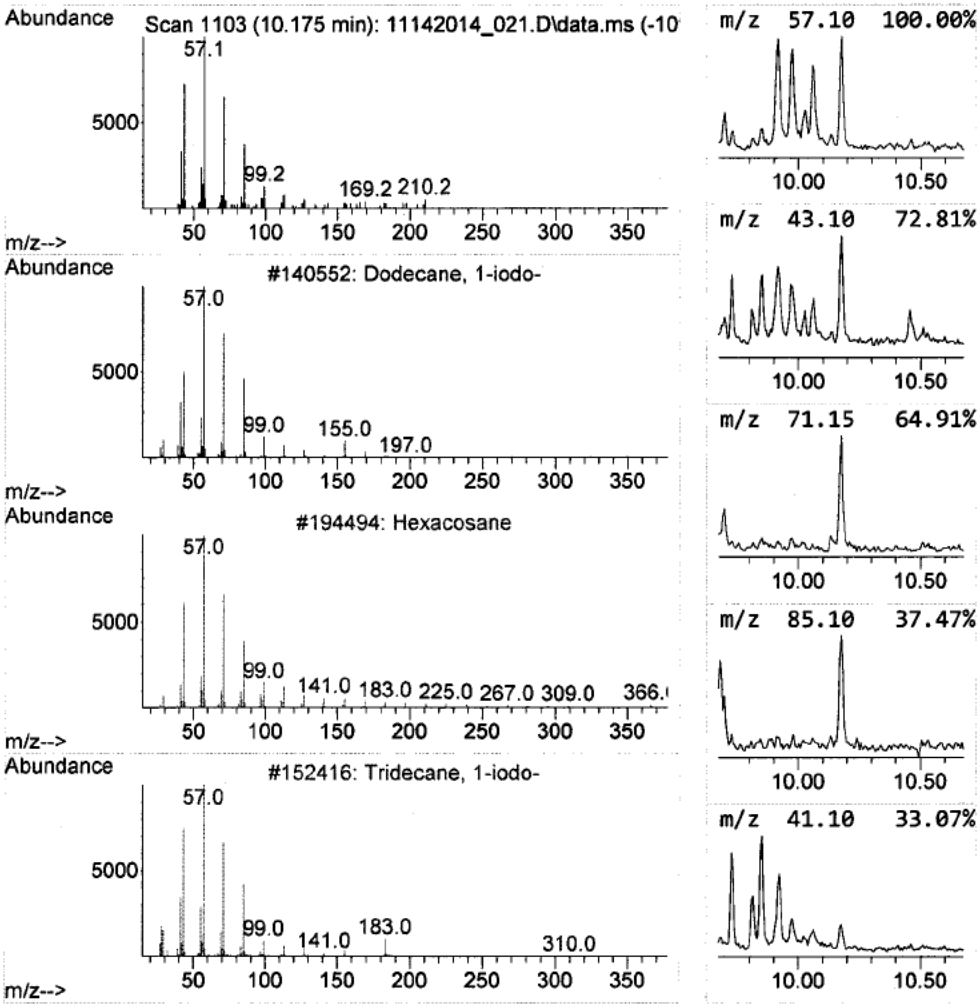
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 18 Dodecane, 1-iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.175	0.56 ug/mL	124659	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
2	Hexacosane	366	C26H54	000630-01-3	86
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	80



