Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

Quant Time: Nov 17 11:09:32 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	5.075	152	432381	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1886857	20.00 ug/mL	# 0.00
5) Acenaphthene-d10	8.216	164	1058879	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.681	188	1605101	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	1000261	20.00 ug/mL	0.00
12) Perylene-d12	16.804	264	614455	20.00 ug/mL	0.01
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	561441	8.63 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery =	~~69.04%~~	
Target Compounds					Qvalue
2) MCHM	5.716	55	114080m	2.77 ug/mL	
4) PPH	6.857	94	76882m	1.85 ug/mL	
6) 1,4-CHDM	0.000		0	N.D. d	
8) DM-1,4-CHDC	0.000		0	N.D. d	
9) di-PPH	8.534	59	180912m	4.75 ug/mL	

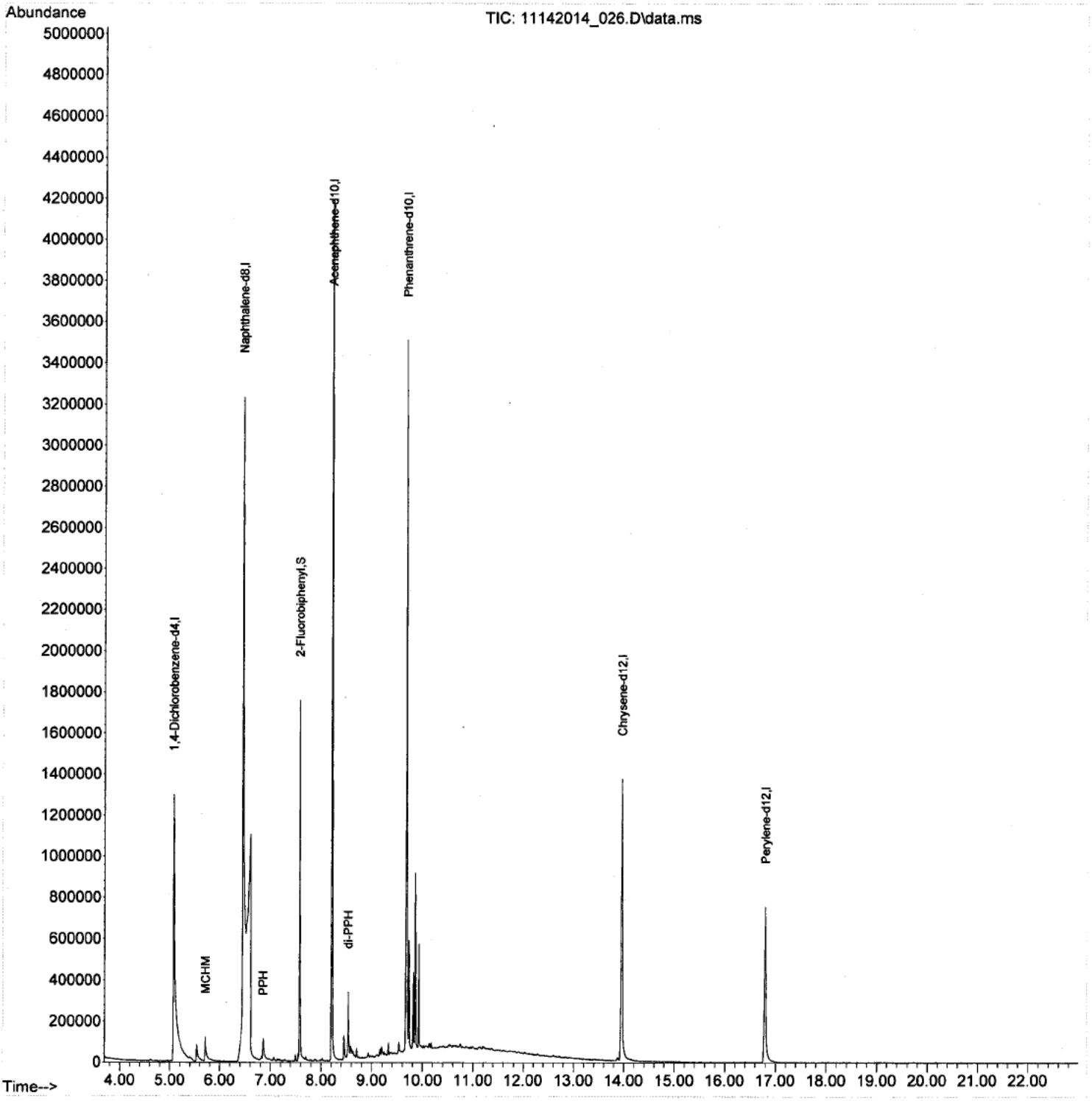
see Analyst Narrative, Surrogate Recovery [redacted] 1/7/11

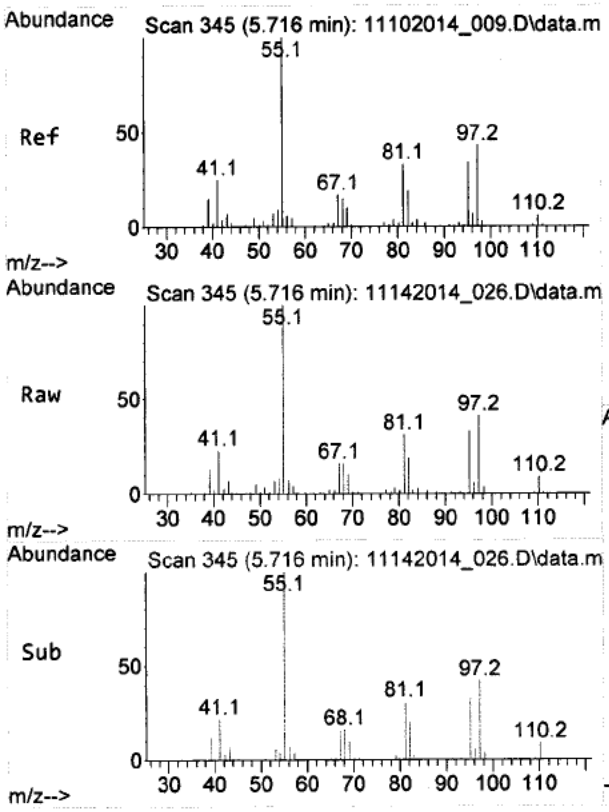
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

Quant Time: Nov 17 11:09:32 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

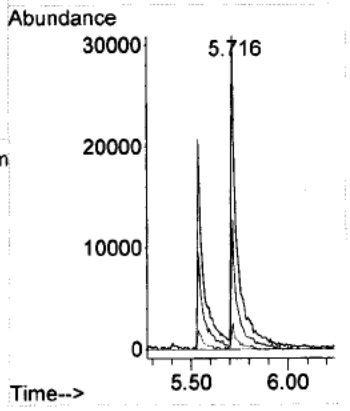


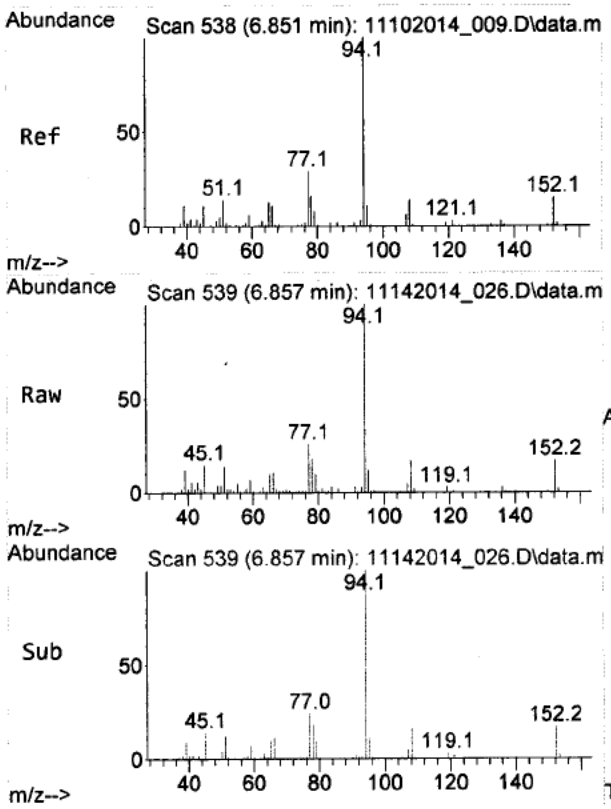


#2
MCHM
Concen: 2.77 ug/mL m
RT: 5.716 min Scan# 345
Delta R.T. 0.000 min
Lab File: 11142014_026.D
Acq: 14 Nov 2014 10:05 pm

Tgt Ion: 55 Resp: 114080

Ion	Ratio	Lower	Upper
55	100		
97	19.7	34.6	51.8#
110	3.2	4.8	7.2#

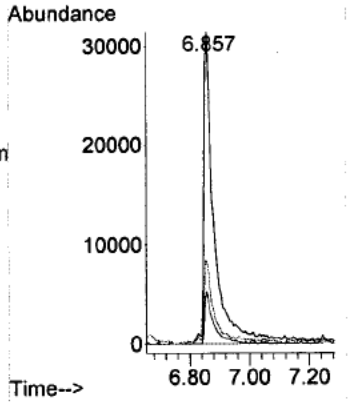


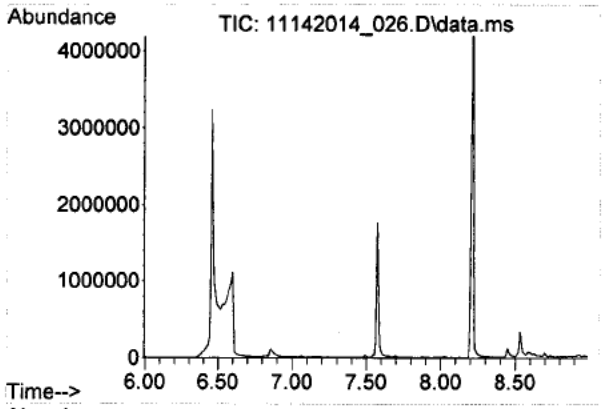


#4
PPH
Concen: 1.85 ug/mL m
RT: 6.857 min Scan# 539
Delta R.T. 0.000 min
Lab File: 11142014_026.D
Acq: 14 Nov 2014 10:05 pm

Tgt Ion: 94 Resp: 76882

Ion	Ratio	Lower	Upper
94	100		
152	14.1	13.4	20.0
77	23.3	21.2	31.8



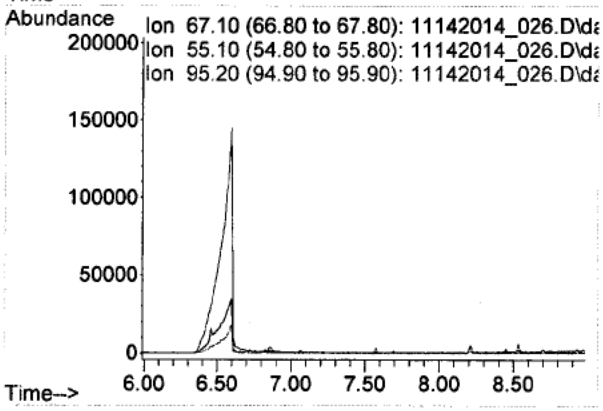


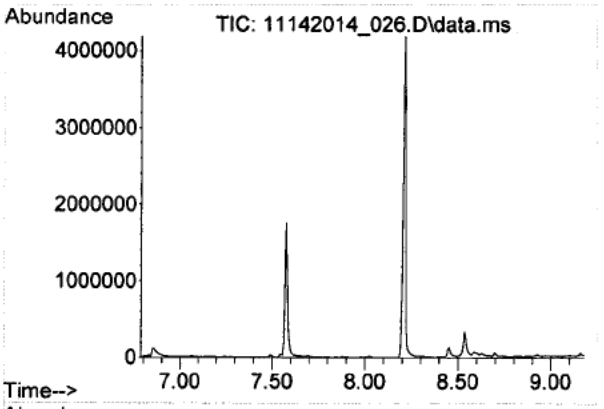
#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_026.D
Acq: 14 Nov 2014 10:05 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8



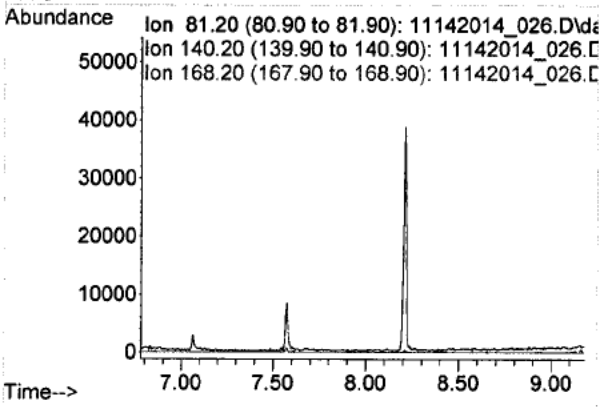


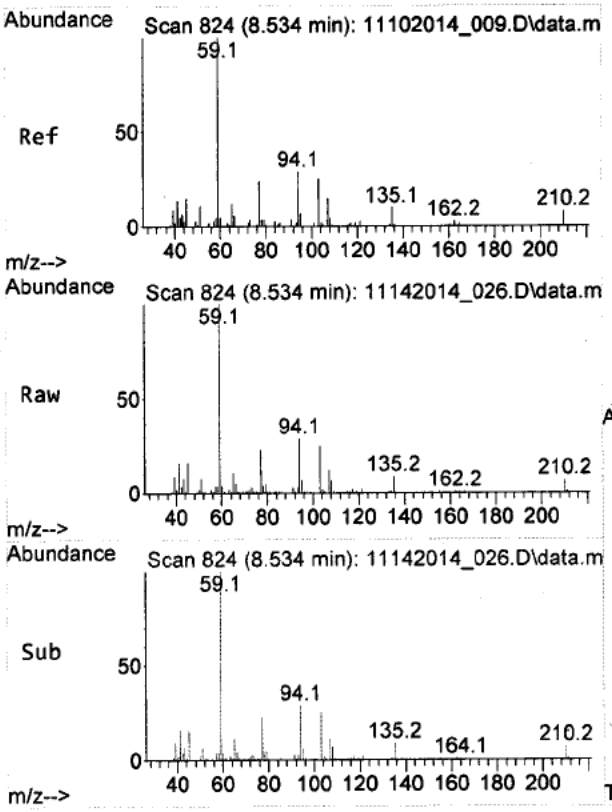
#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_026.D
Acq: 14 Nov 2014 10:05 pm

Tgt Ion: 81

Sig	Exp Ratio
81	100
140	61.8
168	17.7

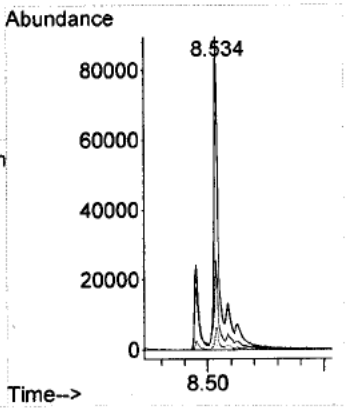




#9
di-PPH
Concen: 4.75 ug/mL m
RT: 8.534 min Scan# 824
Delta R.T. -0.006 min
Lab File: 11142014_026.D
Acq: 14 Nov 2014 10:05 pm

Tgt Ion: 59 Resp: 180912

Ion	Ratio	Lower	Upper
59	100		
94	19.0	23.0	34.6#
210	4.7	6.1	9.1#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 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_026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	229	236	289	rBV	1294104	3199305	53.79%	9.495%
2	5.540	309	315	339	rBV	79443	176295	2.96%	0.523%
3	5.716	339	345	401	rVB	118134	269136	4.52%	0.799%
4	6.457	449	471	481	rBV	3229798	5947785	100.00%	17.651%
5	6.599	481	495	527	rVB	1096853	4372788	73.52%	12.977%
6	6.857	527	539	567	rVB	105743	273926	4.61%	0.813%
7	7.575	653	661	679	rBV	1753893	1776391	29.87%	5.272%
8	8.210	759	769	797	rBV	4186103	4650706	78.19%	13.802%
9	8.451	797	810	817	rBV	116380	151557	2.55%	0.450%
10	8.534	817	824	831	rVV	318315	388134	6.53%	1.152%
11	8.587	831	833	849	rVB3	55721	150787	2.54%	0.447%
12	8.698	849	852	857	rBV	45166	38461	0.65%	0.114%
13	8.928	877	891	895	rBV2	24347	37171	0.62%	0.110%
14	9.163	927	931	933	rBV	36263	36841	0.62%	0.109%
15	9.193	933	936	943	rVV	44238	55387	0.93%	0.164%
16	9.328	953	959	963	rBV	60339	53067	0.89%	0.157%
17	9.534	987	994	1007	rBV	55841	107239	1.80%	0.318%
18	9.681	1007	1019	1025	rVV2	3460378	4316825	72.58%	12.811%
19	9.728	1025	1027	1035	rVV	542034	547965	9.21%	1.626%
20	9.851	1035	1048	1055	rVV	864712	1216526	20.45%	3.610%
21	9.928	1055	1061	1073	rVV	518869	621806	10.45%	1.845%
22	10.022	1073	1077	1081	rVV7	20661	42247	0.71%	0.125%
23	10.057	1081	1083	1093	rVV10	17909	62469	1.05%	0.185%
24	10.134	1093	1096	1101	rVV5	27468	44752	0.75%	0.133%
25	10.339	1119	1131	1139	rVV5	8236	34017	0.57%	0.101%
26	10.534	1157	1164	1173	rVB5	14394	40451	0.68%	0.120%
27	10.875	1217	1222	1239	rVV5	9612	46804	0.79%	0.139%
28	10.998	1239	1243	1257	rVV5	14132	40434	0.68%	0.120%
29	11.145	1257	1268	1273	rVV5	14658	52286	0.88%	0.155%
30	11.204	1273	1278	1301	rVV5	18328	99529	1.67%	0.295%
31	11.375	1301	1307	1319	rVV5	13033	46478	0.78%	0.138%
32	11.534	1319	1334	1341	rVV5	9713	43639	0.73%	0.130%
33	13.963	1737	1747	1813	rVB	1369149	2934359	49.34%	8.708%
34	16.804	2215	2230	2291	rBV	754952	1820398	30.61%	5.402%

LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 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

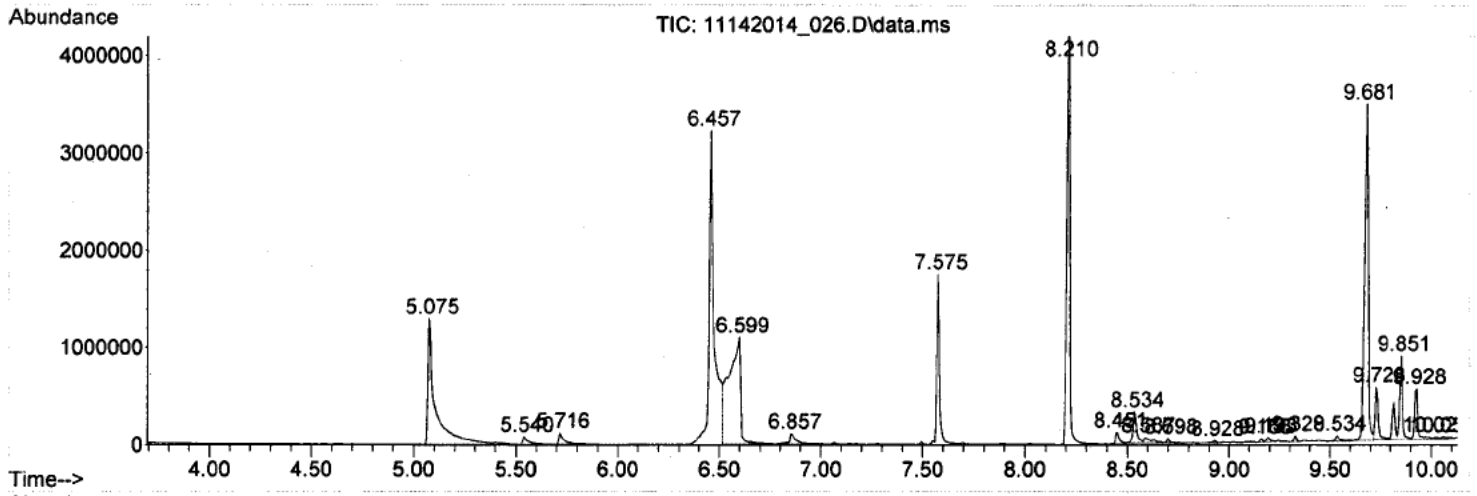
Sum of corrected areas: 33695961

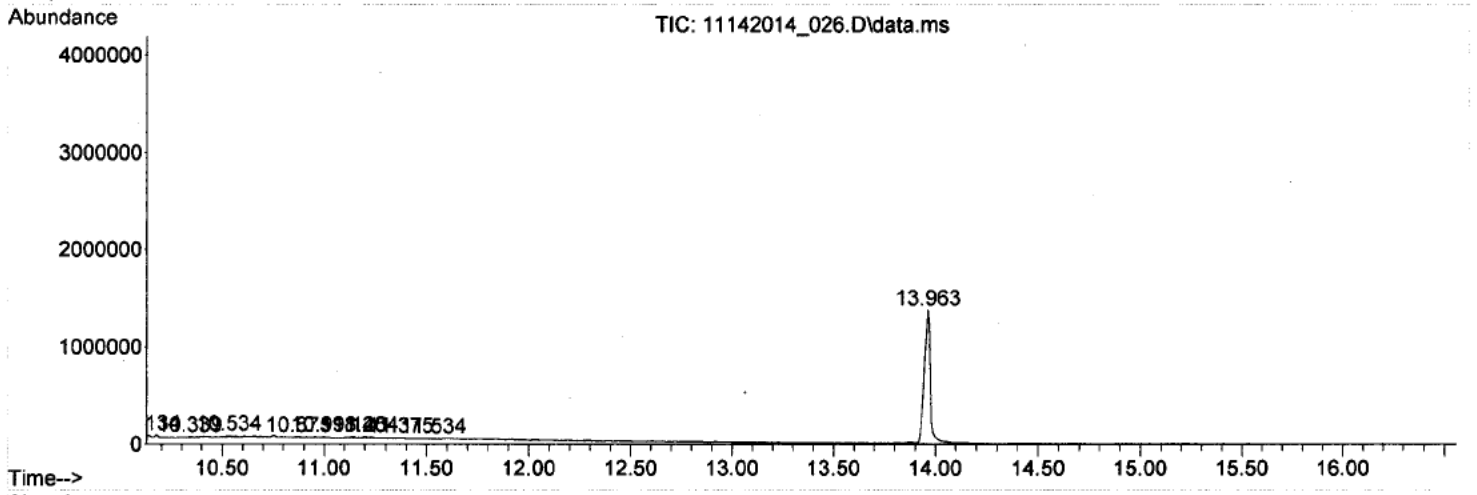
LSC Report - Integrated Chromatogram

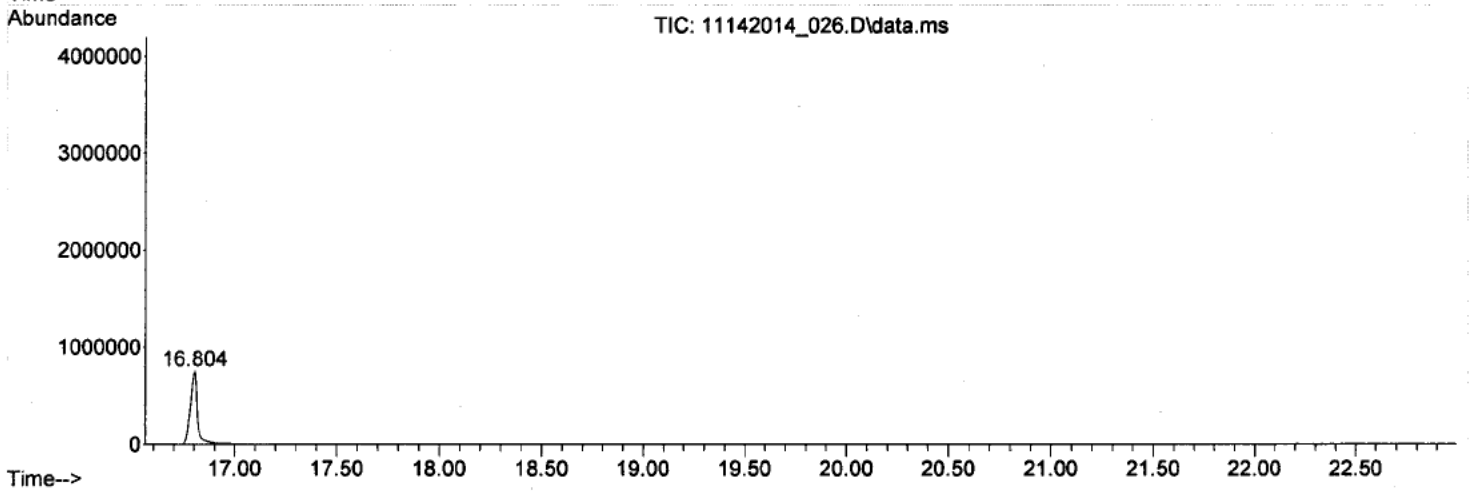
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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







Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

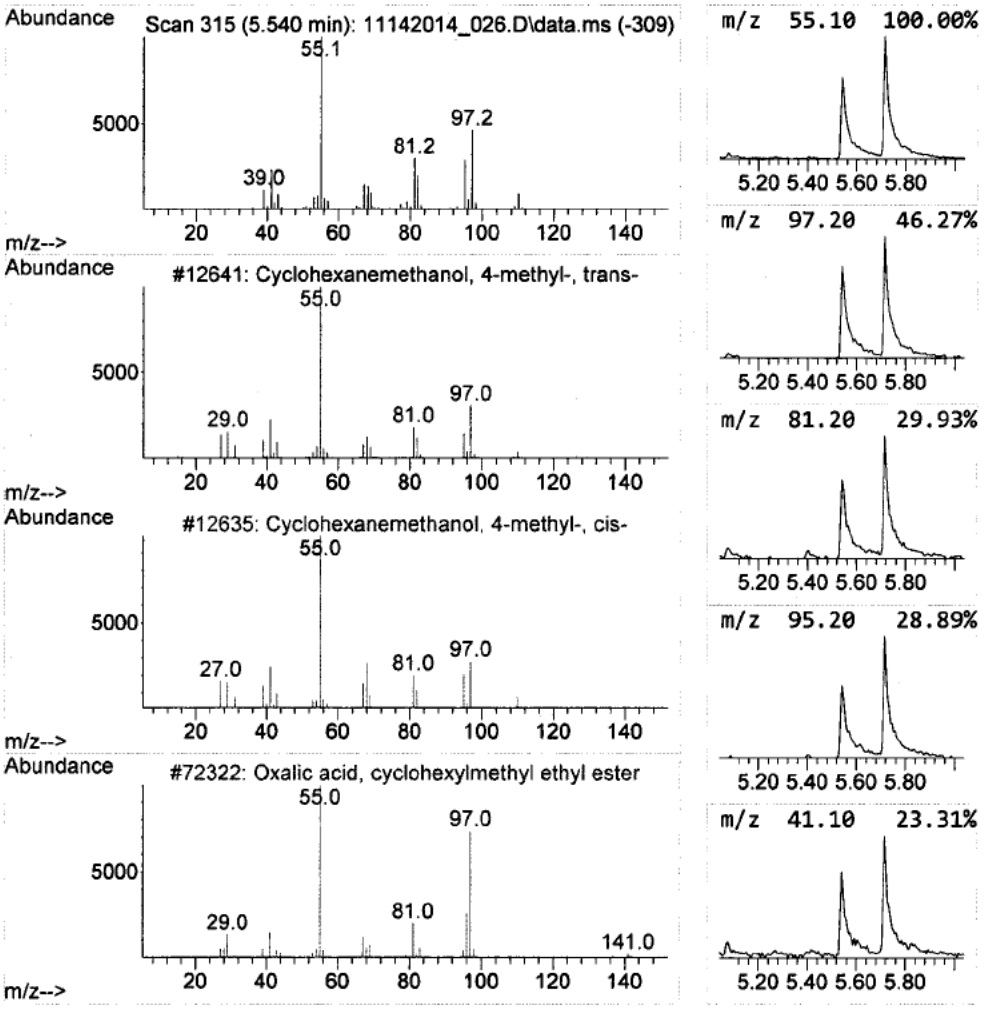
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 1 Cyclohexanemethanol, 4-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.540	1.10 ug/mL	176295	1,4-Dichlorobenzene-d4	5.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	78
2	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	53
3	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	50
4	Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	50
5	1,1'-Bicycloheptyl	194	C14H26	023183-11-1	47



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

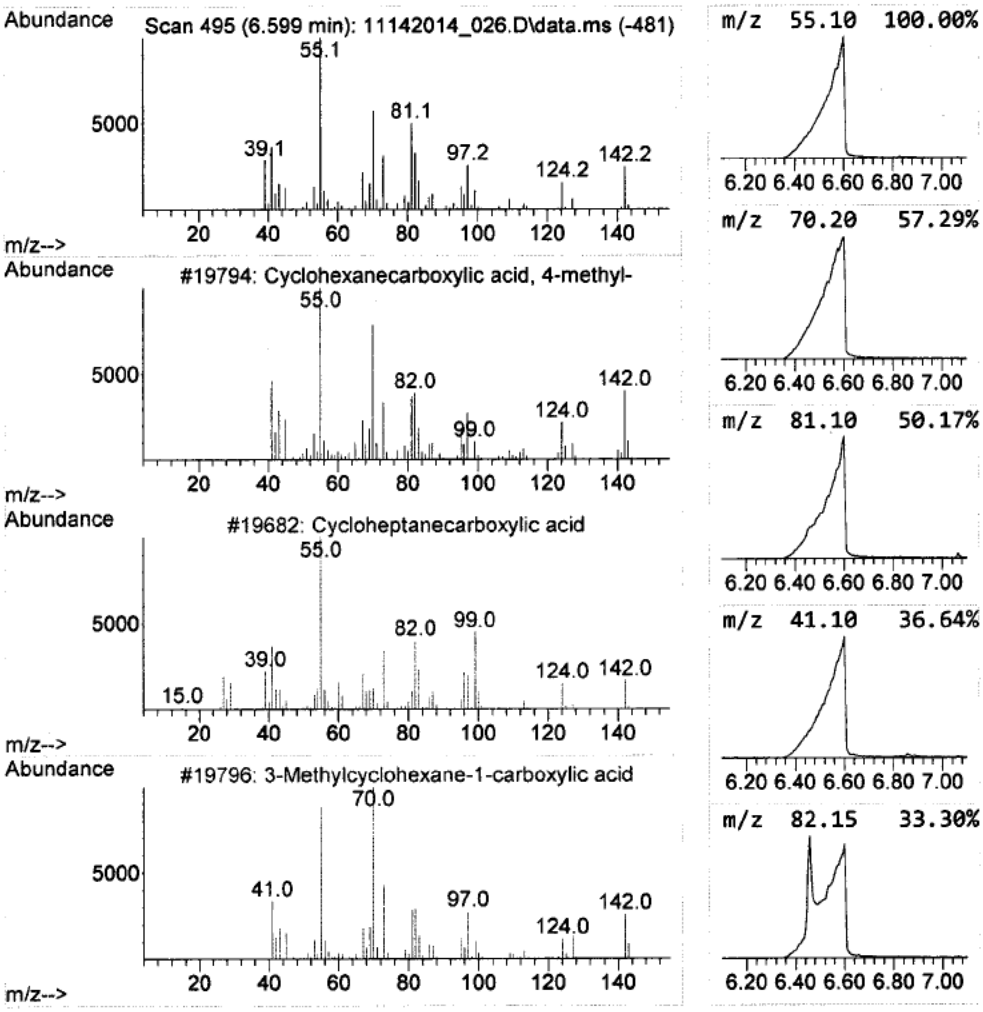
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 2 Cyclohexanecarboxylic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.599	14.70 ug/mL	4372790	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	94
2	Cycloheptanecarboxylic acid	142	C8H14O2	001460-16-8	53
3	3-Methylcyclohexane-1-carboxylic...	142	C8H14O2	1000132-15-7	45
4	1,14-Tetradecanediol	230	C14H30O2	019812-64-7	14
5	Cyclopentanone, oxime	99	C5H9NO	001192-28-5	14



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

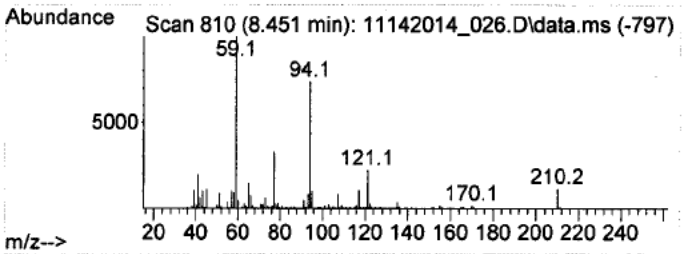
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

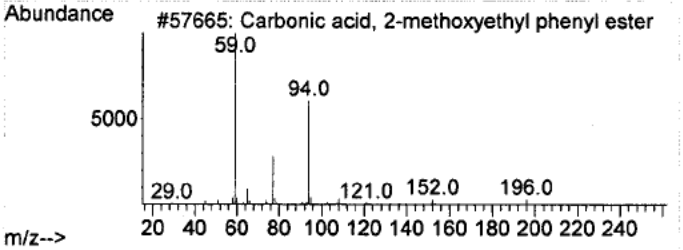
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

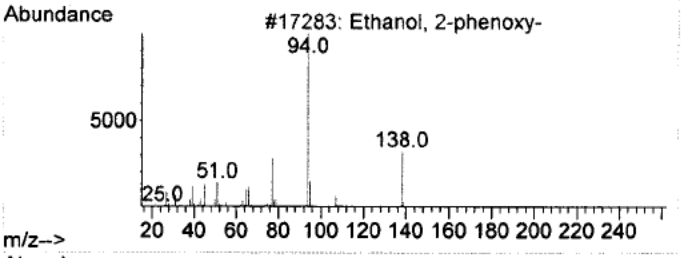
****
Peak Number 3 Carbonic acid, 2-methoxyeth... Concentration Rank 5

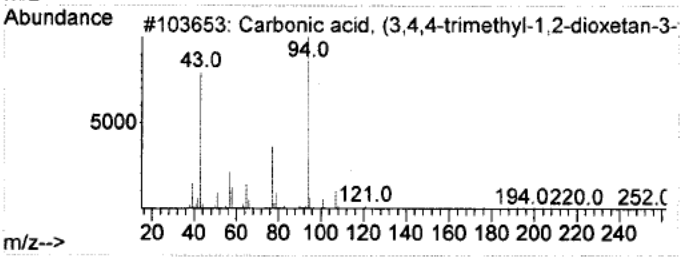
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	0.65 ug/mL	151557	Acenaphthene-d10	8.216

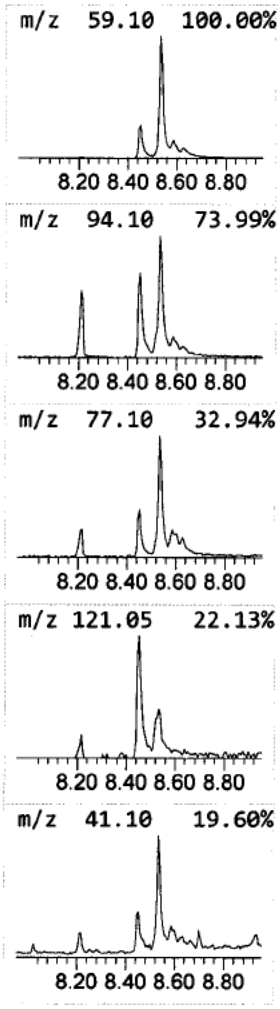
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	72
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	35
3	Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	32
4	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	27
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	27











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

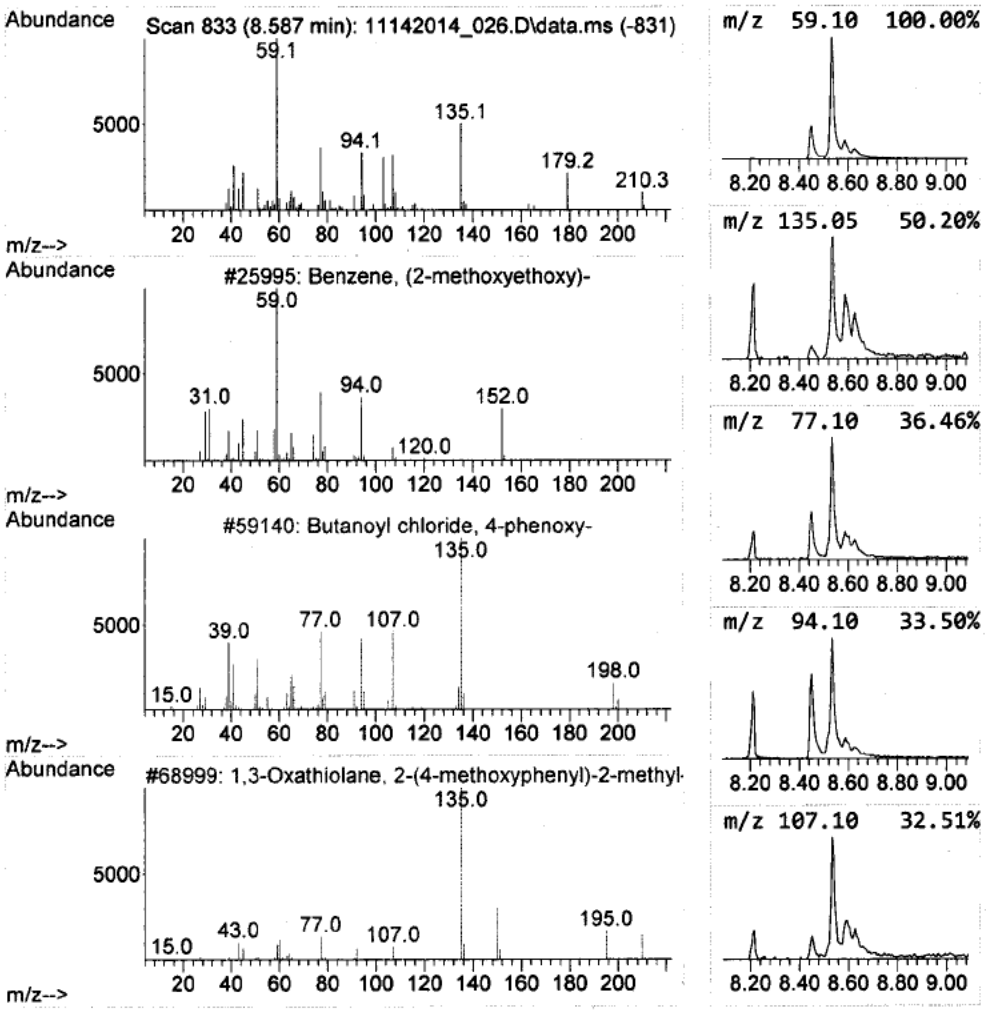
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 4 Benzene, (2-methoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.587	0.65 ug/mL	150787	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methoxyethoxy)-	152	C9H12O2	041532-81-4	32
2	Butanoyl chloride, 4-phenoxy-	198	C10H11ClO2	005139-89-9	27
3	1,3-Oxathiolane, 2-(4-methoxyphe...	210	C11H14O2S	100058-73-9	22
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	16
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	16



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

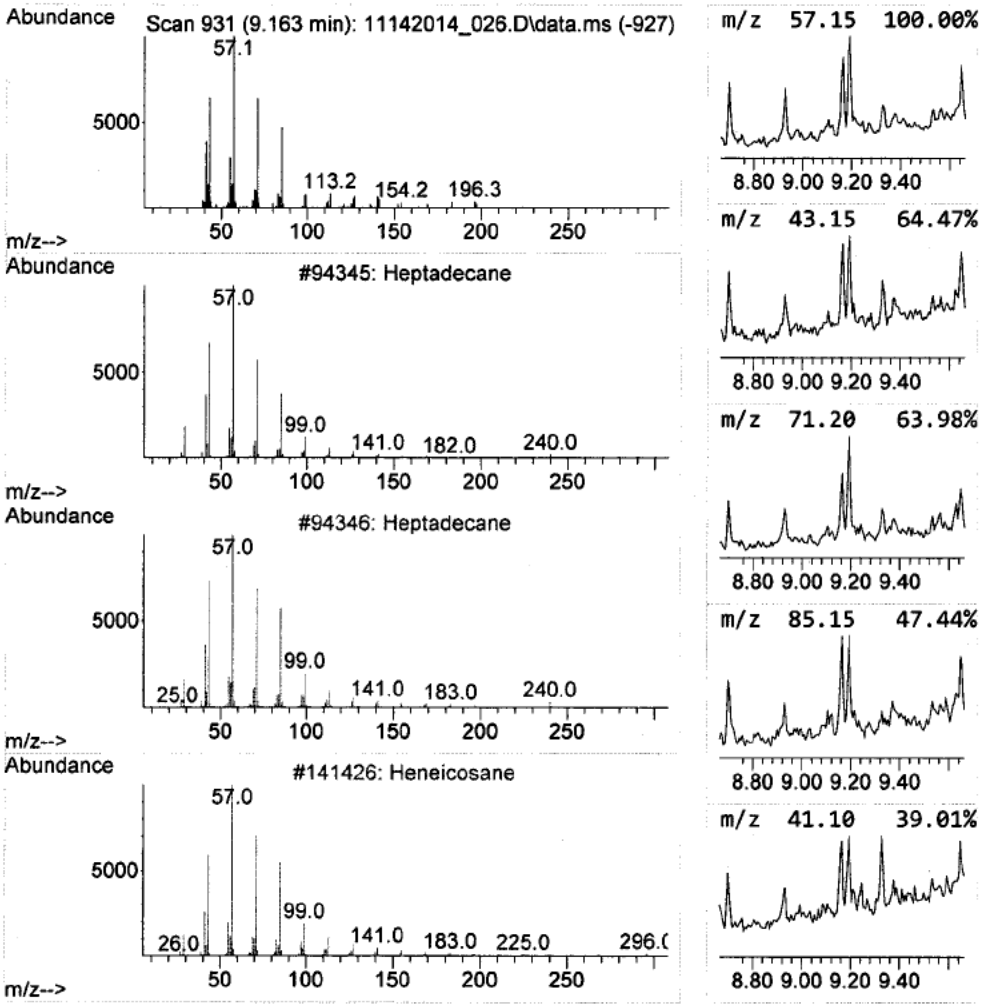
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 5 Heptadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.163	0.17 ug/mL	36841	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Tetracosane	338	C24H50	000646-31-1	80
5	Octadecane	254	C18H38	000593-45-3	80



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

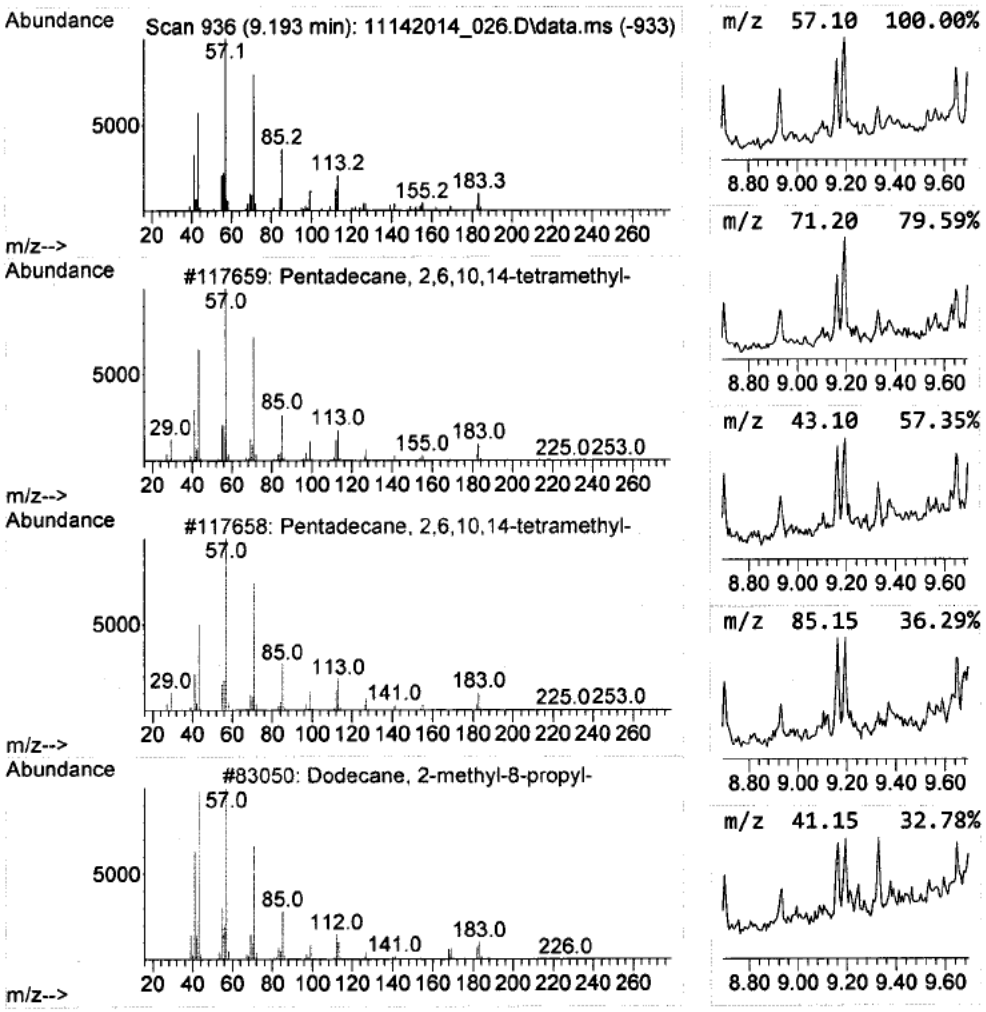
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 6 Pentadecane, 2,6,10,14-tetr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.193	0.26 ug/mL	55387	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
3	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	78
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	72
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59



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Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