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

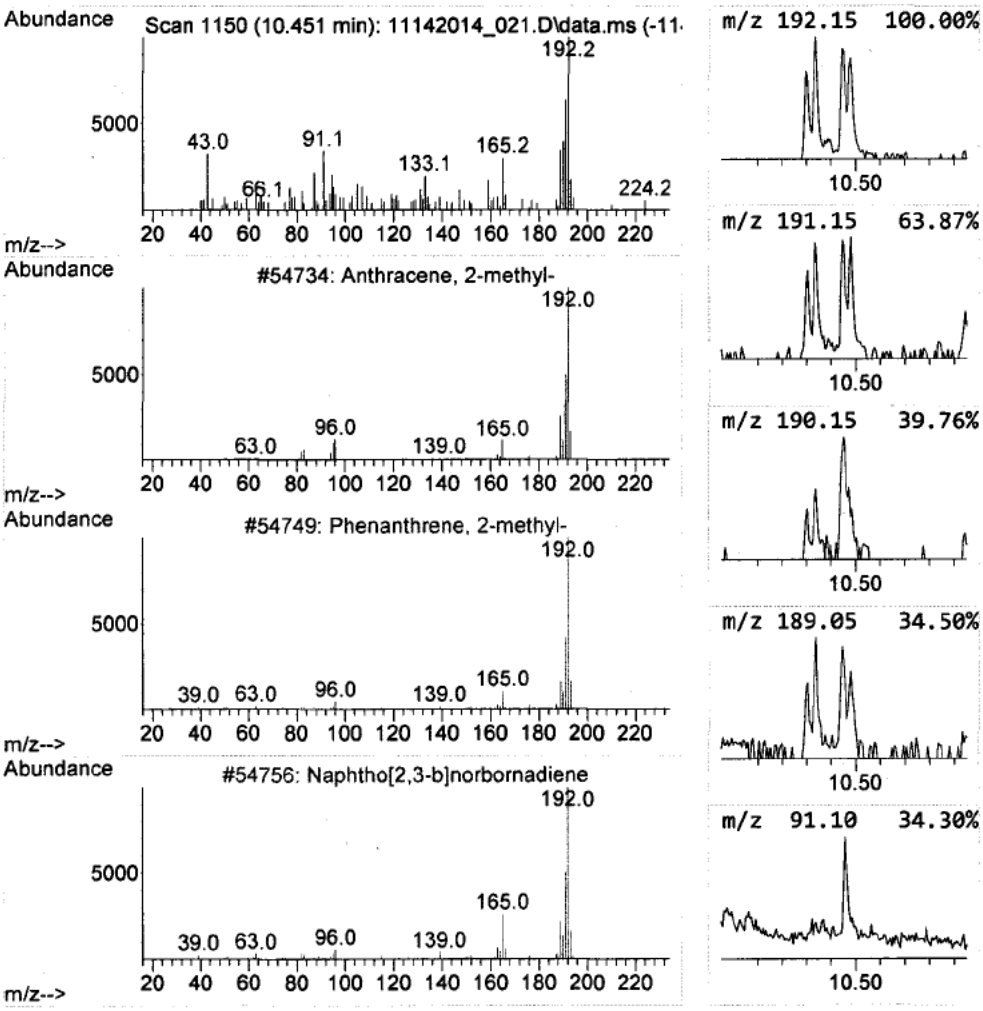
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 19 Anthracene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	0.81 ug/mL	181711	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	55
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	55
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	50