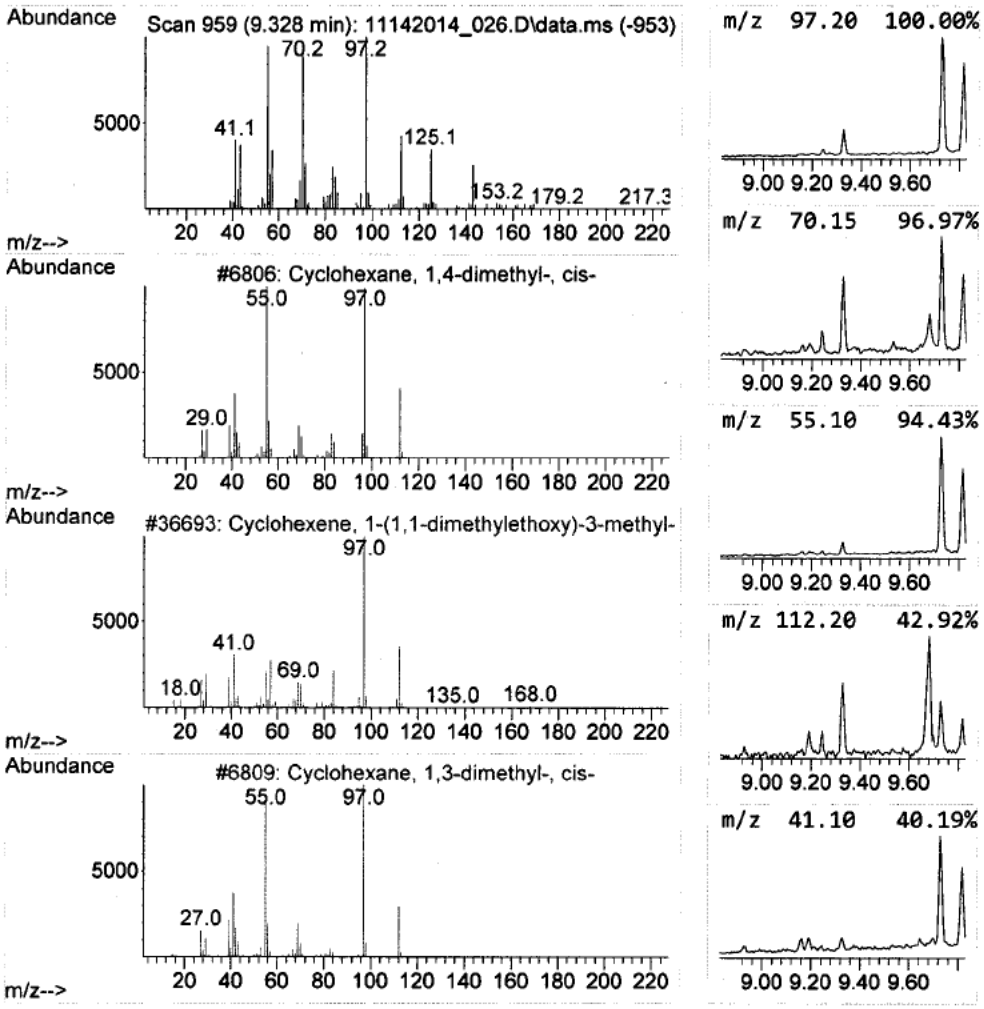
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 7 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	0.25 ug/mL	53067	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	45
2	Cyclohexene, 1-(1,1-dimethyletho...	168	C11H20O	040648-24-6	43
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	38
4	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	38
5	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	38



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Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

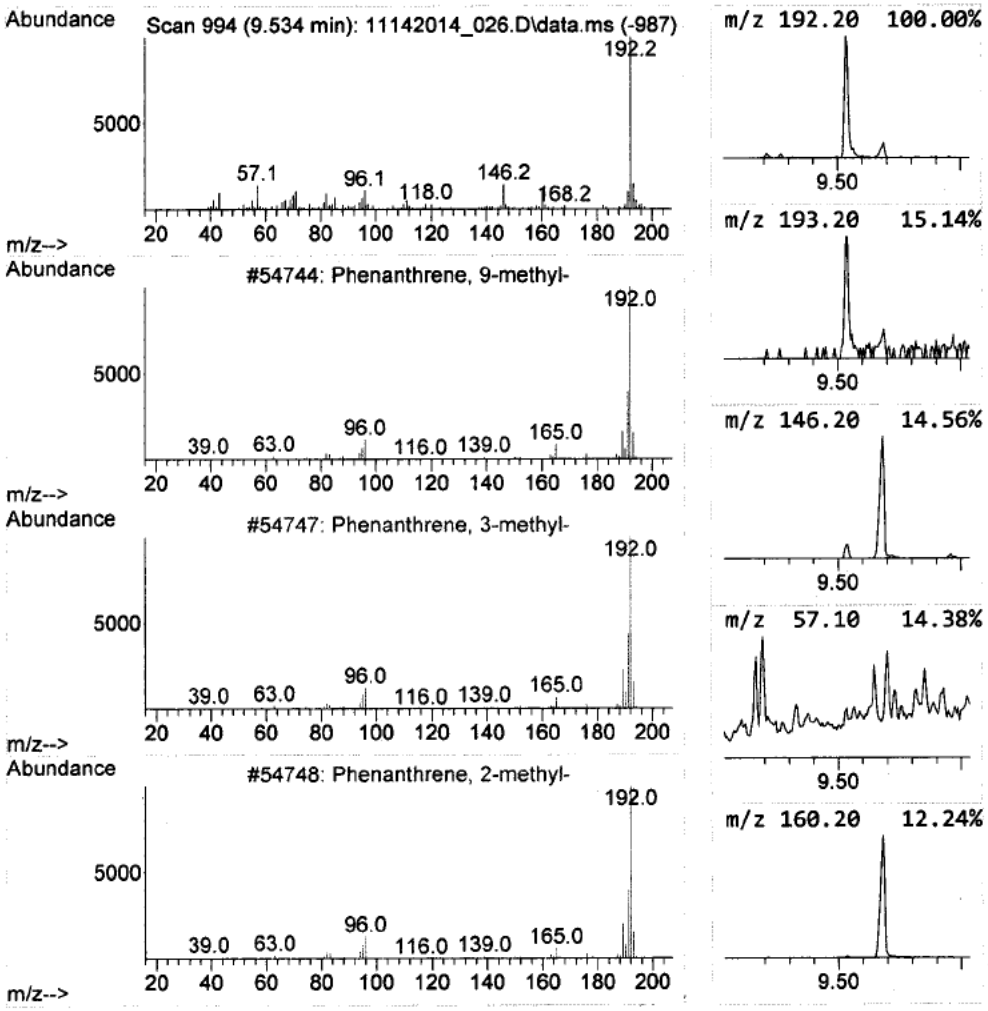
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 8 Phenanthrene, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.534	0.50 ug/mL	107239	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	58
2	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	58
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	58
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	53



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Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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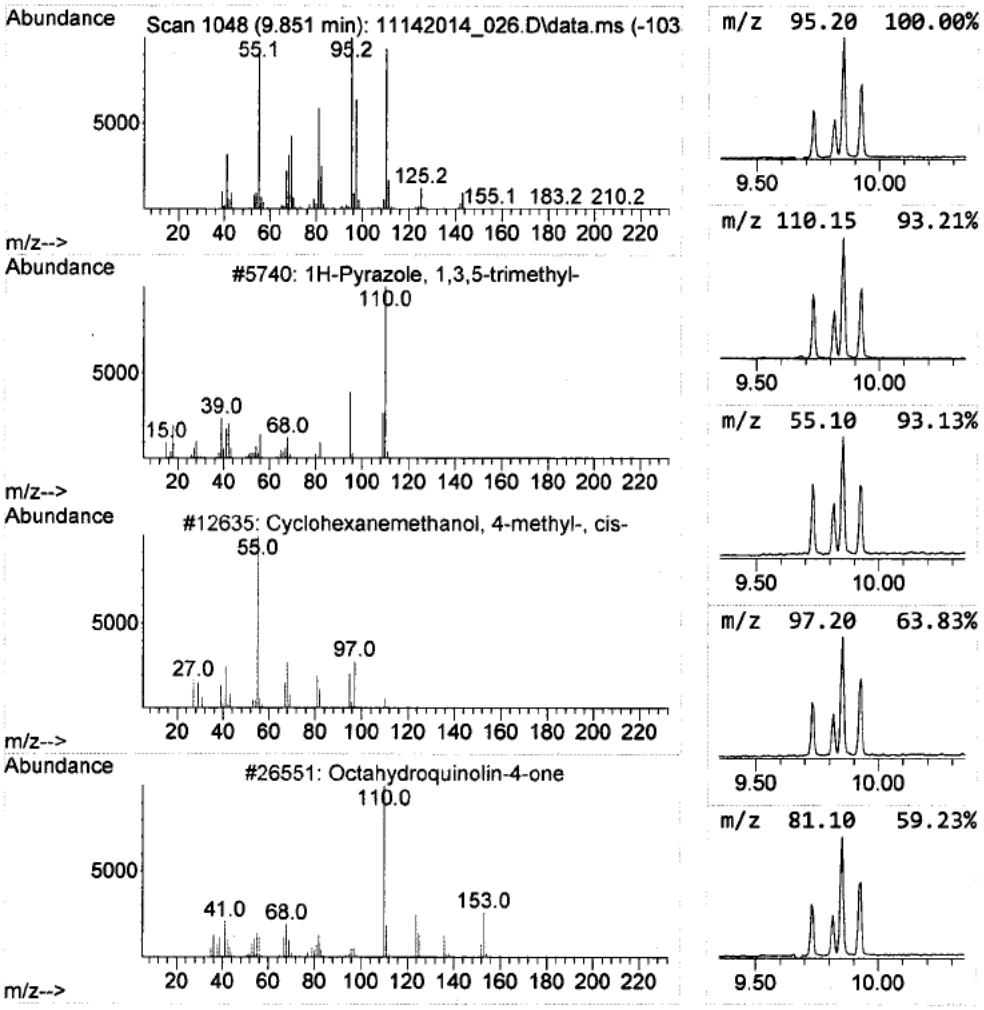
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 9 1H-Pyrazole, 1,3,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	5.64 ug/mL	1216530	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	58
2	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	43
3	Octahydroquinolin-4-one	153	C9H15NO	1000302-88-0	38
4	2-Furancarboxylic acid, 2-ethylc...	222	C13H18O3	1000278-83-7	35
5	4H-Cyclopenta[b]pyridin-4-one, o...	139	C8H13NO	1000327-57-3	35



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Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

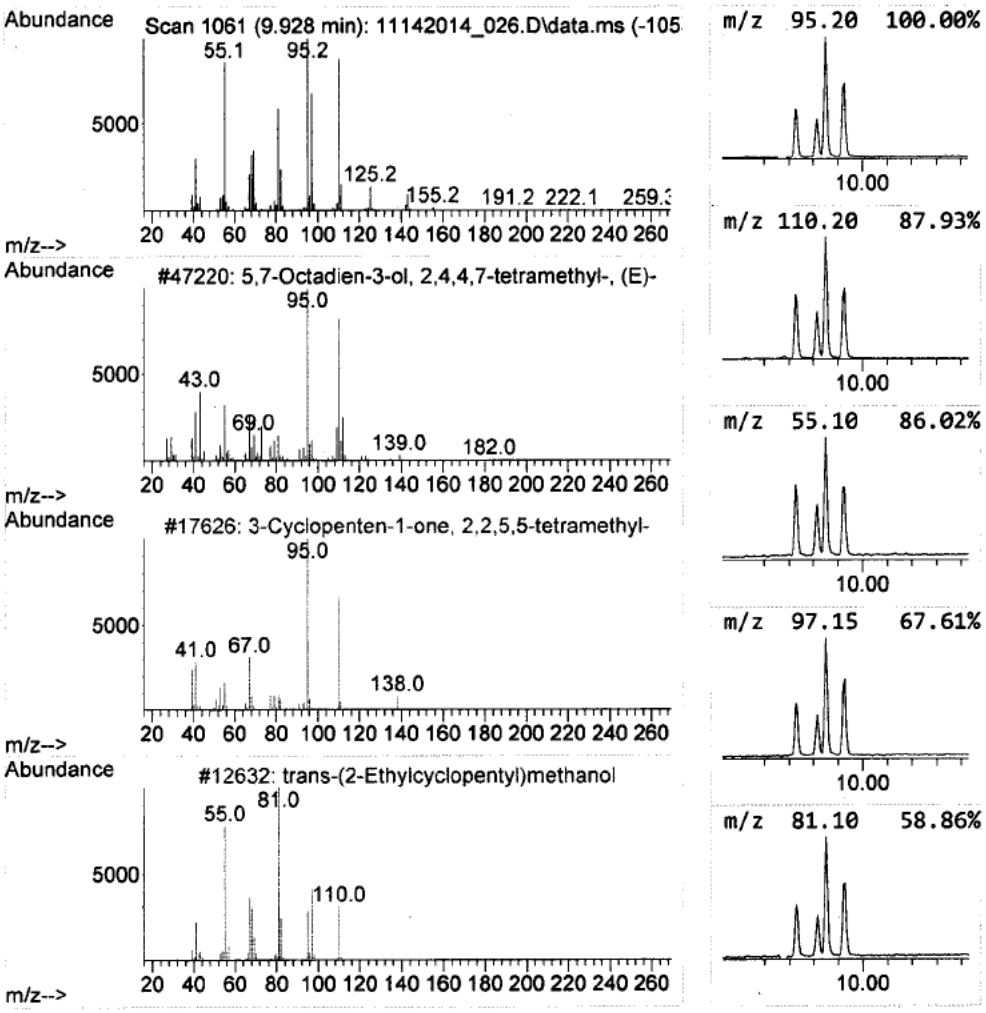
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 10 5,7-Octadien-3-ol, 2,4,4,7-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	2.88 ug/mL	621806	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	50
2	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	47
3	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	47
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	47
5	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43



Library Search Compound Report

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Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

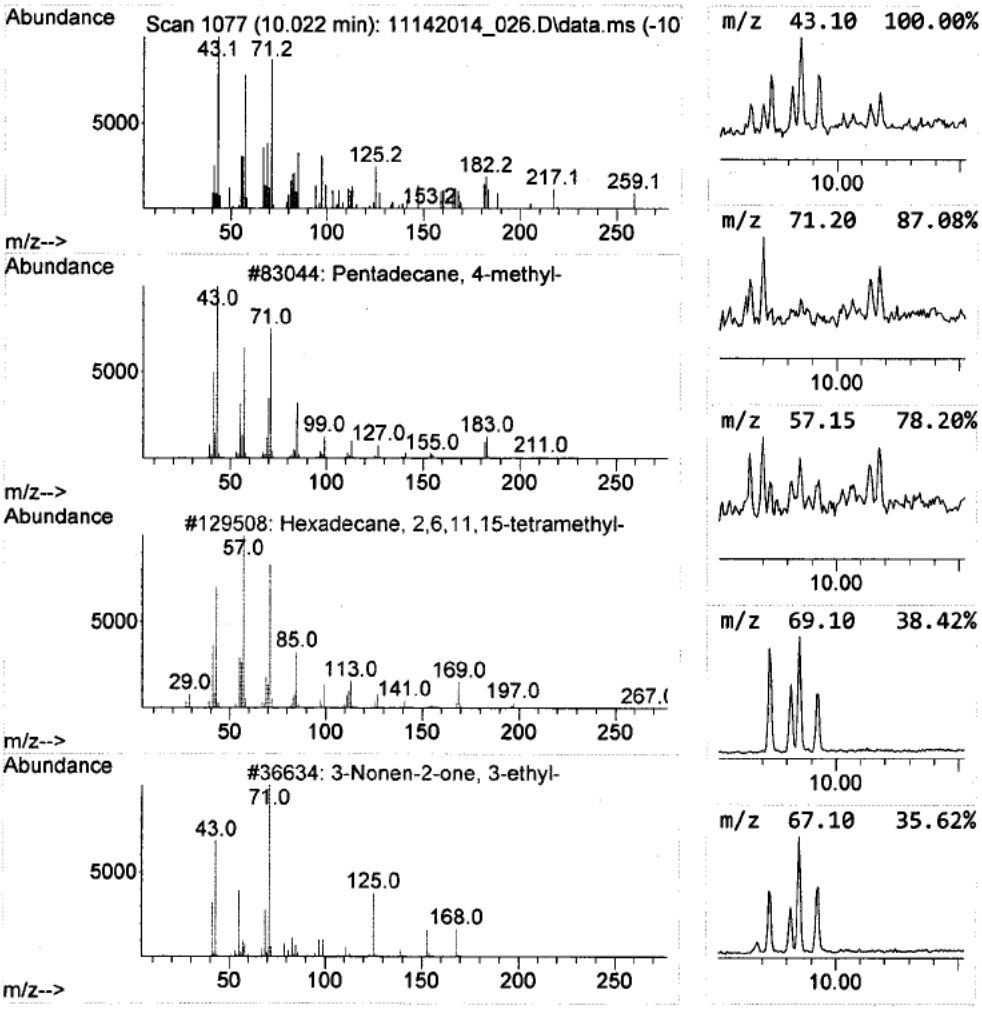
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 11 Pentadecane, 4-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	0.20 ug/mL	42247	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	50
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	43
3	3-Nonen-2-one, 3-ethyl-	168	C11H20O	056312-56-2	43
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	43
5	tert-Nonyl mercaptan	160	C9H20S	025360-10-5	43



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Acq On : 14 Nov 2014 10:05 pm
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Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

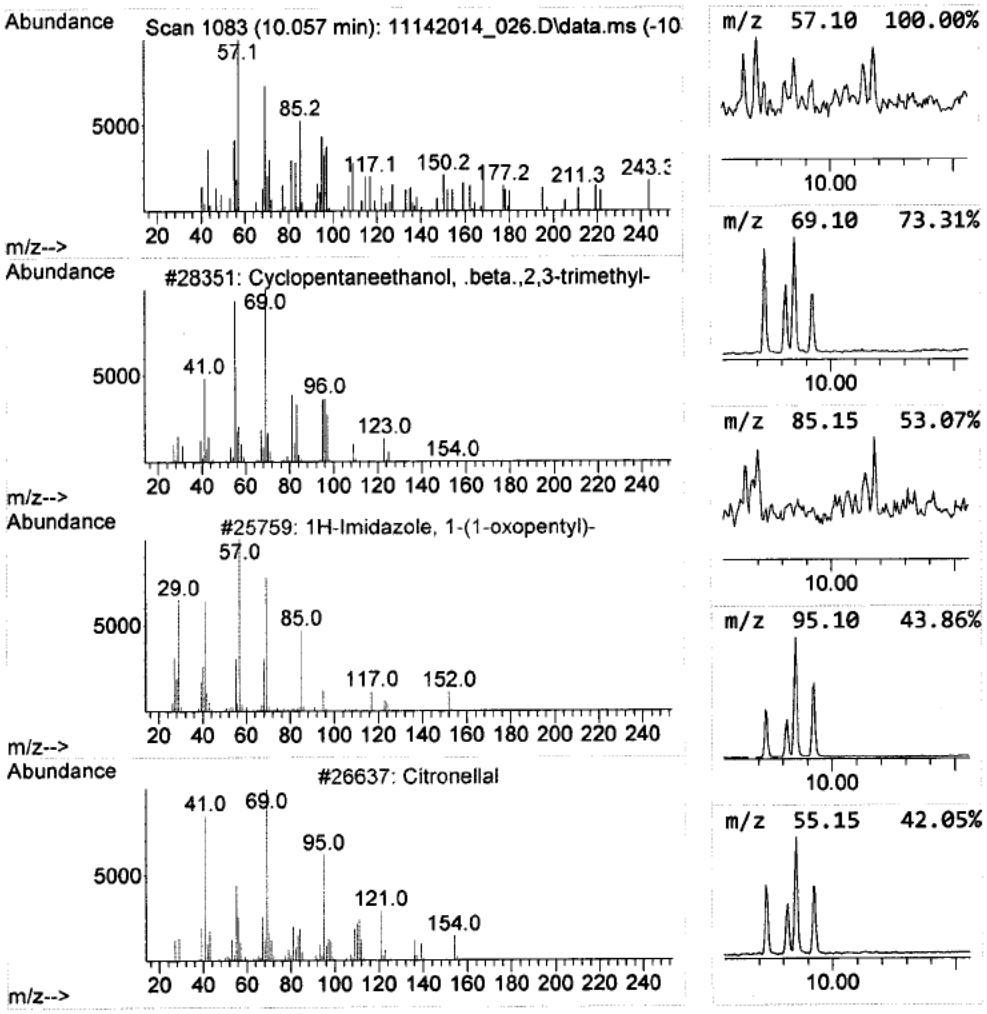
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 12 Cyclopentaneethanol, .beta.... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.057	0.29 ug/mL	62469	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	38
2	1H-Imidazole, 1-(1-oxopentyl)-	152	C8H12N2O	069393-13-1	35
3	Citronellal	154	C10H18O	000106-23-0	35
4	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	27
5	1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	27



Library Search Compound Report

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Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

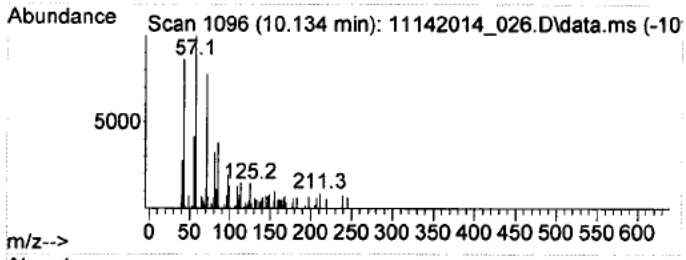
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

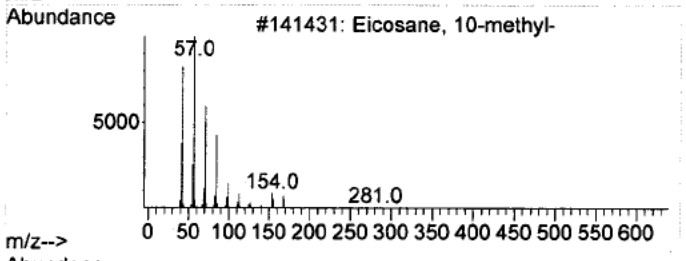
****

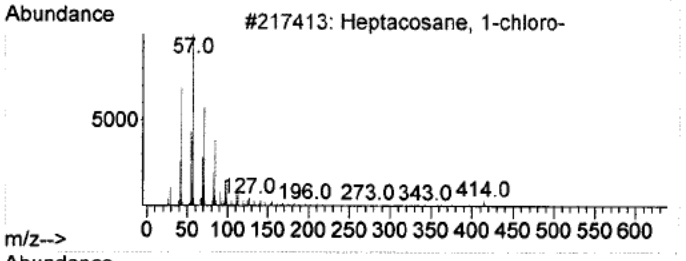
Peak Number 13 Eicosane, 10-methyl- Concentration Rank 15

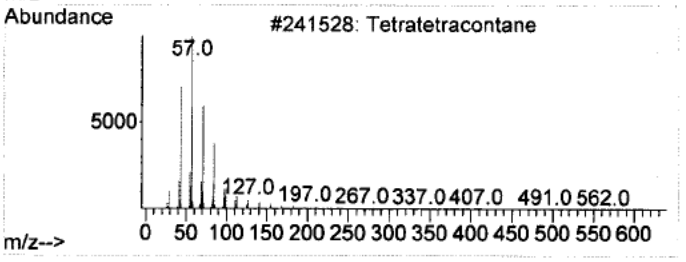
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	0.21 ug/mL	44752	Phenanthrene-d10	9.681

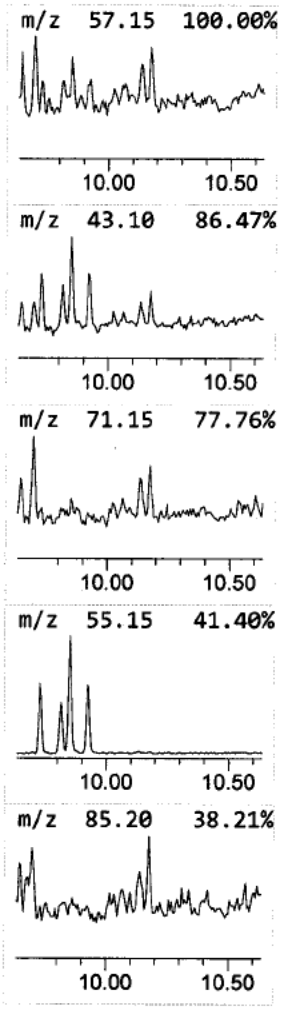
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
3	Tetratetracontane	619	C44H90	007098-22-8	64
4	Tetracosane	338	C24H50	000646-31-1	59
5	Octacosane	394	C28H58	000630-02-4	59











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Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