Tentatively Identified Compound (LSC) summary

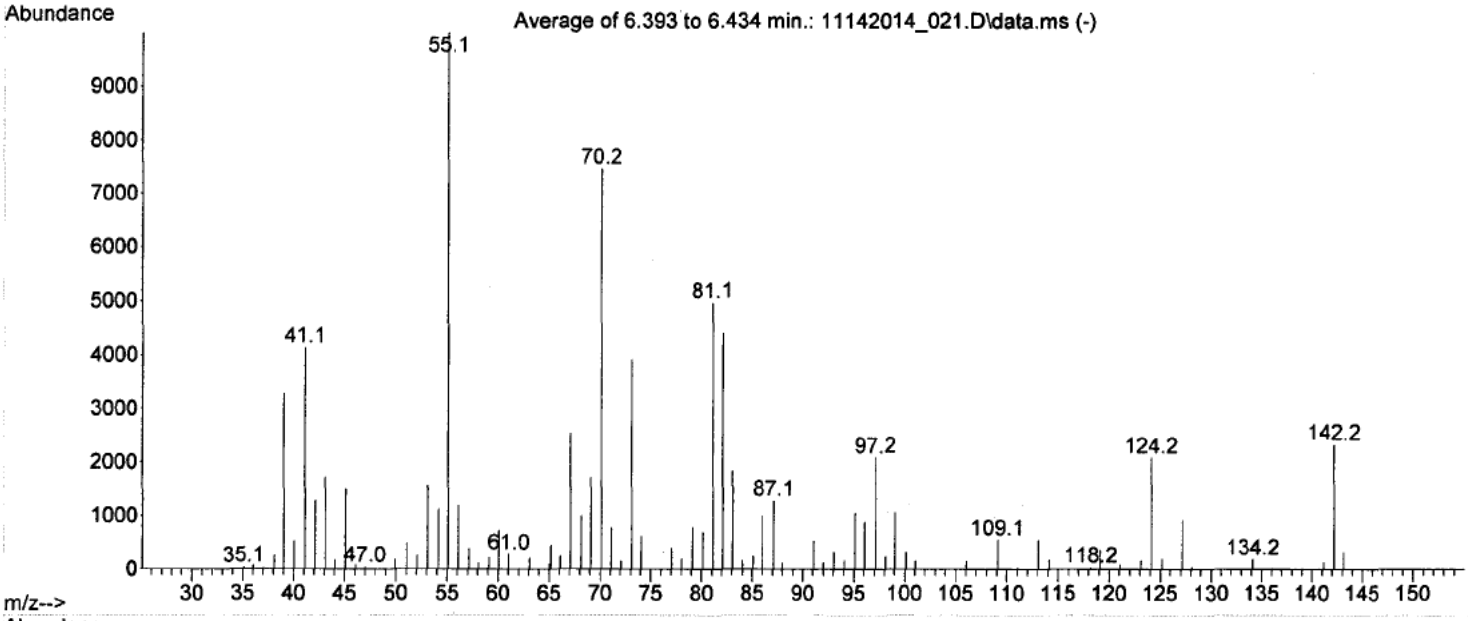
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_021.D
Acq On : 14 Nov 2014 07:39 pm
Operator : [redacted]
Sample : NE36694
Misc : Tag # NE36694, 1X
ALS Vial : 20 Sample Multiplier: 1

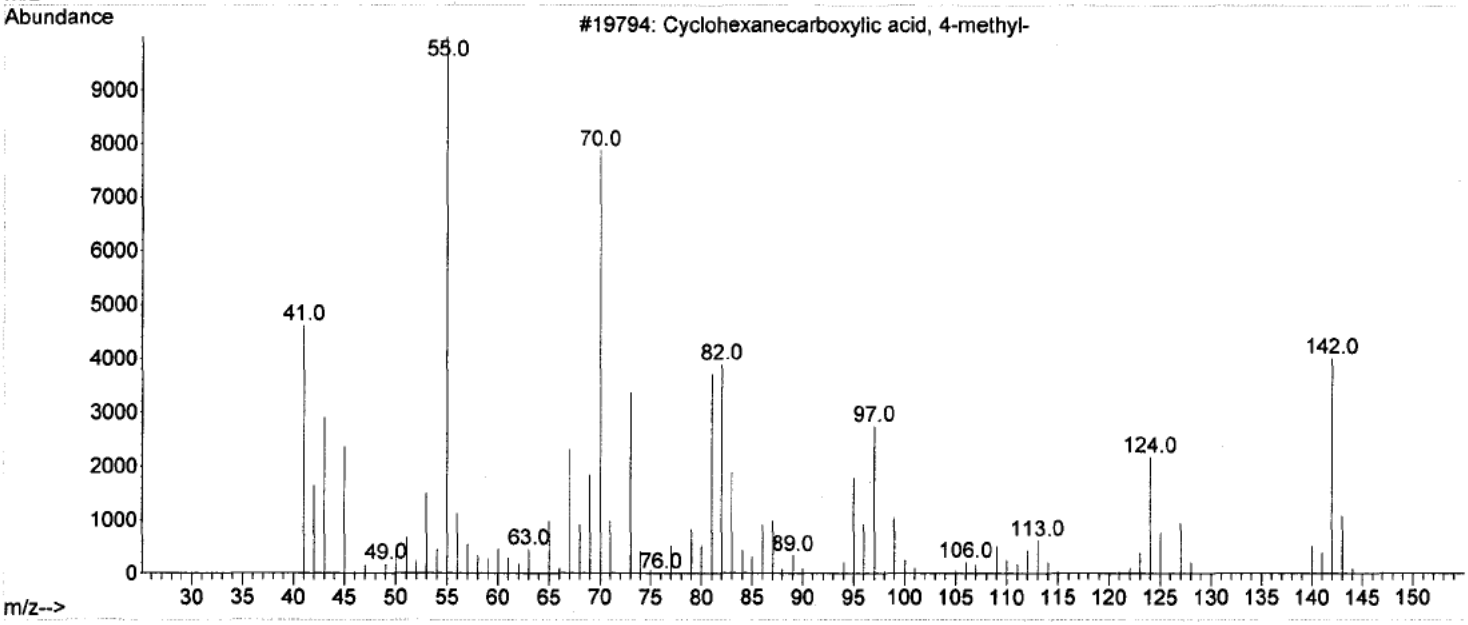
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

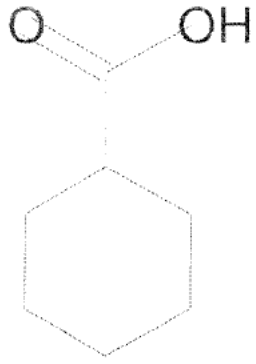
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
o-Xylene	3.793	0.8	ug/mL	128354	1	5.081	3191720	20.0
7-Oxabicyclo[4....	5.404	0.8	ug/mL	131421	1	5.081	3191720	20.0
Cyclohexanemeth...	5.716	3.3	ug/mL	530409	1	5.081	3191720	20.0
2-Propanone, 1-...	6.663	1.3	ug/mL	326547	2	6.457	5100040	20.0
Naphthalene, 2-...	7.175	0.9	ug/mL	234025	2	6.457	5100040	20.0
Naphthalene, 2-...	7.275	0.5	ug/mL	130875	2	6.457	5100040	20.0
Naphthalene, 1,...	7.881	0.7	ug/mL	170210	3	8.216	4641180	20.0
Carbonic acid, ...	8.451	1.6	ug/mL	371151	3	8.216	4641180	20.0
Benzene, nitroso-	8.604	5.6	ug/mL	1302890	3	8.216	4641180	20.0
Naphthalene, 1,...	8.739	0.7	ug/mL	158737	3	8.216	4641180	20.0
Disulfide, bis(...	8.928	0.8	ug/mL	186723	3	8.216	4641180	20.0
Decane, 2-methyl-	9.192	1.2	ug/mL	257964	4	9.681	4472970	20.0
Phenanthrene, 9...	9.534	0.7	ug/mL	157222	4	9.681	4472970	20.0
1H-Imidazole, 2...	9.851	2.2	ug/mL	485055	4	9.681	4472970	20.0
Cyclohexene, 1,...	9.922	1.5	ug/mL	333765	4	9.681	4472970	20.0
Allyl(allyloxy)...	9.975	0.8	ug/mL	176257	4	9.681	4472970	20.0
Glutaric acid, ...	10.057	1.1	ug/mL	249613	4	9.681	4472970	20.0
Dodecane, 1-iodo-	10.175	0.6	ug/mL	124659	4	9.681	4472970	20.0
Anthracene, 2-m...	10.451	0.8	ug/mL	181711	4	9.681	4472970	20.0