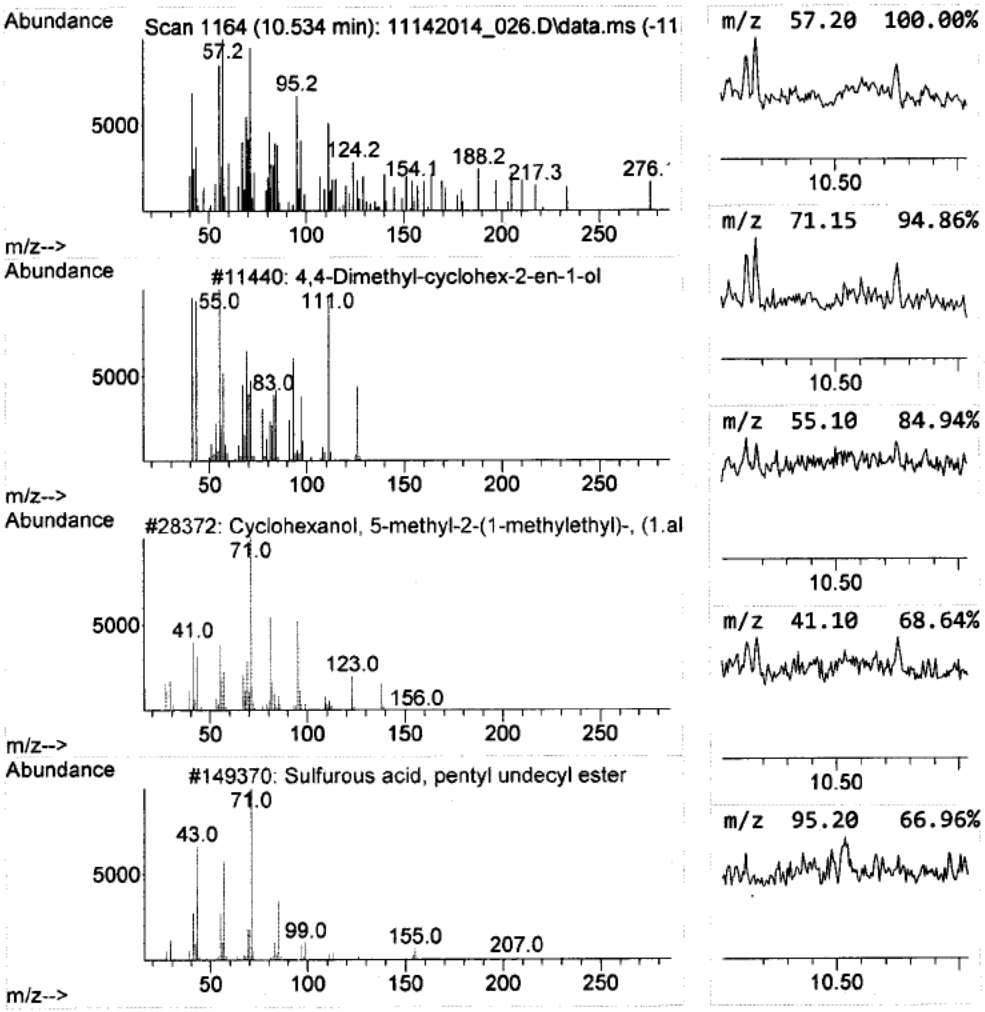
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 14 4,4-Dimethyl-cyclohex-2-en-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.534	0.19 ug/mL	40451	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	1000143-72-5	30
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000490-99-3	27
3	Sulfurous acid, pentyl undecyl e...	306	C16H34O3S	1000309-14-4	27
4	Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	27
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	22



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Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

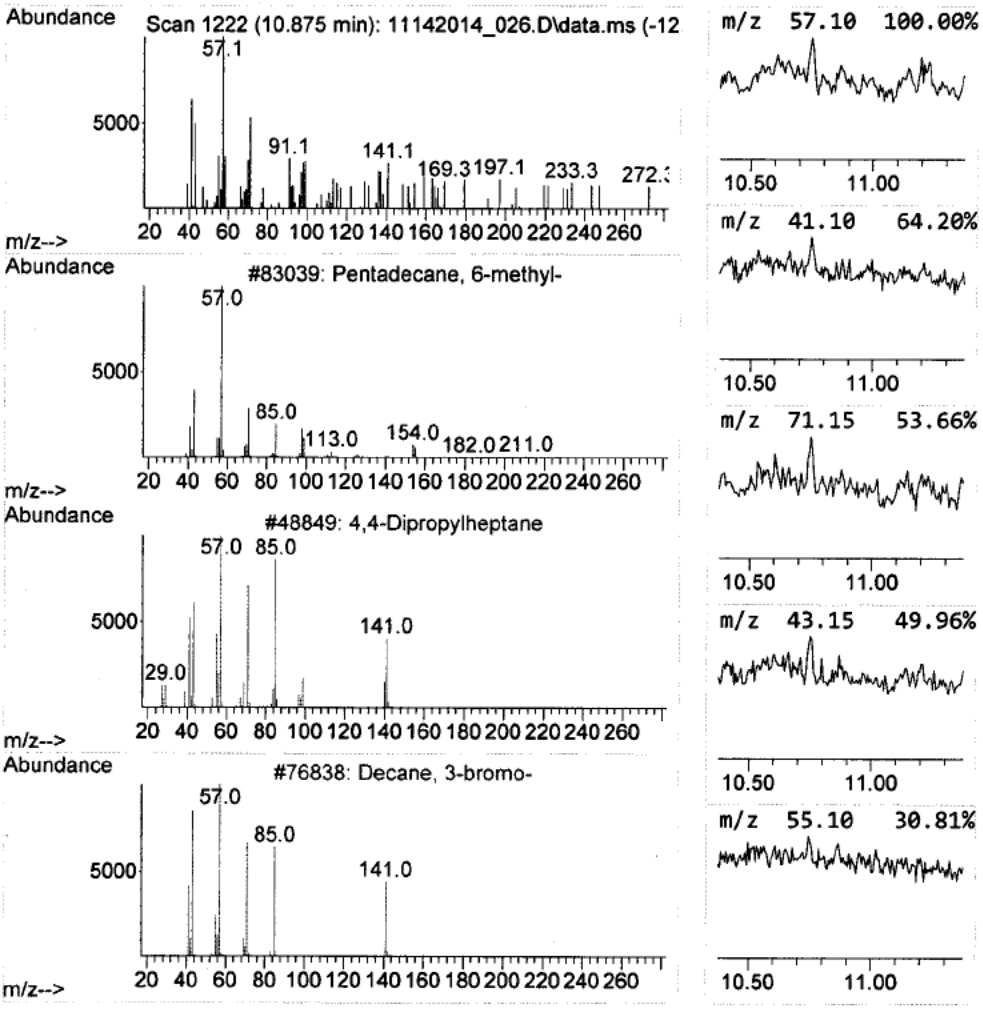
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 15 Pentadecane, 6-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	0.22 ug/mL	46804	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 6-methyl-	226	C16H34	010105-38-1	25
2	4,4-Dipropylheptane	184	C13H28	017312-72-0	16
3	Decane, 3-bromo-	220	C10H21Br	030571-71-2	14
4	Nonane, 4-methyl-	142	C10H22	017301-94-9	12
5	Diaziridinone, bis(1,1-dimethylp...	198	C11H22N2O	019656-75-8	10



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Data File : 11142014_026.D
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Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

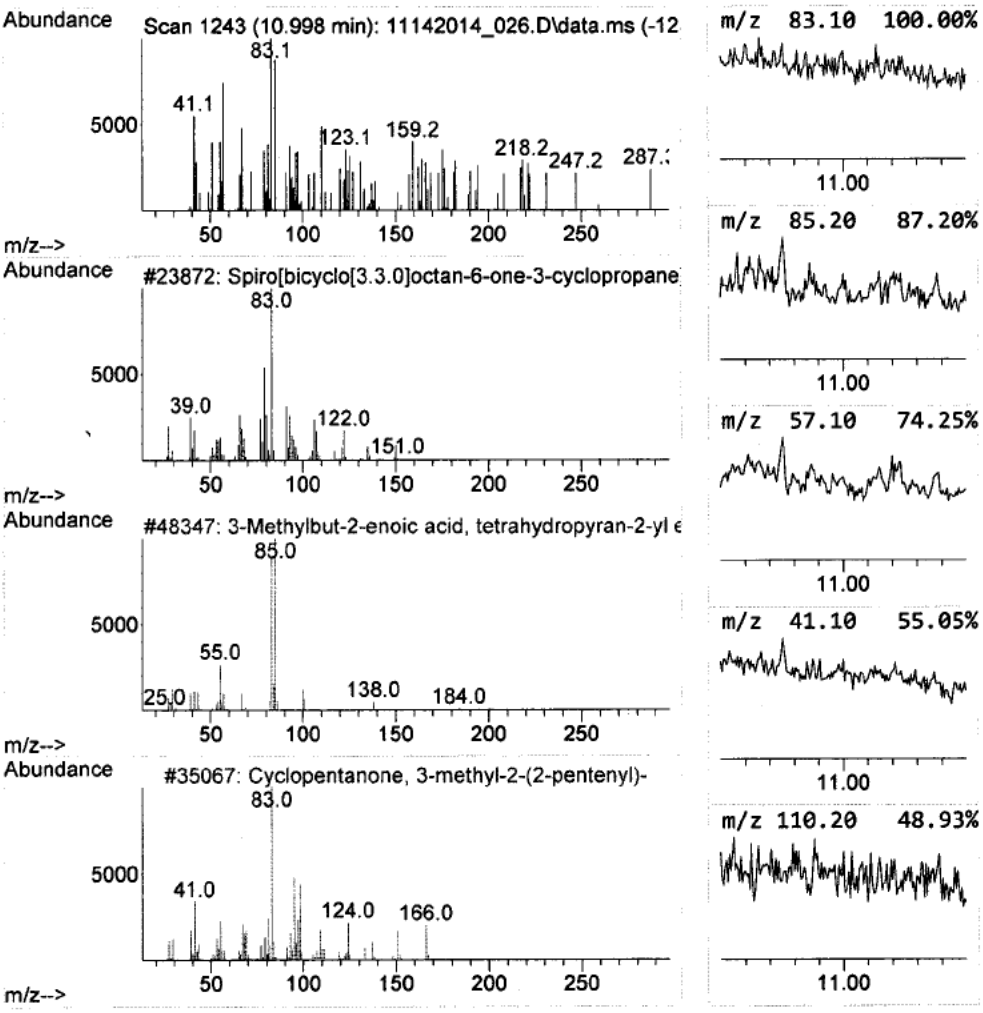
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 16 Spiro[bicyclo[3.3.0]octan-6... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	0.19 ug/mL	40434	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[bicyclo[3.3.0]octan-6-one-...	150	C10H14O	1000152-21-9	12
2	3-Methylbut-2-enoic acid, tetrah...	184	C10H16O3	1000187-32-6	12
3	Cyclopentanone, 3-methyl-2-(2-pe...	166	C11H18O	007051-39-0	11
4	1-Cyclohexylethanol, heptafluoro...	324	C12H15F7O2	1000365-15-8	10
5	8-Azabicyclo[3.2.1]octan-3-ol, 8...	217	C14H19NO	022932-25-8	10



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Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

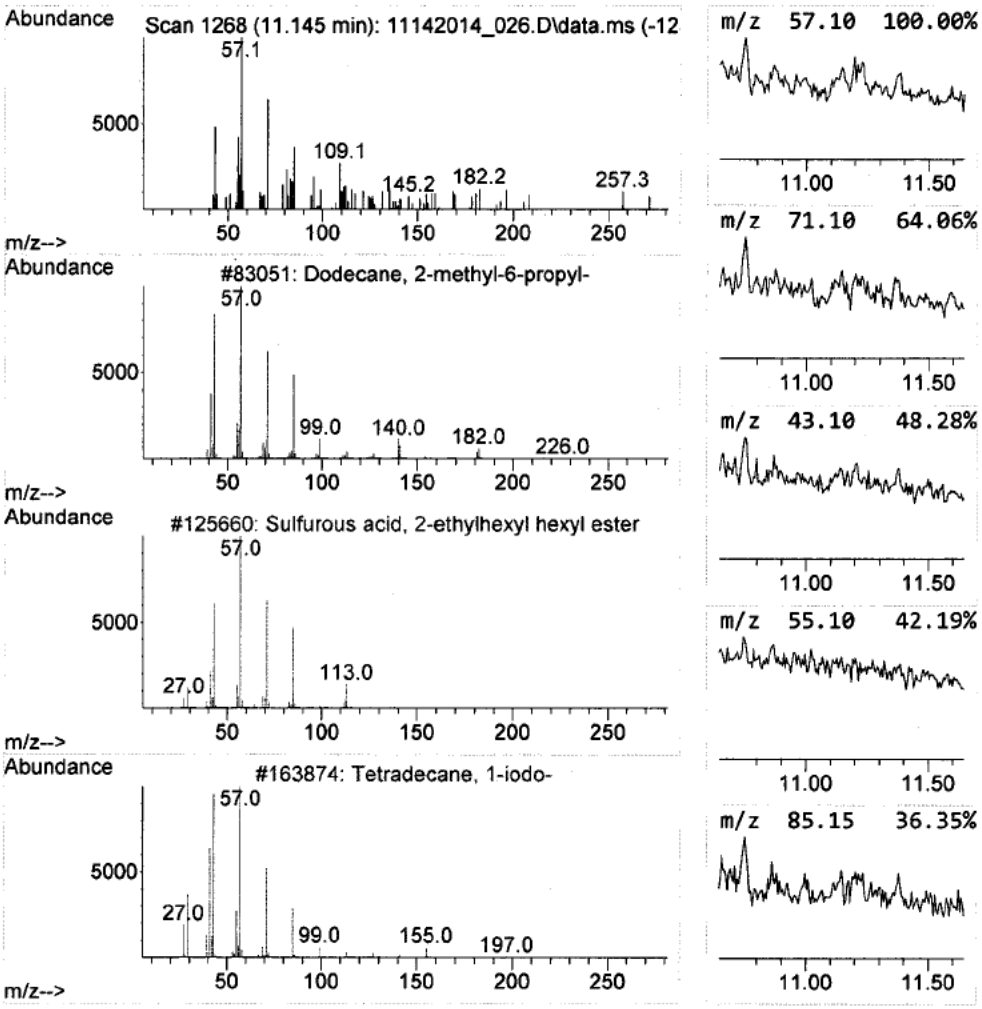
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 17 Dodecane, 2-methyl-6-propyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	0.24 ug/mL	52286	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	27
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H3003S	1000309-20-2	22
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	22
4	Undecane	156	C11H24	001120-21-4	22
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	22



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Data File : 11142014_026.D
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Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

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

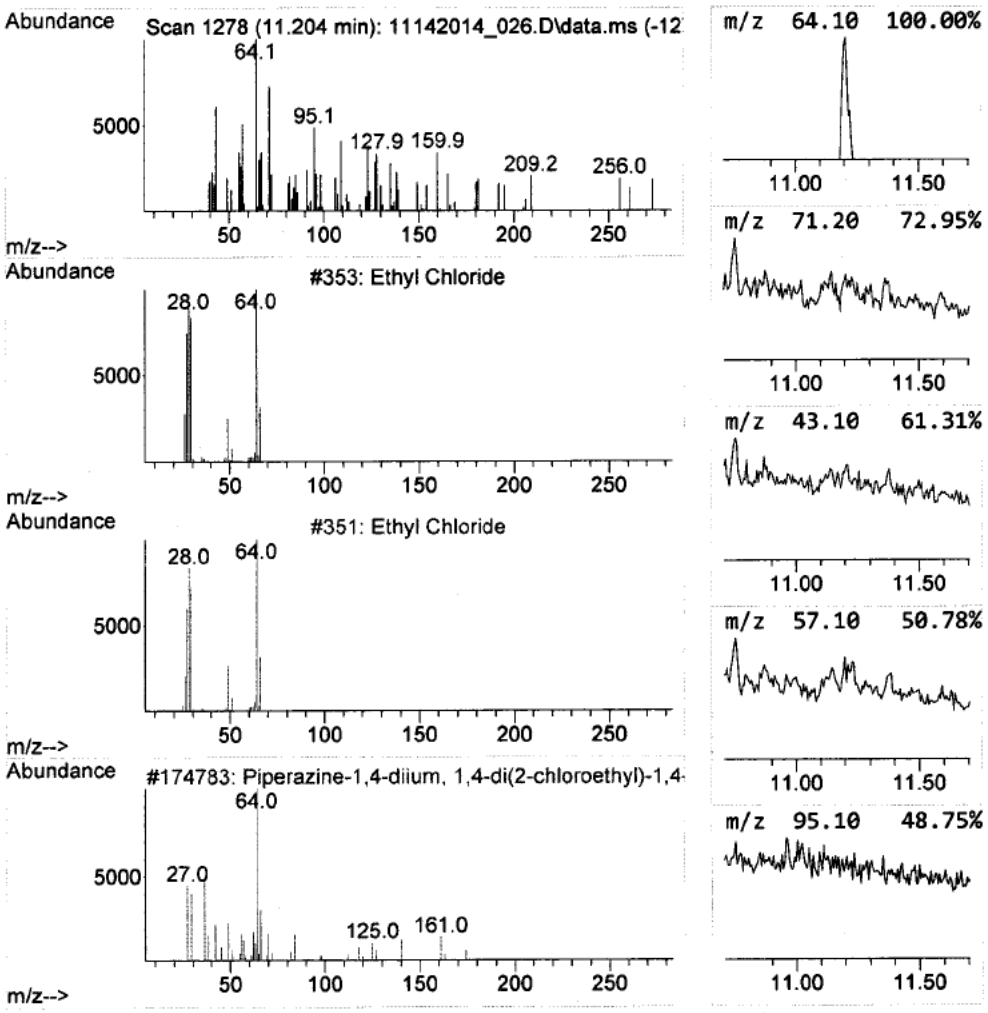
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 18 Ethyl Chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	0.46 ug/mL	99529	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Chloride	64	C2H5Cl	000075-00-3	64
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	59
3	Piperazine-1,4-diium, 1,4-di(2-c...	338	C12H26Cl4N2	1000273-25-4	38
4	2-Nitrobenzenesulfonyl fluoride	205	C6H4FNO4S	000433-98-7	37
5	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	23



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Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

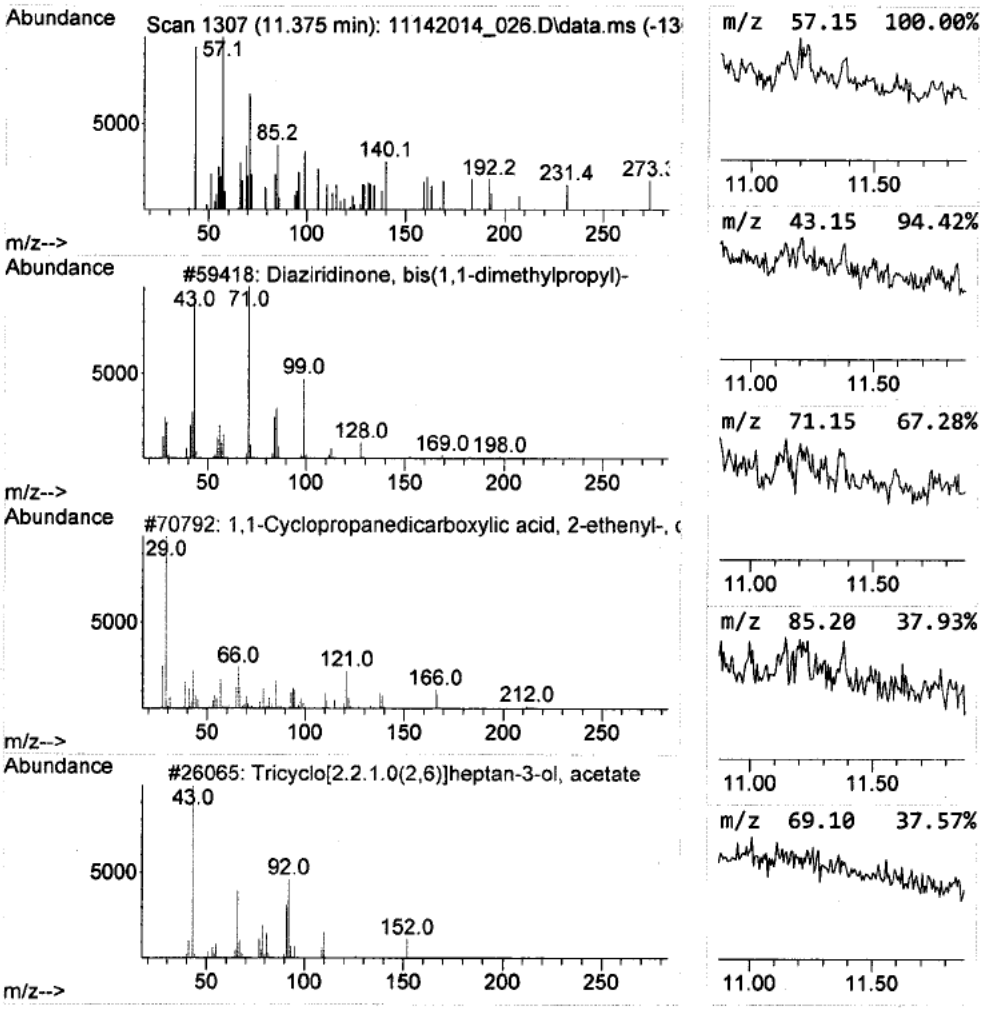
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 19 Diaziridinone, bis(1,1-dime... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.375	0.22 ug/mL	46478	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diaziridinone, bis(1,1-dimethylp...	198	C11H22N2O	019656-75-8	10
2	1,1-Cyclopropanedicarboxylic aci...	212	C11H16O4	007686-78-4	10
3	Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C9H12O2	006555-48-2	10
4	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	10
5	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	10



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

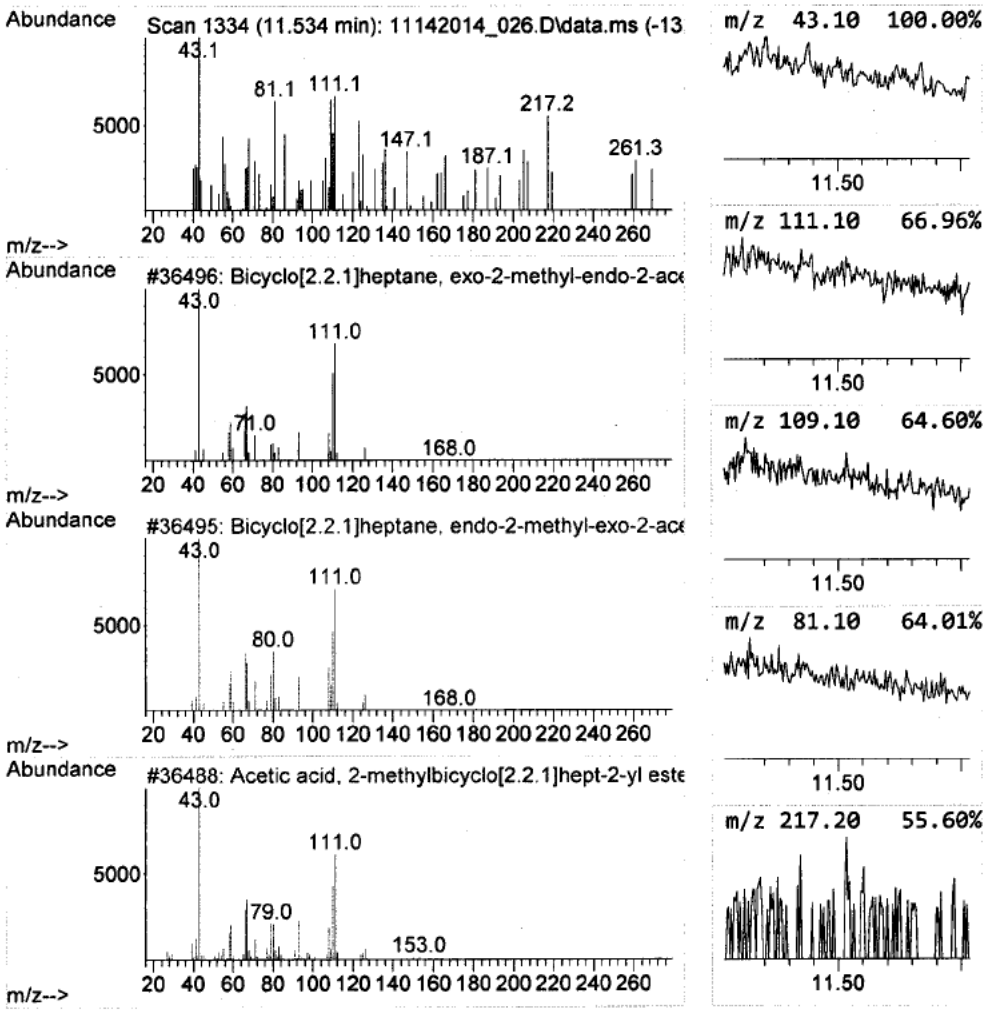
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 20 Bicyclo[2.2.1]heptane, exo-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.534	0.20 ug/mL	43639	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, exo-2-met...	168	C10H16O2	1000138-90-3	27
2	Bicyclo[2.2.1]heptane, endo-2-me...	168	C10H16O2	1000138-90-1	17
3	Acetic acid, 2-methylbicyclo[2.2...	168	C10H16O2	1000191-08-7	16
4	1H-Pyrrole-2,5-dione, 1-ethenyl-	123	C6H5NO2	007685-94-1	14
5	Pyridine, 3-methoxy-	109	C6H7NO	007295-76-3	10



Tentatively Identified Compound (LSC) summary

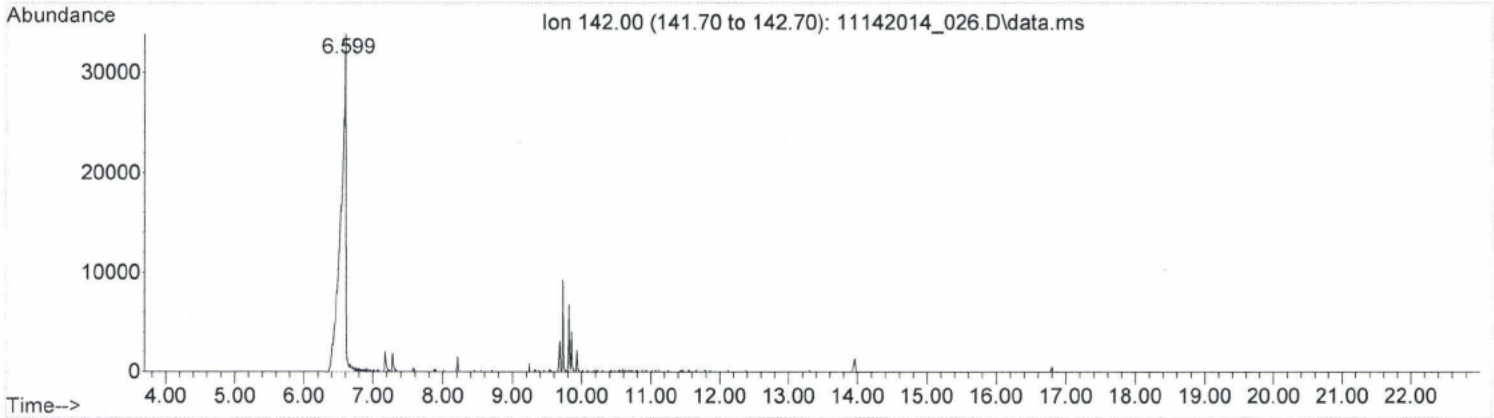
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_026.D
Acq On : 14 Nov 2014 10:05 pm
Operator : [redacted]
Sample : NE36692-MS
Misc : Tag # NE36692-MS, Matrix Spike, 1X
ALS Vial : 25 Sample Multiplier: 1

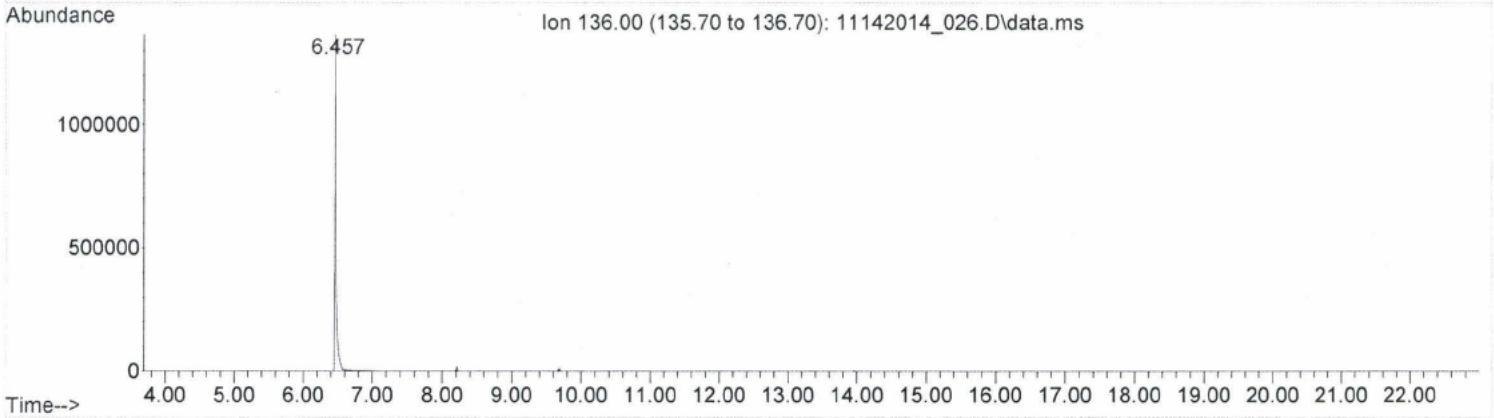
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

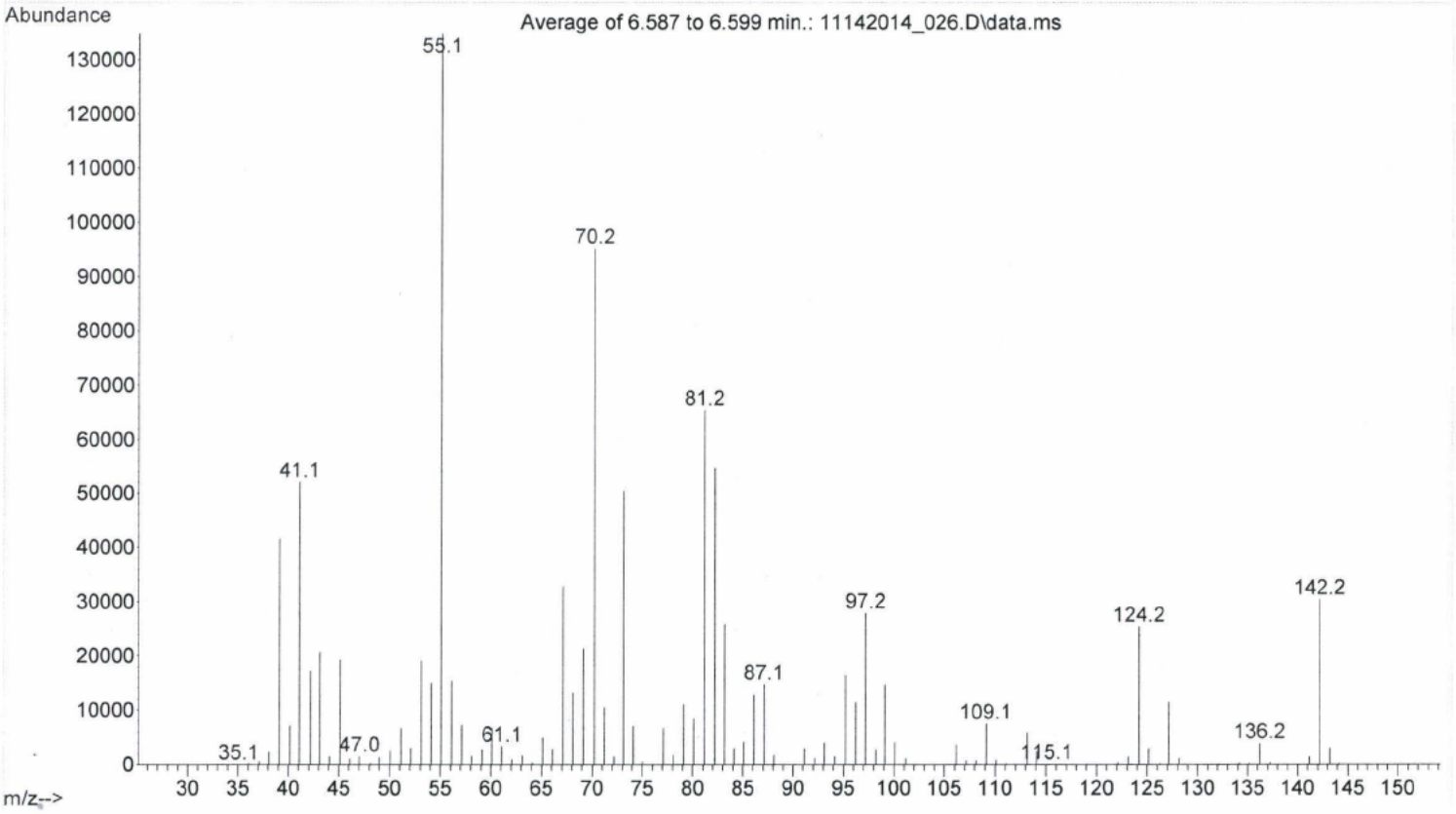
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Cyclohexanemeth...	5.540	1.1	ug/mL	176295	1	5.075	3199310	20.0
Cyclohexanecarb...	6.599	14.7	ug/mL	4372790	2	6.457	5947790	20.0
Carbonic acid, ...	8.451	0.7	ug/mL	151557	3	8.216	4650710	20.0
Benzene, (2-met...	8.587	0.6	ug/mL	150787	3	8.216	4650710	20.0
Heptadecane	9.163	0.2	ug/mL	36841	4	9.681	4316830	20.0
Pentadecane, 2,...	9.193	0.3	ug/mL	55387	4	9.681	4316830	20.0
Cyclohexane, 1,...	9.328	0.2	ug/mL	53067	4	9.681	4316830	20.0
Phenanthrene, 9...	9.534	0.5	ug/mL	107239	4	9.681	4316830	20.0
1H-Pyrazole, 1,...	9.851	5.6	ug/mL	1216530	4	9.681	4316830	20.0
5,7-Octadien-3-...	9.928	2.9	ug/mL	621806	4	9.681	4316830	20.0
Pentadecane, 4-...	10.022	0.2	ug/mL	42247	4	9.681	4316830	20.0
Cyclopentaneeth...	10.057	0.3	ug/mL	62469	4	9.681	4316830	20.0
Eicosane, 10-me...	10.134	0.2	ug/mL	44752	4	9.681	4316830	20.0
4,4-Dimethyl-cy...	10.534	0.2	ug/mL	40451	4	9.681	4316830	20.0
Pentadecane, 6-...	10.875	0.2	ug/mL	46804	4	9.681	4316830	20.0
Spiro[bicyclo[3...	10.998	0.2	ug/mL	40434	4	9.681	4316830	20.0
Dodecane, 2-met...	11.145	0.2	ug/mL	52286	4	9.681	4316830	20.0
Ethyl Chloride	11.204	0.5	ug/mL	99529	4	9.681	4316830	20.0
Diaziridinone, ...	11.375	0.2	ug/mL	46478	4	9.681	4316830	20.0
Bicyclo[2.2.1]h...	11.534	0.2	ug/mL	43639	4	9.681	4316830	20.0

File :D:[redacted]\RP1616\11142014_Run\11142014_026.D
Operator : [redacted]
Acquired : 14 Nov 2014 10:05 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36692-MS
Misc Info : Tag # NE36692-MS, Matrix Spike, 1X
Vial Number: 25







[redacted] RP1616 12/17/14

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Nov 17 11:08:23 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	427851	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1861756	20.00 ug/mL	# 0.00
5) Acenaphthene-d10	8.216	164	1022448	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.681	188	1561524	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	936135	20.00 ug/mL	0.00
12) Perylene-d12	16.804	264	584841	20.00 ug/mL	0.01
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	585637	9.32 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery	= ~~74.56%~~	
Target Compounds					Qvalue
2) MCHM	5.540	55	55953m	1.47 ug/mL	
4) PPH	6.863	94	10205m	0.55 ug/mL	
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	48495m	1.71 ug/mL	

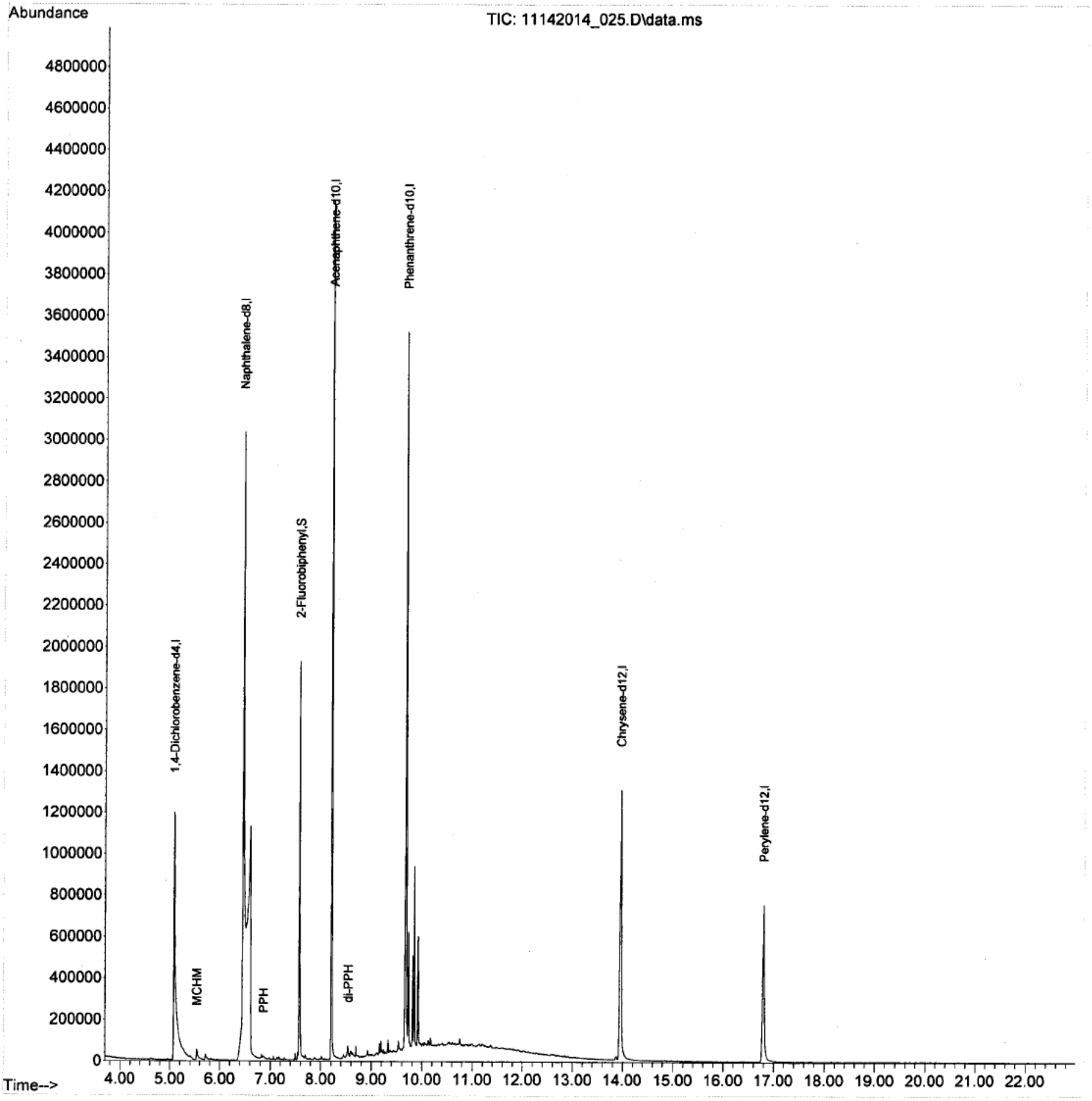
See Analyst Narrative, Surrogate Recovery [redacted] 1/7/15

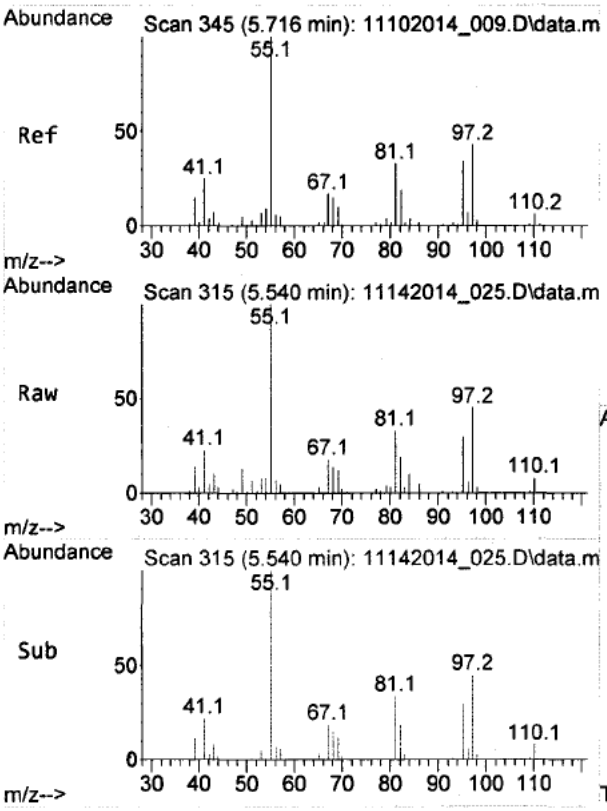
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Nov 17 11:08:23 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

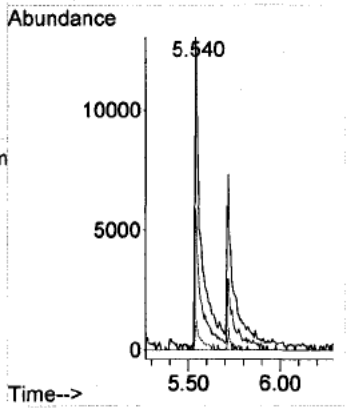


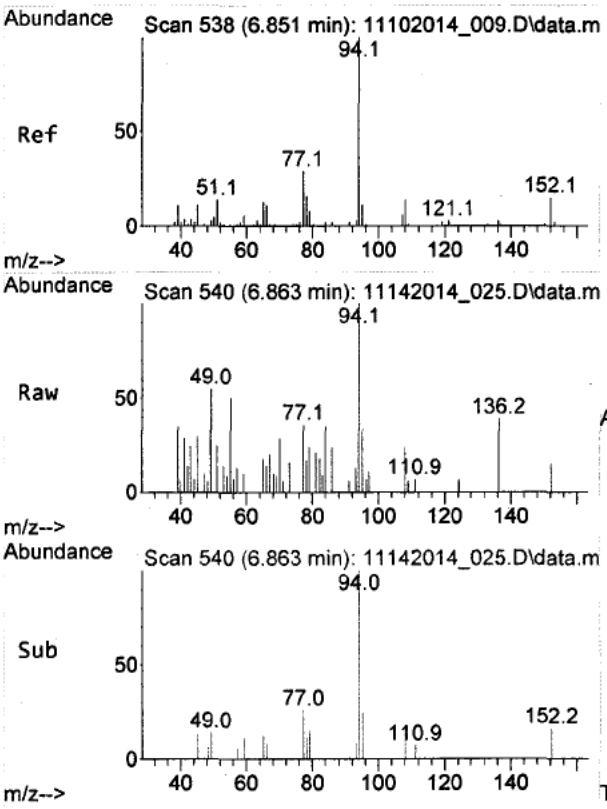


#2
MCHM
Concen: 1.47 ug/mL m
RT: 5.540 min Scan# 315
Delta R.T. -0.176 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 55 Resp: 55953

Ion	Ratio	Lower	Upper
55	100		
97	8.3	34.6	51.8#
110	1.8	4.8	7.2#

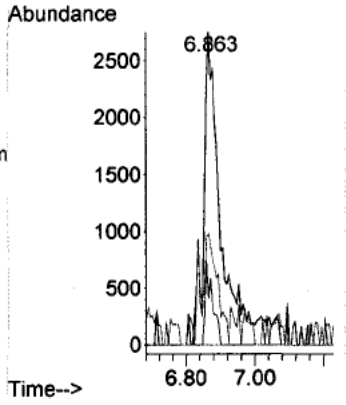


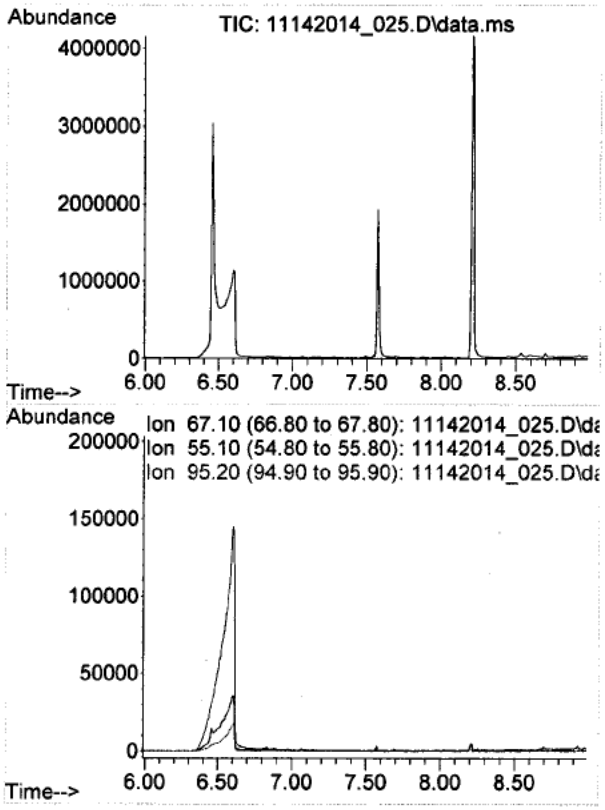


#4
PPH
Concen: 0.55 ug/mL m
RT: 6.863 min Scan# 540
Delta R.T. 0.006 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 94 Resp: 10205