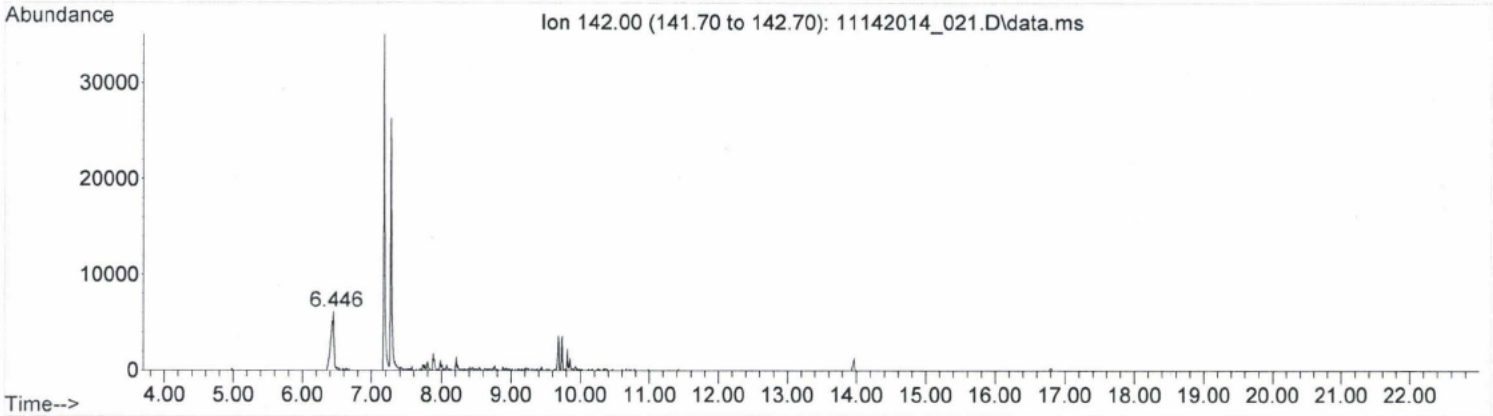
Library Searched : C:\Database\NIST11.L
Quality : 94
ID : Cyclohexanecarboxylic acid, 4-methyl-