Ion	Ratio	Lower	Upper
94	100		
152	10.4	13.4	20.0#
77	23.9	21.2	31.8



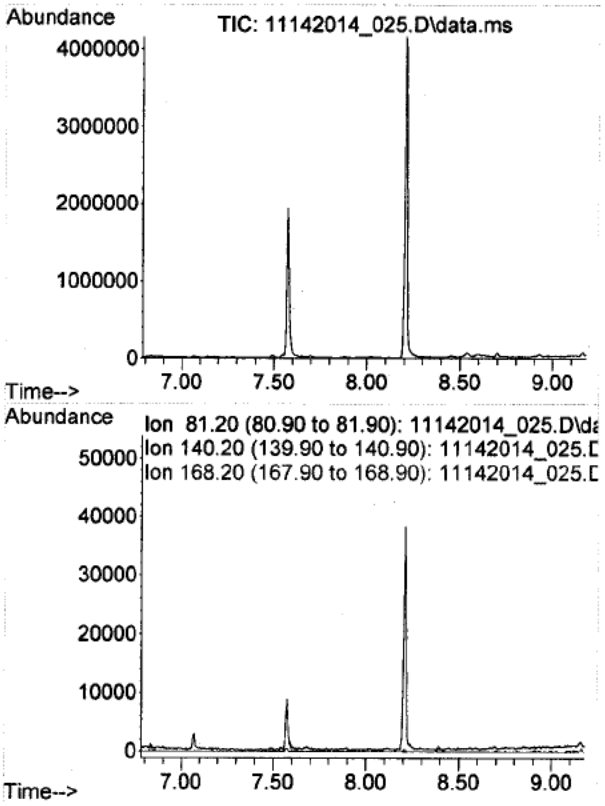


#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8

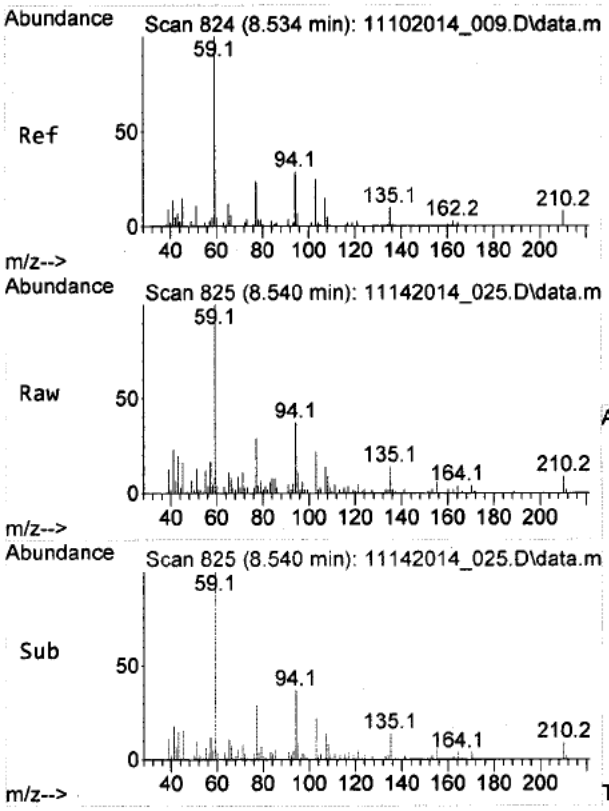


#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 81

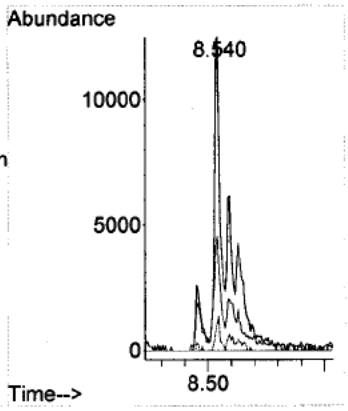
Sig	Exp Ratio
81	100
140	61.8
168	17.7



#9
di-PPH
Concen: 1.71 ug/mL m
RT: 8.540 min Scan# 825
Delta R.T. -0.000 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 59 Resp: 48495

Ion	Ratio	Lower	Upper
59	100		
94	15.8	23.0	34.6#
210	3.7	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Dec 01 12:49:49 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	738919	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1861756	20.00 ug/mL	# 0.00
24) Acenaphthene-d10	8.216	164	1022448	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.681	188	1561524	20.00 ug/mL	0.00
49) Chrysene-d12	13.963	240	936135	20.00 ug/mL	-0.01
58) Perylene-d12	16.804	264	584841	20.00 ug/mL	0.00
Target Compounds					Qvalue
2) Bis(2-chloroethyl) ether	0.000		0	N.D.	
3) n-Decane	0.000		0	N.D. d	
4) 1,3-Dichlorobenzene	0.000		0	N.D. d	
5) 1,4-Dichlorobenzene	0.000		0	N.D. d	
6) 1,2-Dichlorobenzene	0.000		0	N.D. d	
7) Benzyl Alcohol	0.000		0	N.D. d	
8) Bis(2-chloroisopropyl)...	0.000		0	N.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...	6.604	55	838035	63.27 ug/mL	95
14) n-Dodecane	0.000		0	N.D. d	
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	0.000		0	N.D. d	
19) Hexachlorobutadiene	0.000		0	N.D.	
20) 2-Methylnapthalene	7.175	142	5357	0.06 ug/mL	93
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	0.000		0	N.D. d	
23) n-Tetradecane	7.693	57	4125	0.08 ug/mL#	93
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	8.393	168	1239	0.01 ug/mL	88
30) 2,4-Dinitrotoluene	0.000		0	N.D. d	
31) n-Hexadecane	8.698	57	7023	0.12 ug/mL#	92
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	10752	0.19 ug/mL#	98
41) Phenanthrene	9.698	178	4134	0.03 ug/mL#	84
42) Anthracene	0.000		0	N.D. d	
43) Carbazole	0.000		0	N.D. d	
44) Dibutyl Phthalate	0.000		0	N.D. d	
45) n-Eicosane	10.751	57	6650	0.12 ug/mL#	100

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Dec 01 12:49:49 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

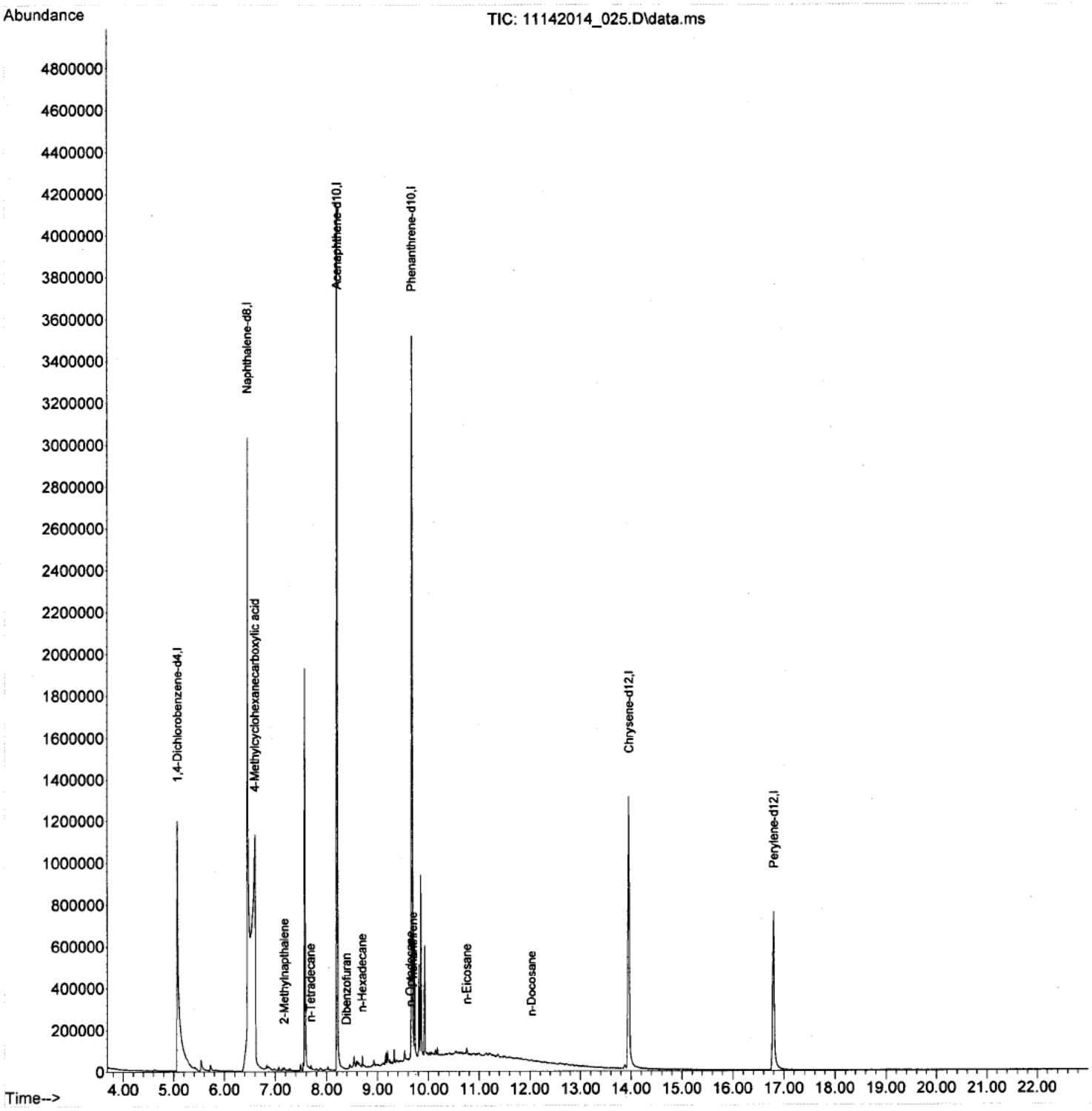
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	0.000		0	N.D. d	
47) Pyrene	0.000		0	N.D. d	
48) n-Docosane	12.034	57	3630	0.07 ug/mL#	91
50) Benzyl Butyl Phthalate	0.000		0	N.D. d	
51) n-Tetracosane	0.000		0	N.D. d	
52) n-Hexacosane	0.000		0	N.D. d	
53) n-Octacosane	0.000		0	N.D. d	
54) Benz[a]anthracene	0.000		0	N.D. d	
55) Chrysene	0.000		0	N.D. d	
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.	
60) Benzo(k)fluoranthene	0.000		0	N.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.	

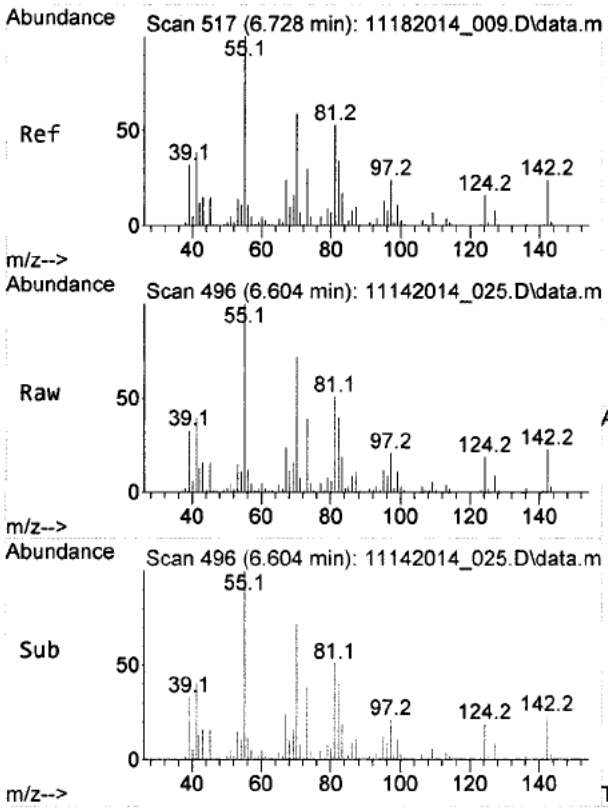
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Dec 01 12:49:49 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

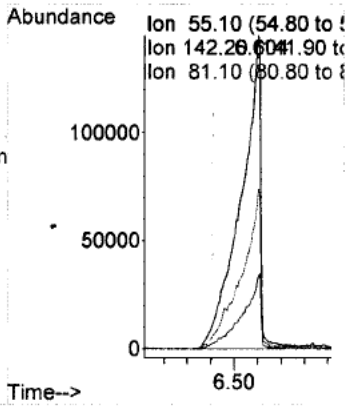


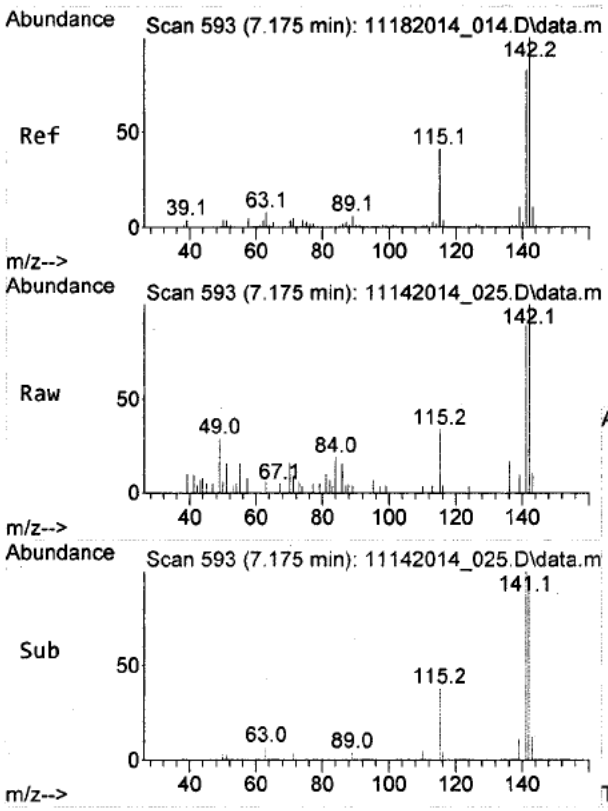


#12
4-Methylcyclohexanecarboxylic acid
Concen: 63.27 ug/mL
RT: 6.604 min Scan# 496
Delta R.T. -0.123 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 55 Resp: 838035

Ion	Ratio	Lower	Upper
55	100		
142	21.8	19.1	28.7
81	49.2	42.3	63.5

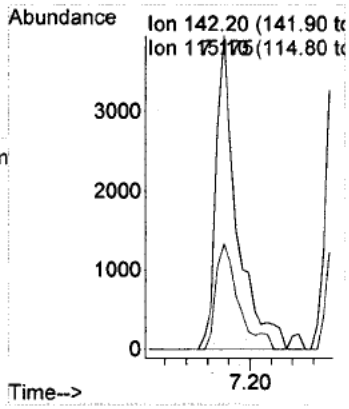


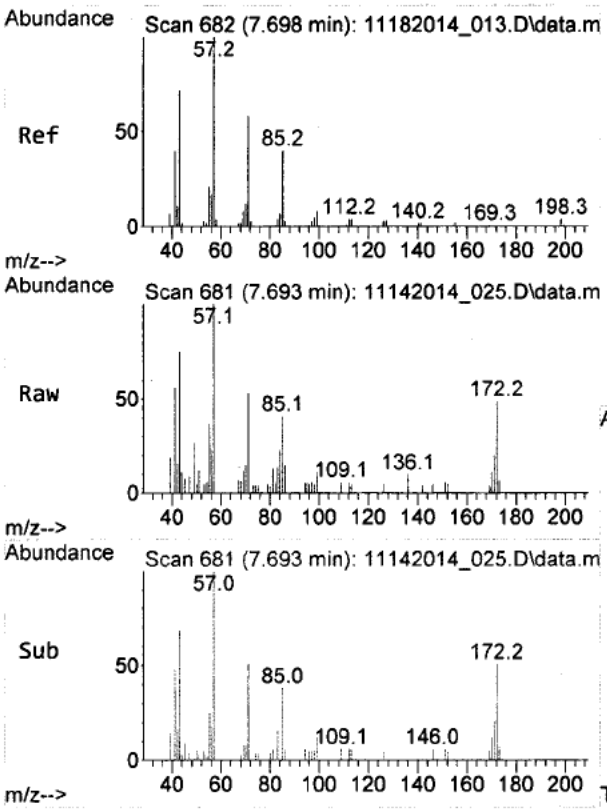


#20
2-Methylnapthalene
Concen: 0.06 ug/mL
RT: 7.175 min Scan# 593
Delta R.T. -0.000 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion:142 Resp: 5357

Ion	Ratio	Lower	Upper
142	100		
115	36.6	33.0	49.4

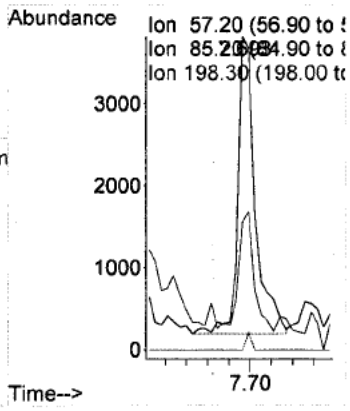


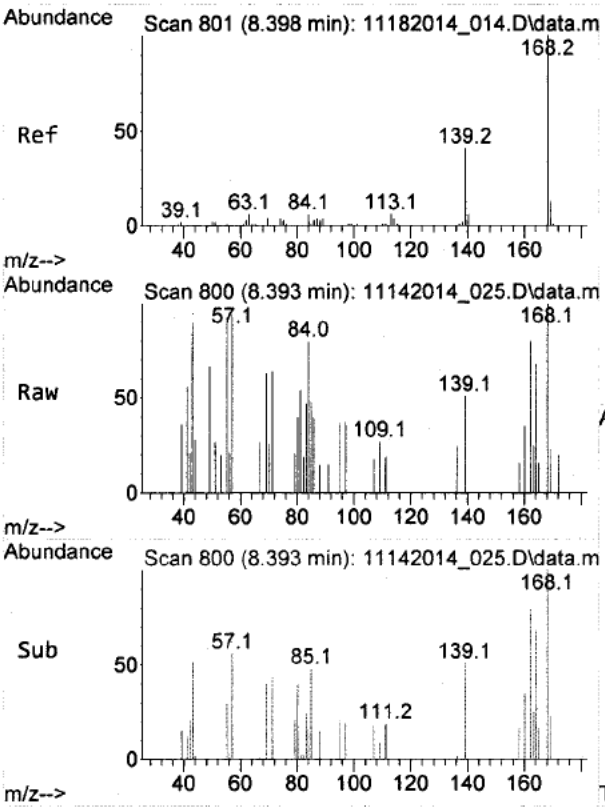


#23
n-Tetradecane
Concen: 0.08 ug/mL
RT: 7.693 min Scan# 681
Delta R.T. -0.005 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 57 Resp: 4125

Ion	Ratio	Lower	Upper
57	100		
85	44.1	31.6	47.4
198	1.8	3.1	4.7#

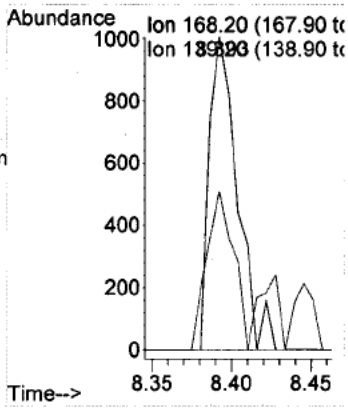


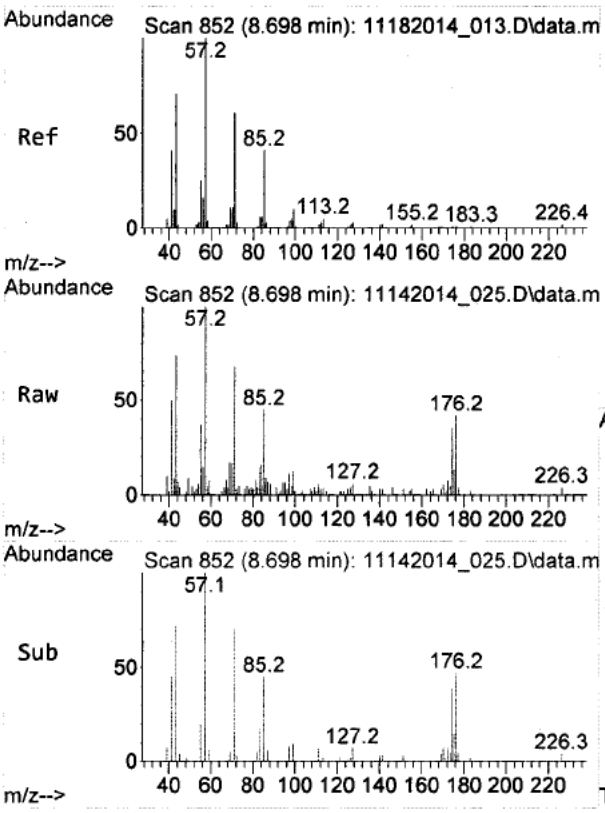


#29
Dibenzofuran
Concen: 0.01 ug/mL
RT: 8.393 min Scan# 800
Delta R.T. -0.005 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion:168 Resp: 1239

Ion	Ratio	Lower	Upper
168	100		
139	48.9	32.9	49.3

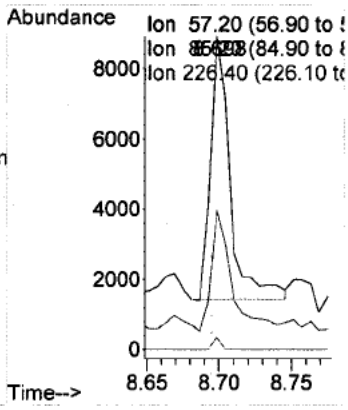


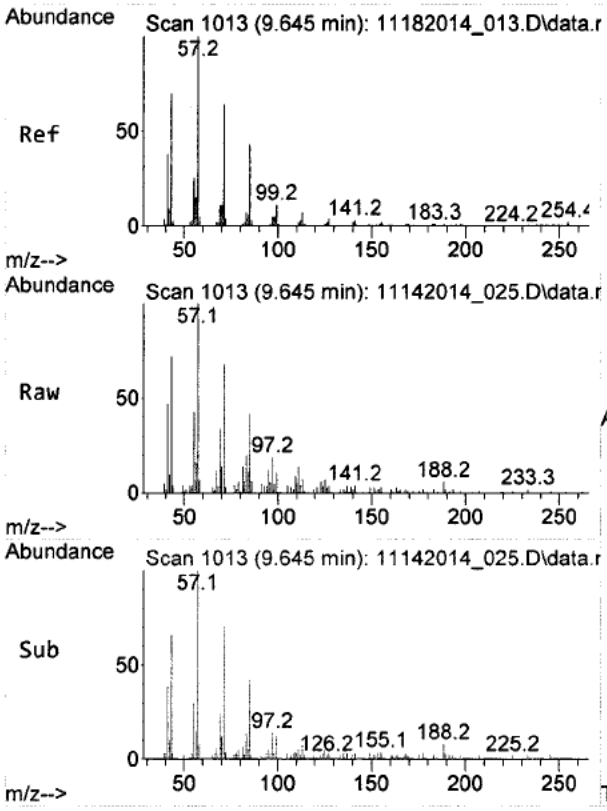


#31
n-Hexadecane
Concen: 0.12 ug/mL
RT: 8.698 min Scan# 852
Delta R.T. 0.000 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 57 Resp: 7023

Ion	Ratio	Lower	Upper
57	100		
85	49.3	35.1	52.7
226	1.8	3.1	4.7#

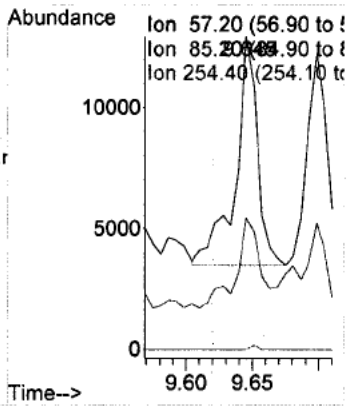


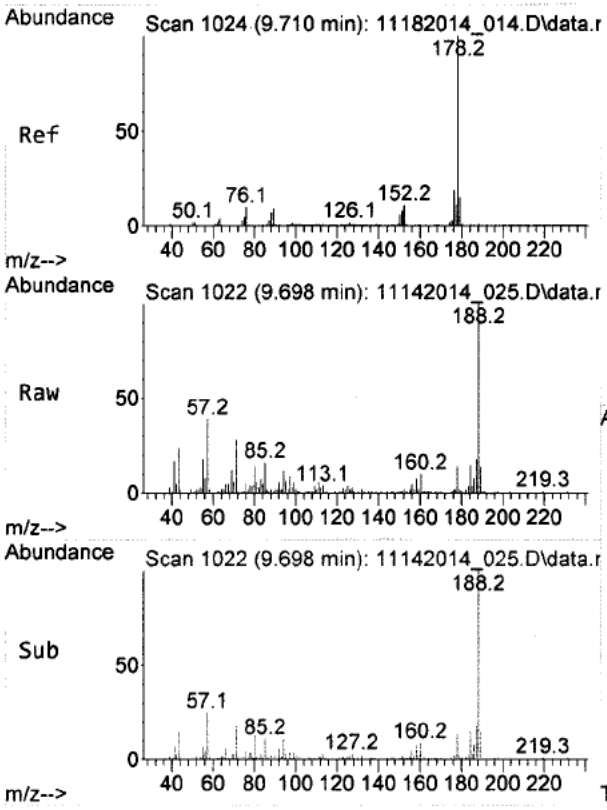


#40
n-Octadecane
Concen: 0.19 ug/mL
RT: 9.645 min Scan# 1013
Delta R.T. 0.000 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 57 Resp: 10752