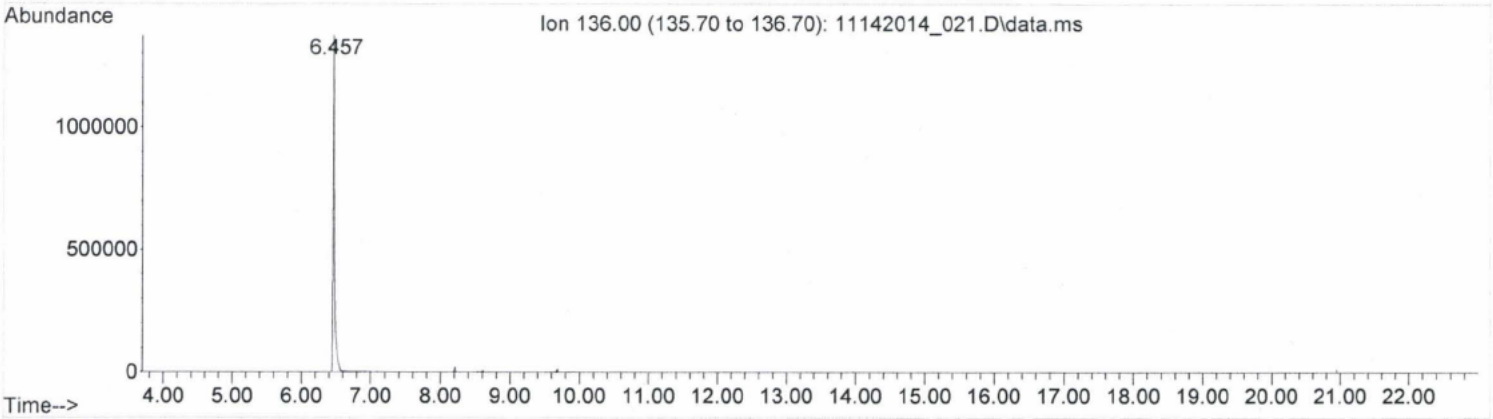


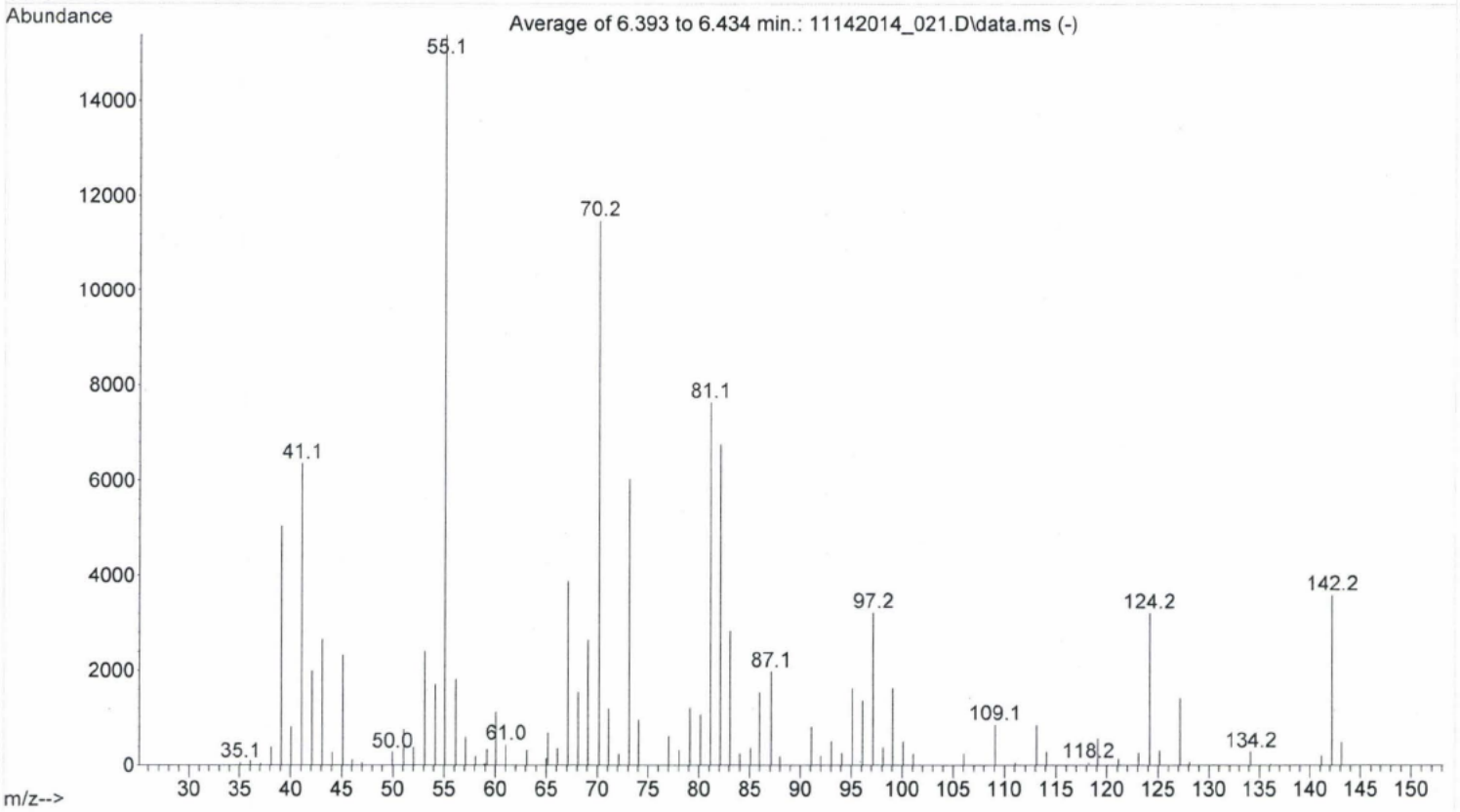




File :D:[redacted]\RP1616\11142014_Run\11142014_021.D
Operator : [redacted]
Acquired : 14 Nov 2014 07:39 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36694
Misc Info : Tag # NE36694, 1X
Vial Number: 20







[redacted] RP1616 12/17/14