Ion	Ratio	Lower	Upper
57	100		
85	44.4	34.5	51.7
254	0.5	1.4	2.2#

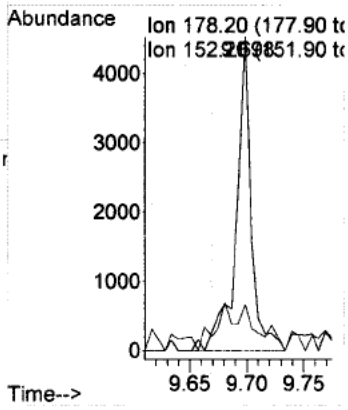


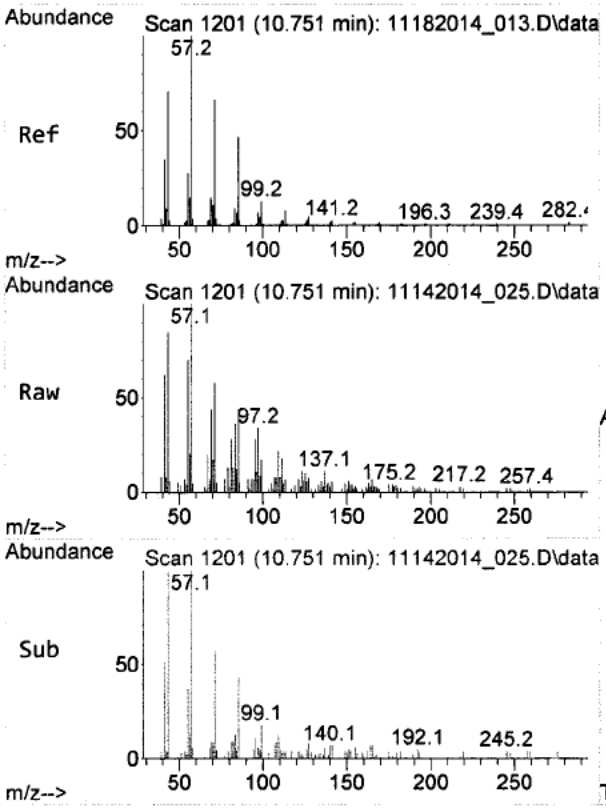


#41
Phenanthrene
Concen: 0.03 ug/mL
RT: 9.698 min Scan# 1022
Delta R.T. -0.012 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion:178 Resp: 4134

Ion	Ratio	Lower	Upper
178	100		
152	16.8	8.5	12.7#

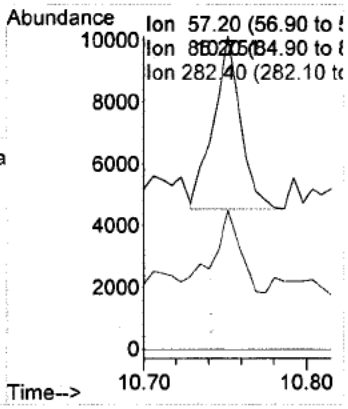


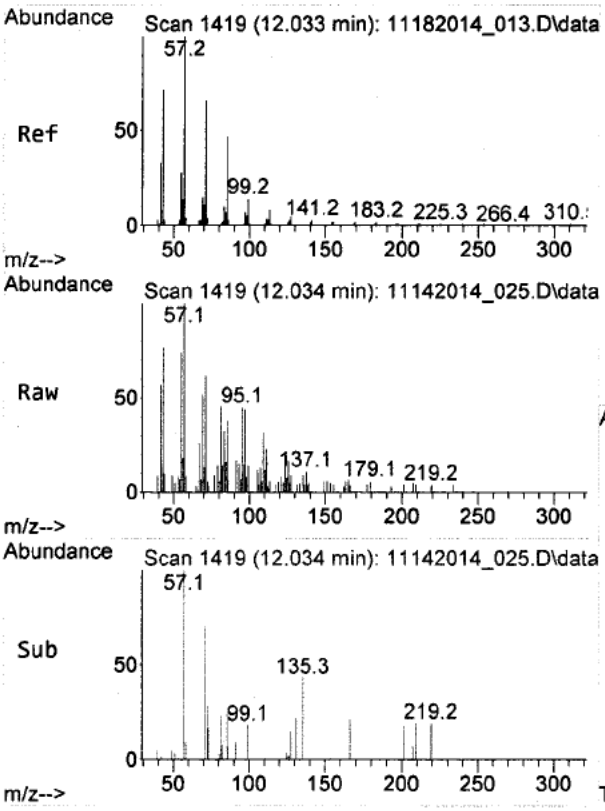


#45
n-Eicosane
Concen: 0.12 ug/mL
RT: 10.751 min Scan# 1201
Delta R.T. 0.000 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 57 Resp: 6650

Ion	Ratio	Lower	Upper
57	100		
85	47.2	37.8	56.8
282	0.0	1.4	2.2#

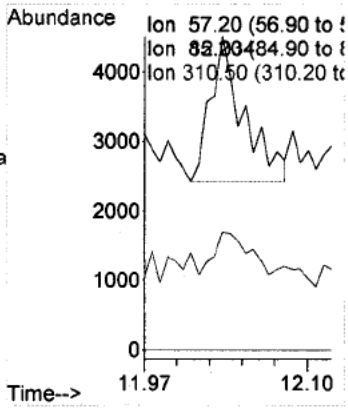




#48
n-Docosane
Concen: 0.07 ug/mL
RT: 12.034 min Scan# 1419
Delta R.T. 0.001 min
Lab File: 11142014_025.D
Acq: 14 Nov 2014 09:36 pm

Tgt Ion: 57 Resp: 3630

Ion	Ratio	Lower	Upper
57	100		
85	40.7	37.5	56.3
311	0.0	0.9	1.3#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 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_025.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.787	13	17	59	rVB	10069	75975	1.30%	0.226%
2	5.075	229	236	289	rBV	1193322	3163172	54.10%	9.398%
3	5.405	289	292	309	rVB8	18508	64126	1.10%	0.191%
4	5.540	309	315	339	rBV	51184	116761	2.00%	0.347%
5	5.716	339	345	361	rVV	26338	58065	0.99%	0.173%
6	6.457	447	471	481	rBV	3031948	5847387	100.00%	17.374%
7	6.604	481	496	525	rVB2	1121023	4904338	83.87%	14.572%
8	6.834	525	535	555	rVB9	23448	70711	1.21%	0.210%
9	7.575	653	661	679	rBV	1924475	1823154	31.18%	5.417%
10	8.210	761	769	799	rBV	4149004	4584076	78.40%	13.620%
11	8.540	817	825	831	rBV4	56127	96431	1.65%	0.287%
12	8.593	831	834	849	rVB4	27586	91666	1.57%	0.272%
13	8.698	849	852	865	rVB2	54472	61940	1.06%	0.184%
14	9.163	927	931	933	rBV	55511	52298	0.89%	0.155%
15	9.193	933	936	943	rBV	60021	60457	1.03%	0.180%
16	9.328	953	959	963	rBV	66072	55487	0.95%	0.165%
17	9.534	985	994	1001	rBV	52270	81997	1.40%	0.244%
18	9.681	1007	1019	1025	rBV	3469100	4251015	72.70%	12.630%
19	9.728	1025	1027	1035	rVV	553612	560185	9.58%	1.664%
20	9.851	1035	1048	1055	rVV2	869515	1194172	20.42%	3.548%
21	9.928	1055	1061	1073	rVV	530152	583069	9.97%	1.732%
22	10.534	1149	1164	1175	rVV	24543	146978	2.51%	0.437%
23	10.657	1175	1185	1193	rVV	22664	116160	1.99%	0.345%
24	10.751	1193	1201	1215	rVV4	44888	154952	2.65%	0.460%
25	10.881	1215	1223	1231	rVV4	20003	98659	1.69%	0.293%
26	10.992	1239	1242	1257	rVV4	24314	114584	1.96%	0.340%
27	11.145	1257	1268	1273	rVV4	26293	116368	1.99%	0.346%
28	11.198	1273	1277	1301	rVV4	28820	197355	3.38%	0.586%
29	11.369	1301	1306	1317	rVV8	26557	100550	1.72%	0.299%
30	11.481	1319	1325	1335	rVV8	18327	86767	1.48%	0.258%
31	11.586	1335	1343	1363	rVV8	17352	132973	2.27%	0.395%
32	11.739	1363	1369	1393	rVV8	16511	126607	2.17%	0.376%
33	13.963	1737	1747	1801	rVV	1304165	2752379	47.07%	8.178%
34	16.804	2213	2230	2271	rBV	758493	1716115	29.35%	5.099%

LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 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

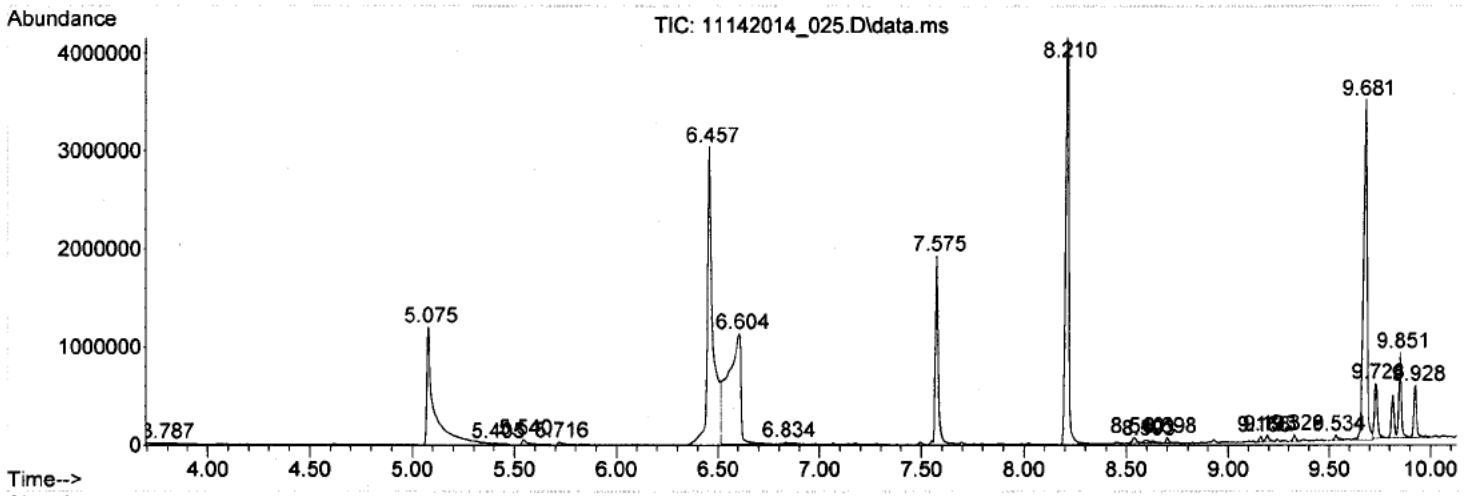
Sum of corrected areas: 33656929

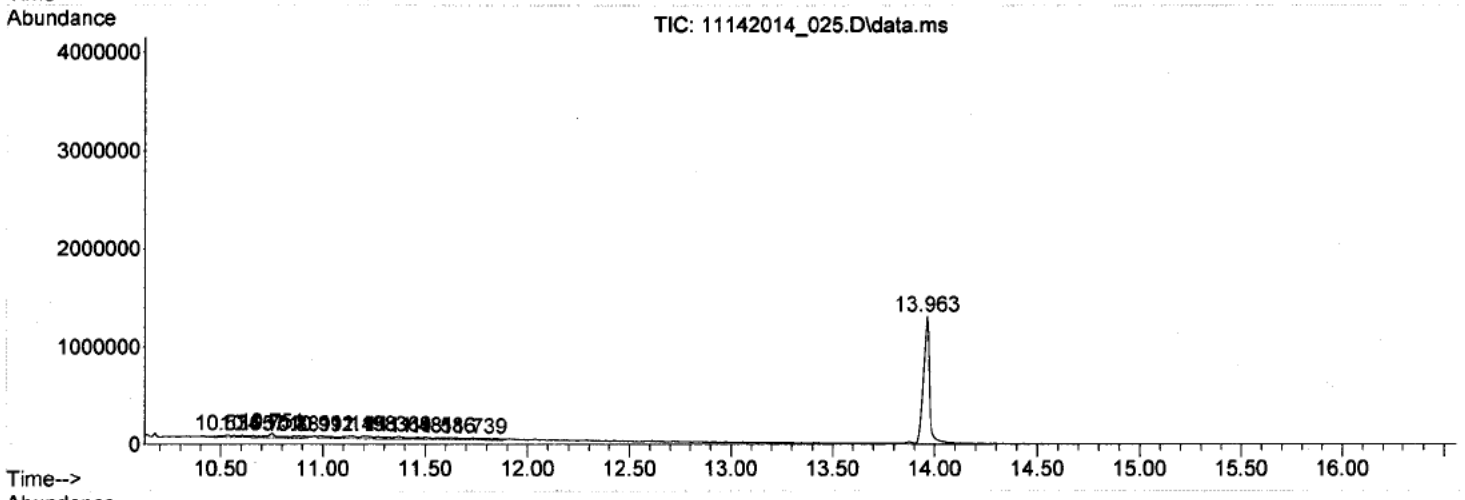
LSC Report - Integrated Chromatogram

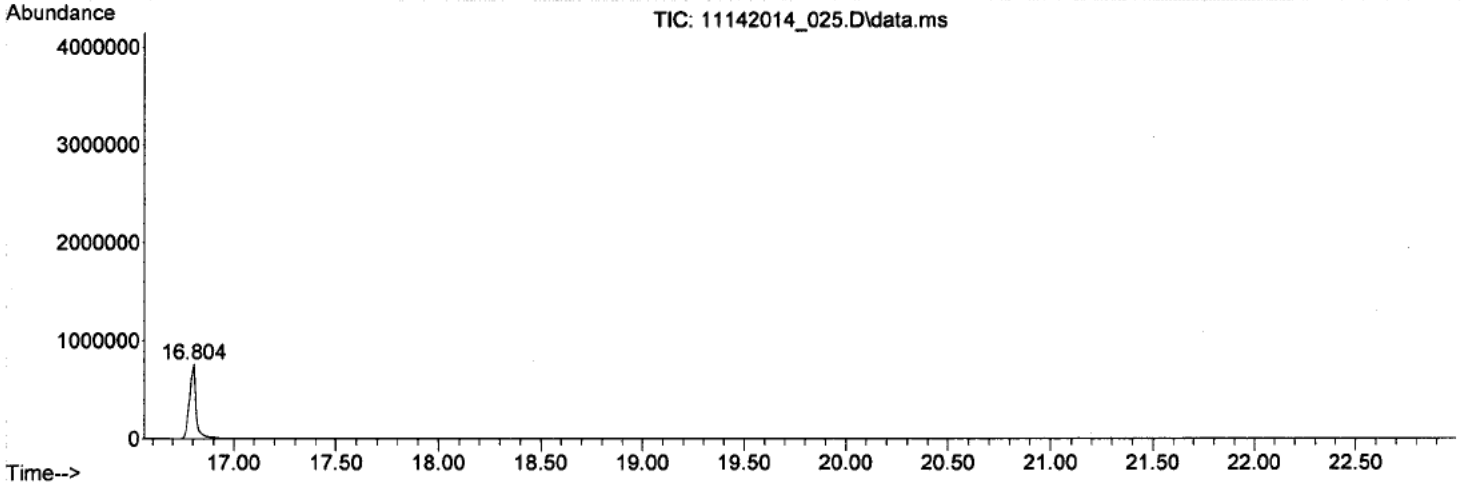
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

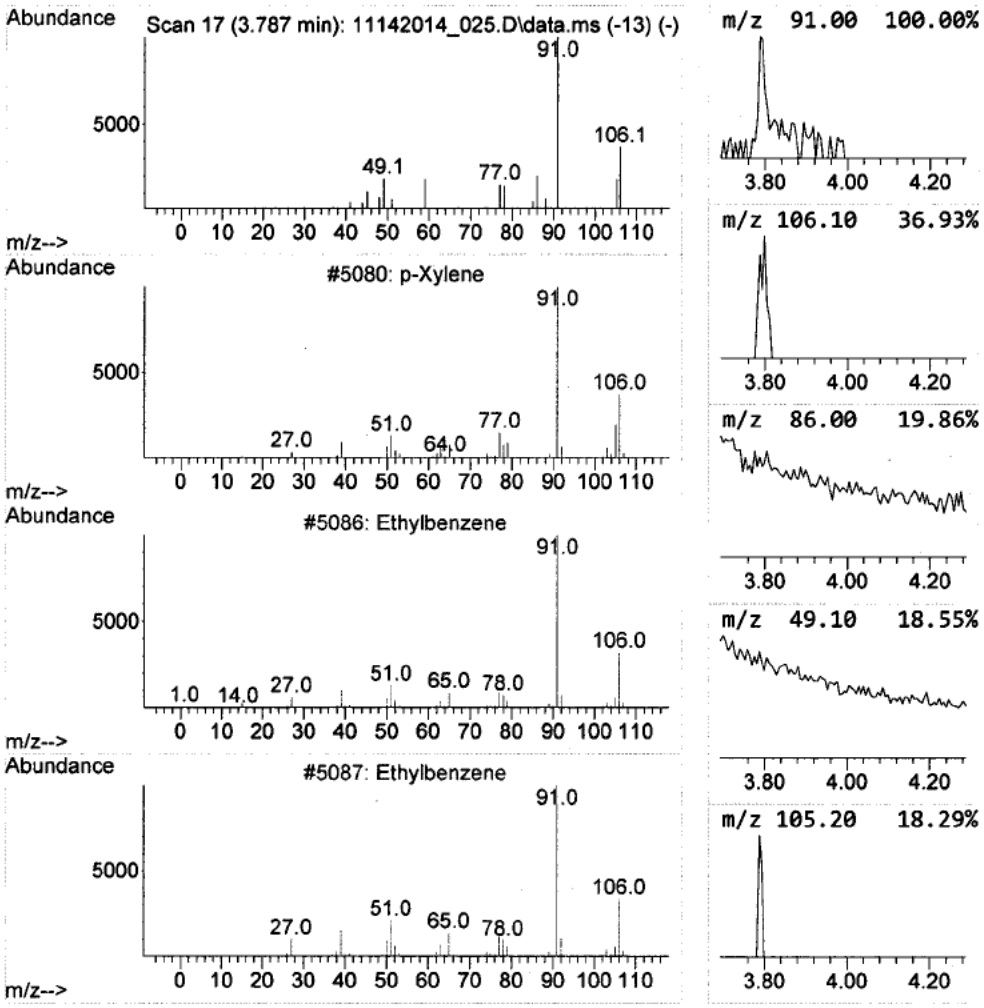
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 1 p-Xylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.787	0.48 ug/mL	75975	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	38
2	Ethylbenzene	106	C8H10	000100-41-4	9
3	Ethylbenzene	106	C8H10	000100-41-4	7
4	Ethylbenzene	106	C8H10	000100-41-4	5
5	Ethylbenzene	106	C8H10	000100-41-4	5



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

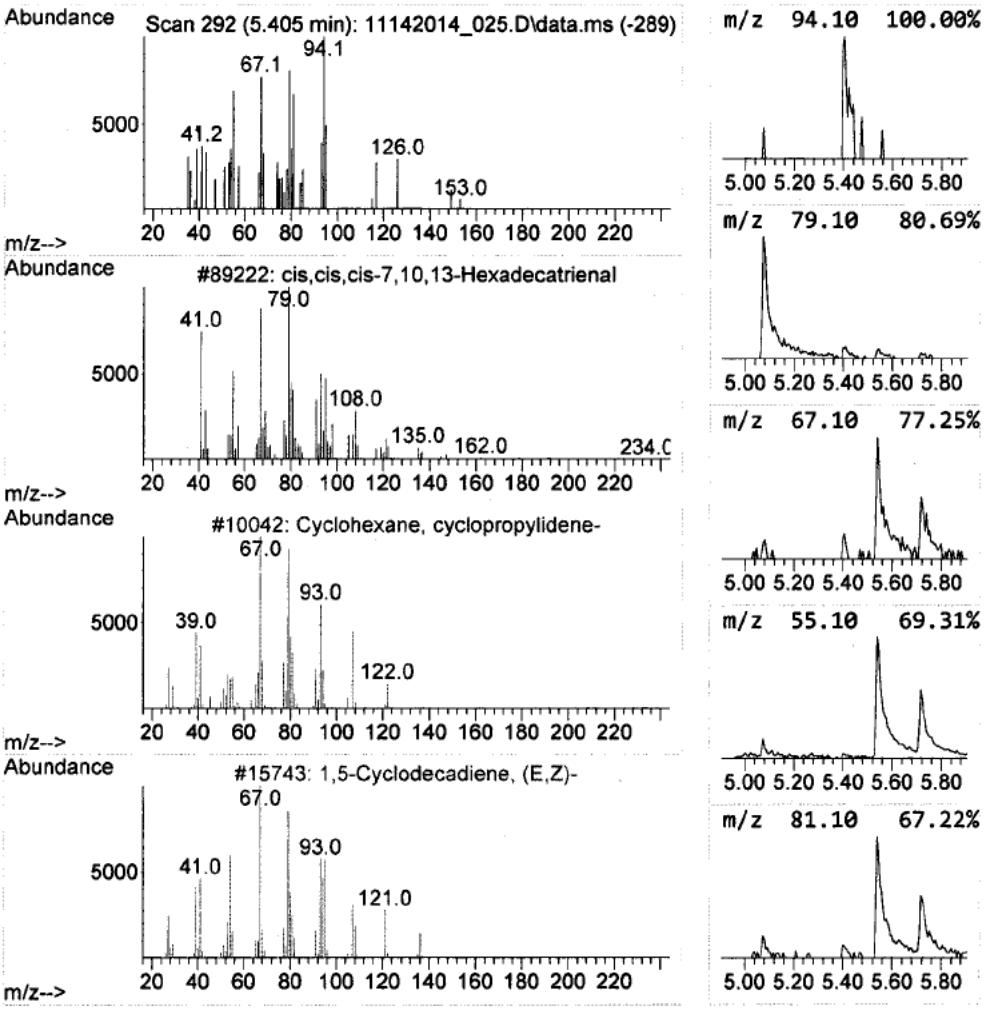
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 2 cis,cis,cis-7,10,13-Hexadec... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.405	0.41 ug/mL	64126	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,cis,cis-7,10,13-Hexadecatrienal	234	C16H26O	056797-43-4	43
2	Cyclohexane, cyclopropylidene-	122	C9H14	014114-06-8	38
3	1,5-Cyclodecadiene, (E,Z)-	136	C10H16	001124-78-3	38
4	4-Cyclopropylnorcarane	136	C10H16	1000222-73-9	35
5	Cyclododecyne	164	C12H20	001129-90-4	35



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

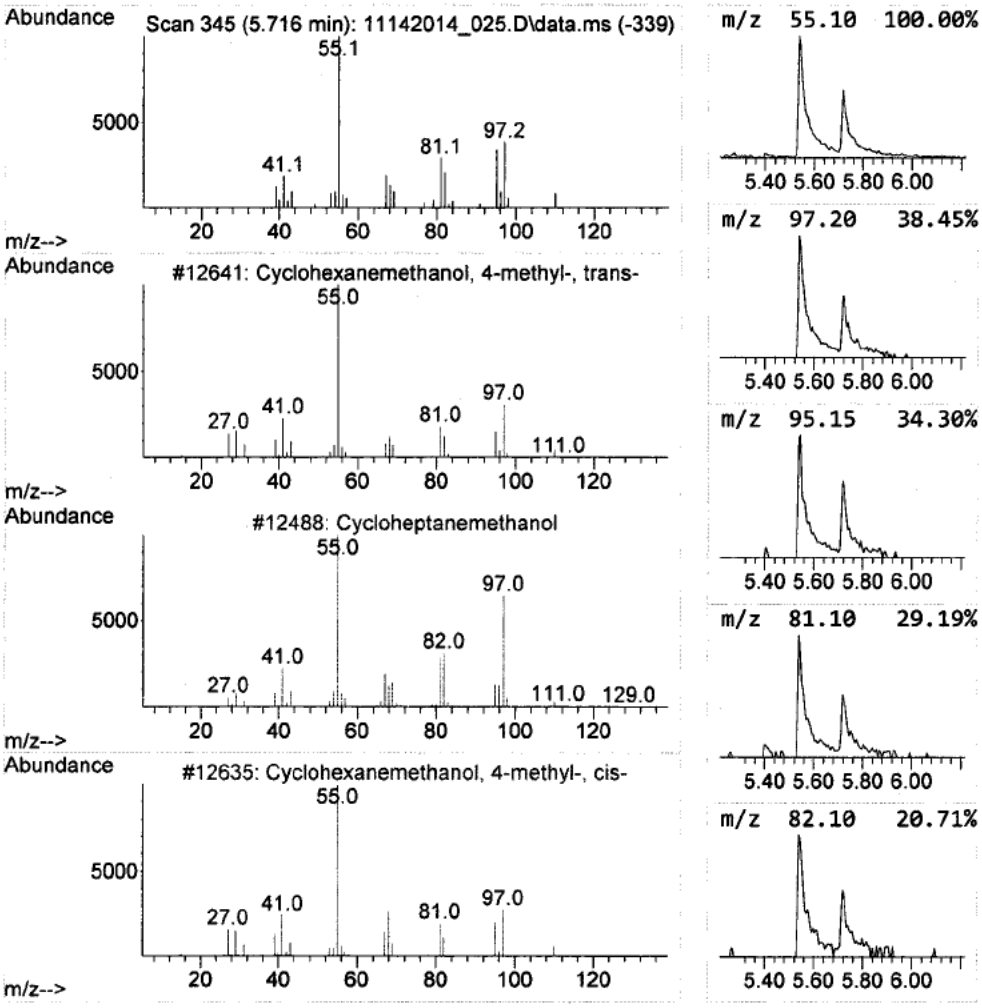
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 3 Cyclohexanemethanol, 4-meth... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	0.37 ug/mL	58065	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	78
2	Cycloheptanemethanol	128	C8H16O	004448-75-3	64
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	59
4	Cycloheptanemethanol	128	C8H16O	004448-75-3	50
5	Cycloheptane, bromo-	176	C7H13Br	002404-35-5	38



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

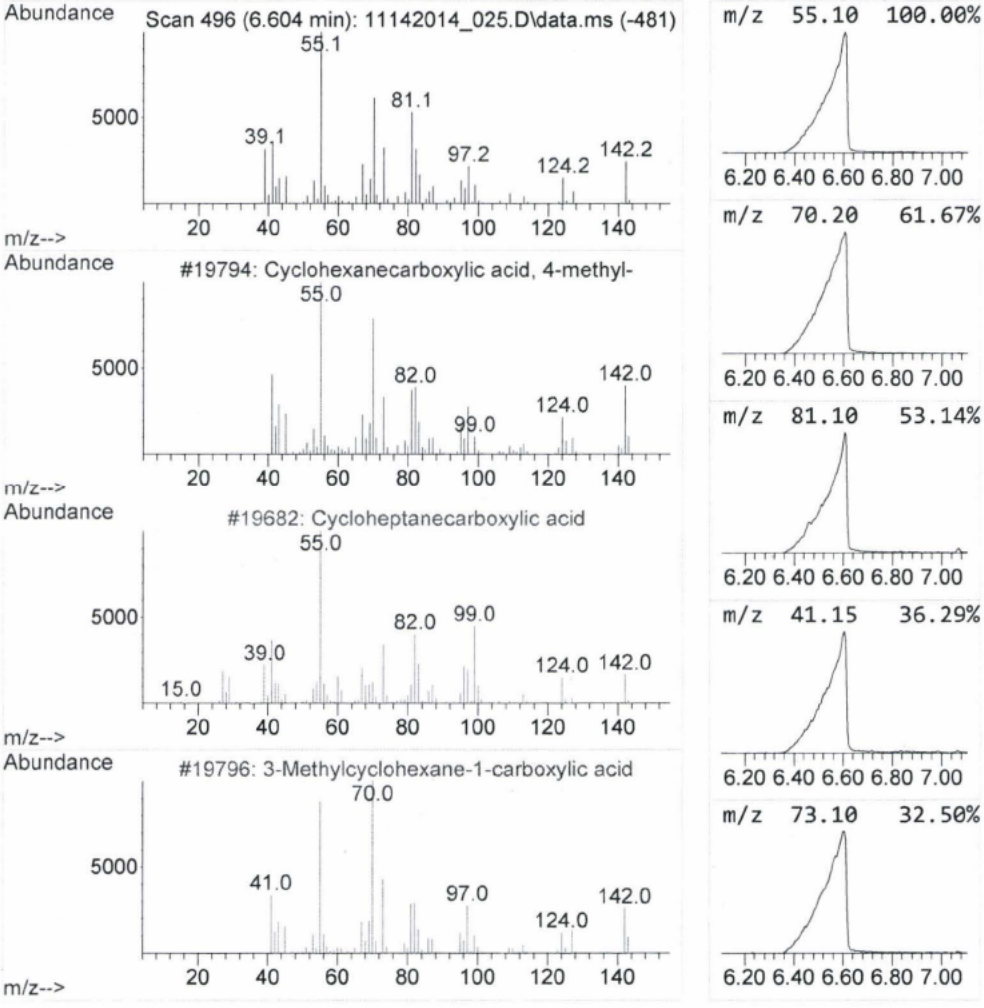
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 4 Cyclohexanecarboxylic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	16.77 ug/mL	4904340	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	94
2	Cycloheptanecarboxylic acid	142	C8H14O2	001460-16-8	60
3	3-Methylcyclohexane-1-carboxylic...	142	C8H14O2	1000132-15-7	22
4	Cycloheptanemethanol	128	C8H16O	004448-75-3	22
5	Dodecyl acrylate	240	C15H28O2	002156-97-0	14



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

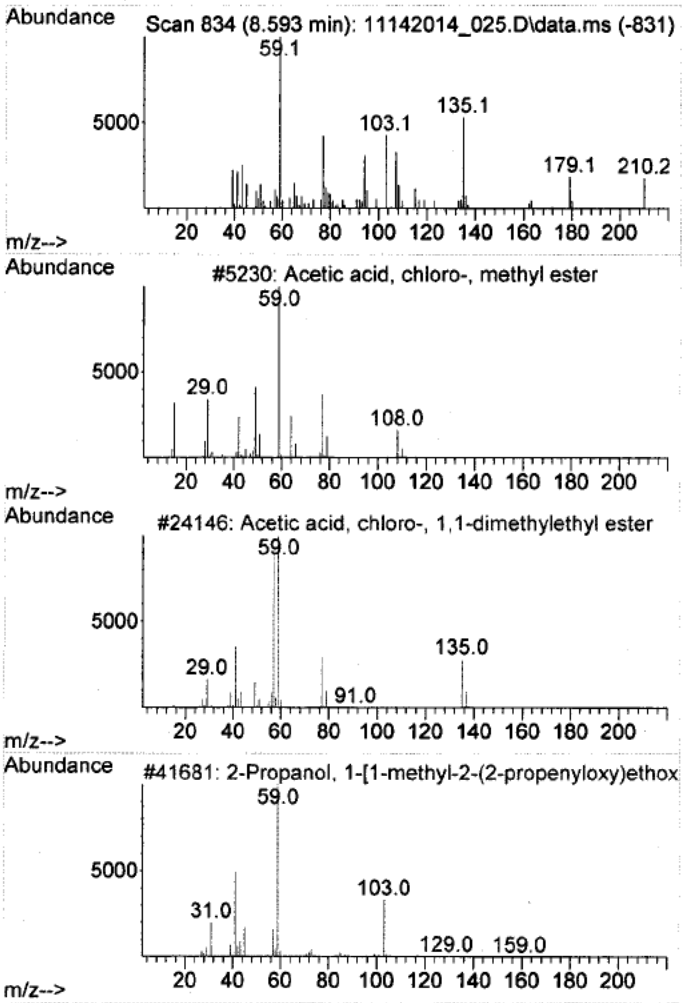
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

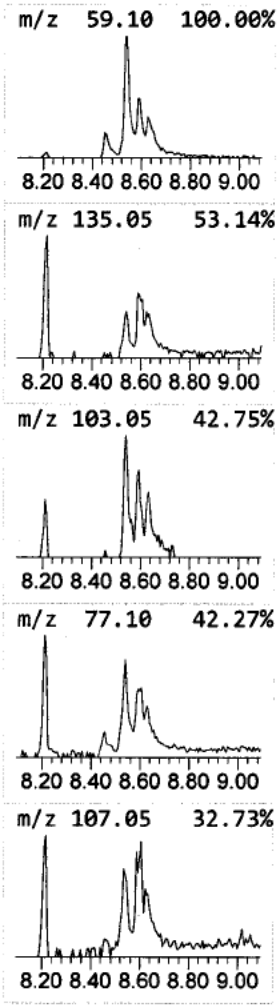
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 5 Acetic acid, chloro-, methy... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.593	0.40 ug/mL	91666	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	27
2	Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	25
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	16
4	Benzene, isothiocyanato-	135	C7H5NS	000103-72-0	14
5	1-Chloro-2-ethoxyethane	108	C4H9ClO	000628-34-2	14





Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

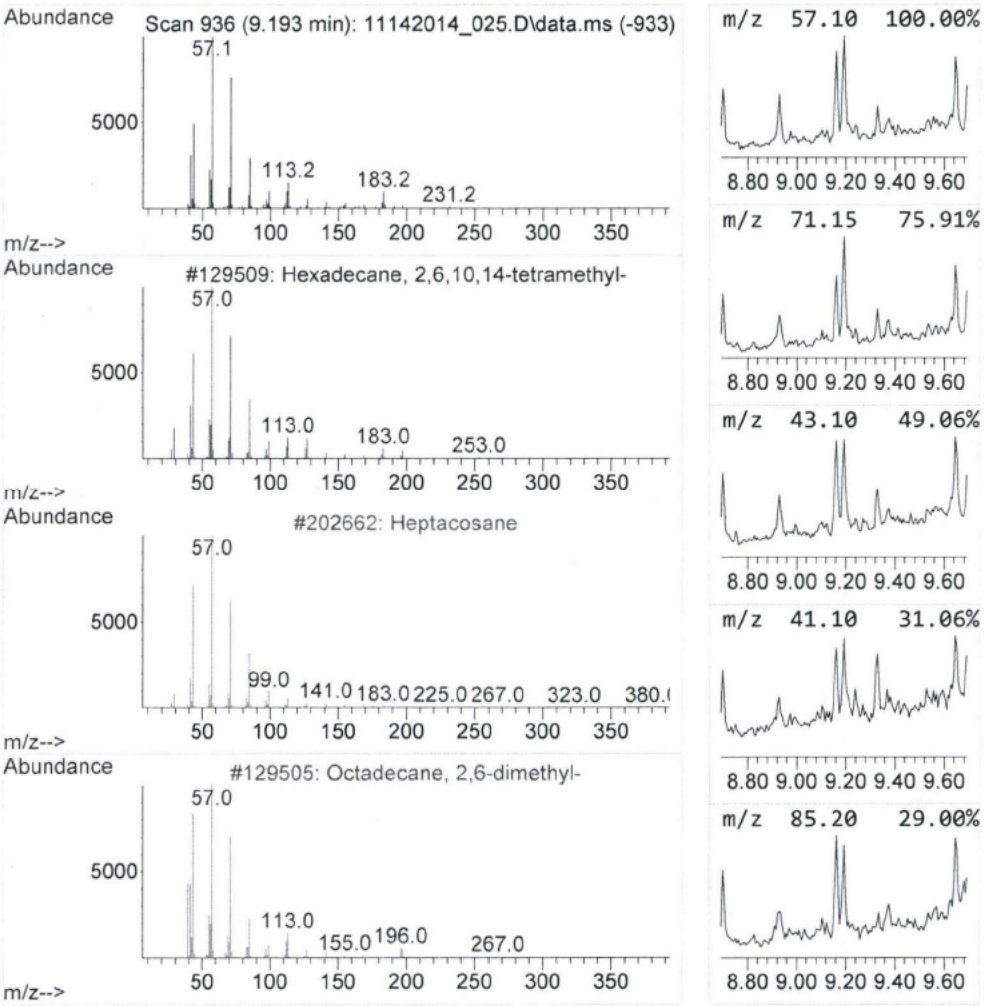
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.193	0.28 ug/mL	60457	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Heptacosane	380	C27H56	000593-49-7	80
3	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	80
4	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	72
5	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	72

Ret time from previous sample indicate the response do possibly be tetramethyl pentadecan[redacted] 12/5/14



Library Search Compound Report

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Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

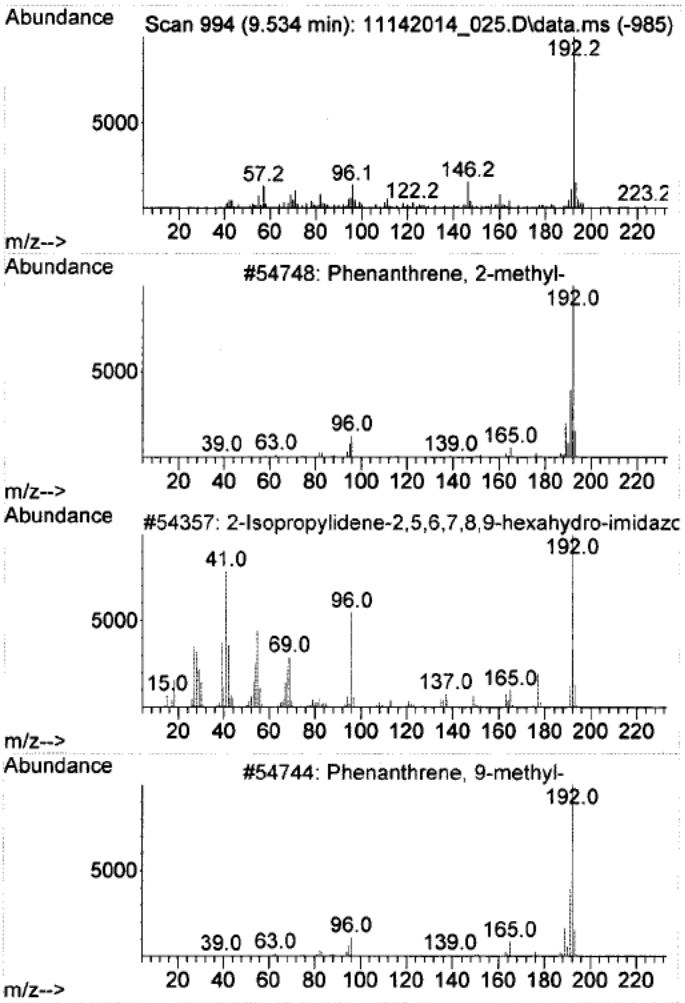
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

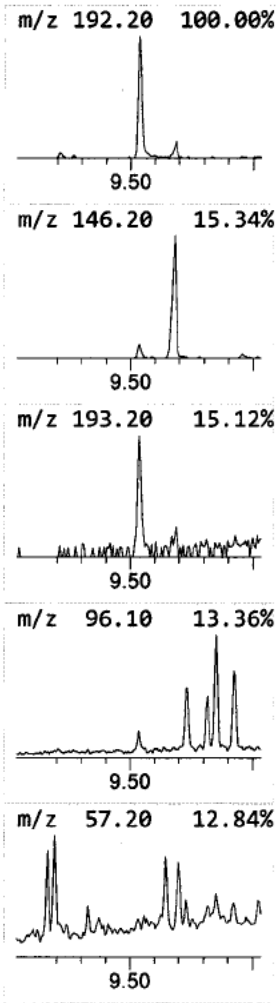
****

Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.534	0.39 ug/mL	81997	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
2	2-Isopropylidene-2,5,6,7,8,9-hex...	192	C11H16N2O	172882-46-1	64
3	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	64
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	59
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	59





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Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

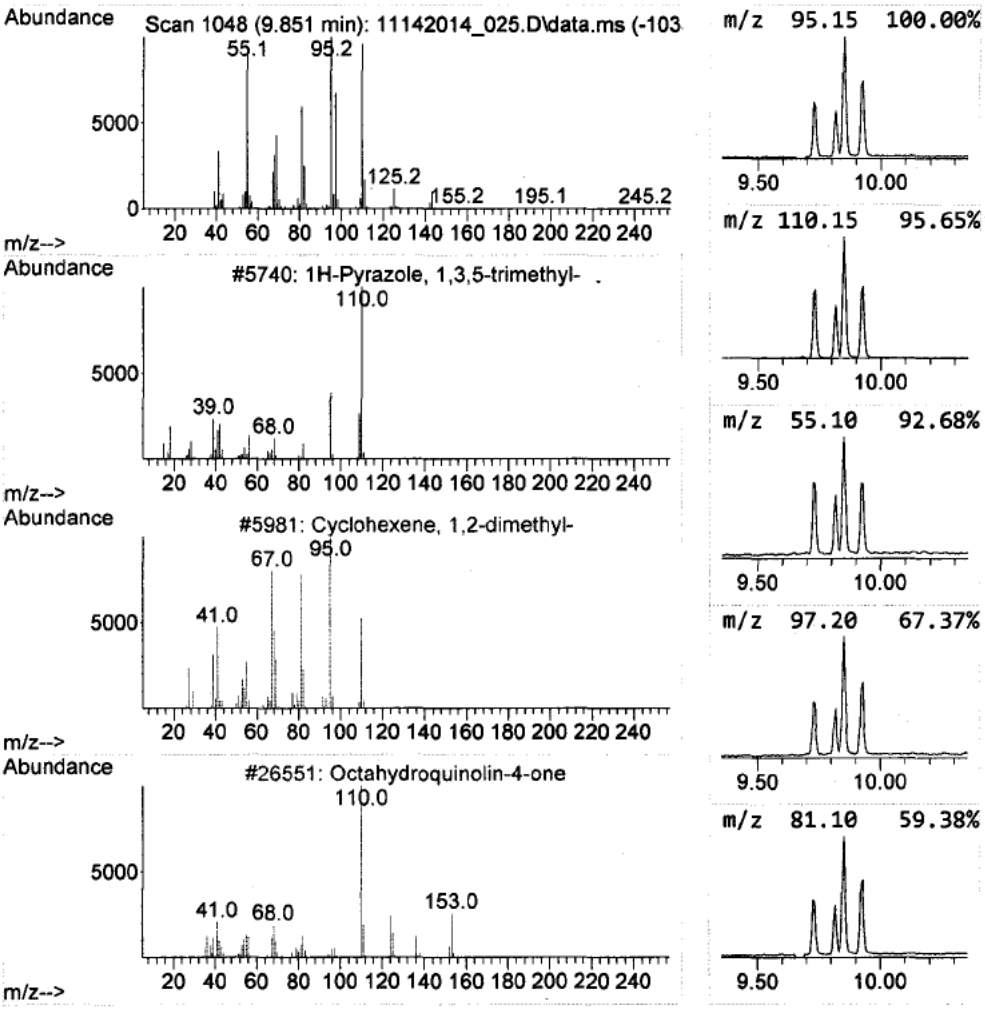
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 8 1H-Pyrazole, 1,3,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	5.62 ug/mL	1194170	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	58
2	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	47
3	Octahydroquinolin-4-one	153	C9H15NO	1000302-88-0	38
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	37
5	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	37



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Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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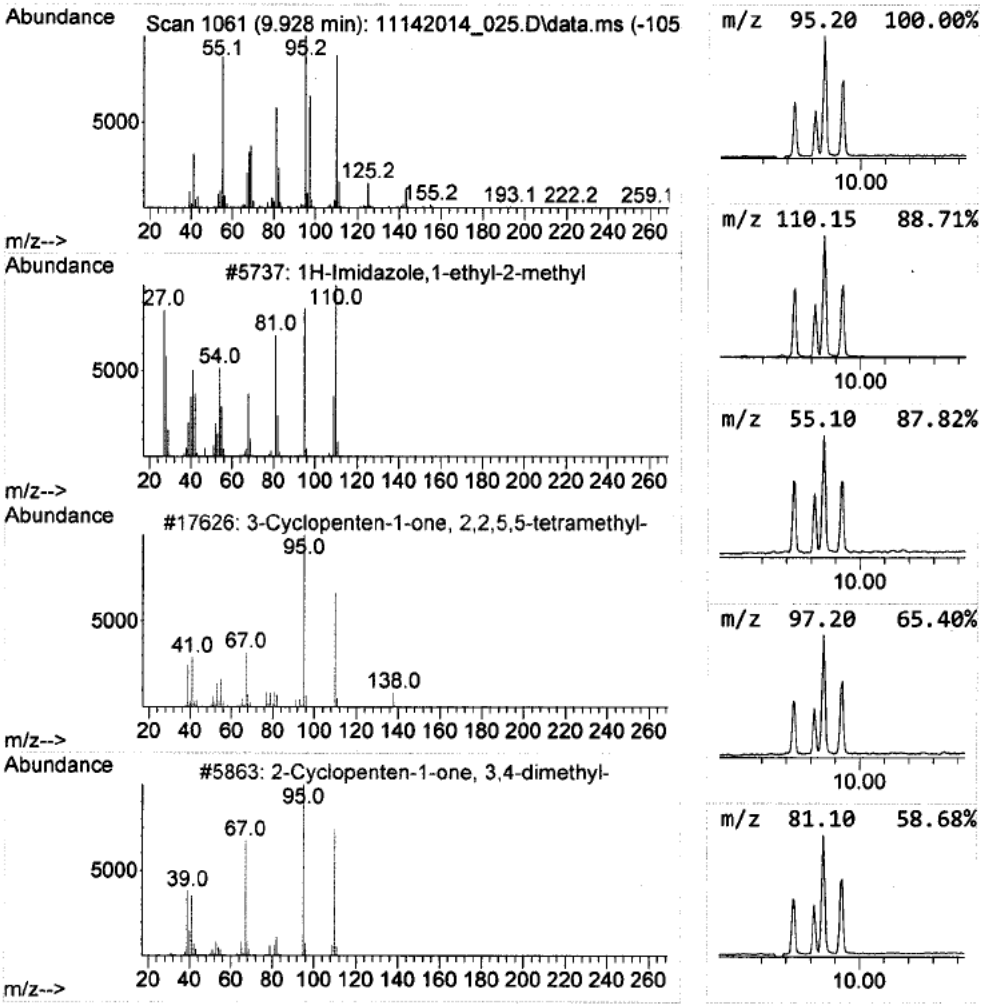
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 9 1H-Imidazole,1-ethyl-2-methyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	2.74 ug/mL	583069	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	52
2	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	47
3	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
4	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	40
5	5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	40



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Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

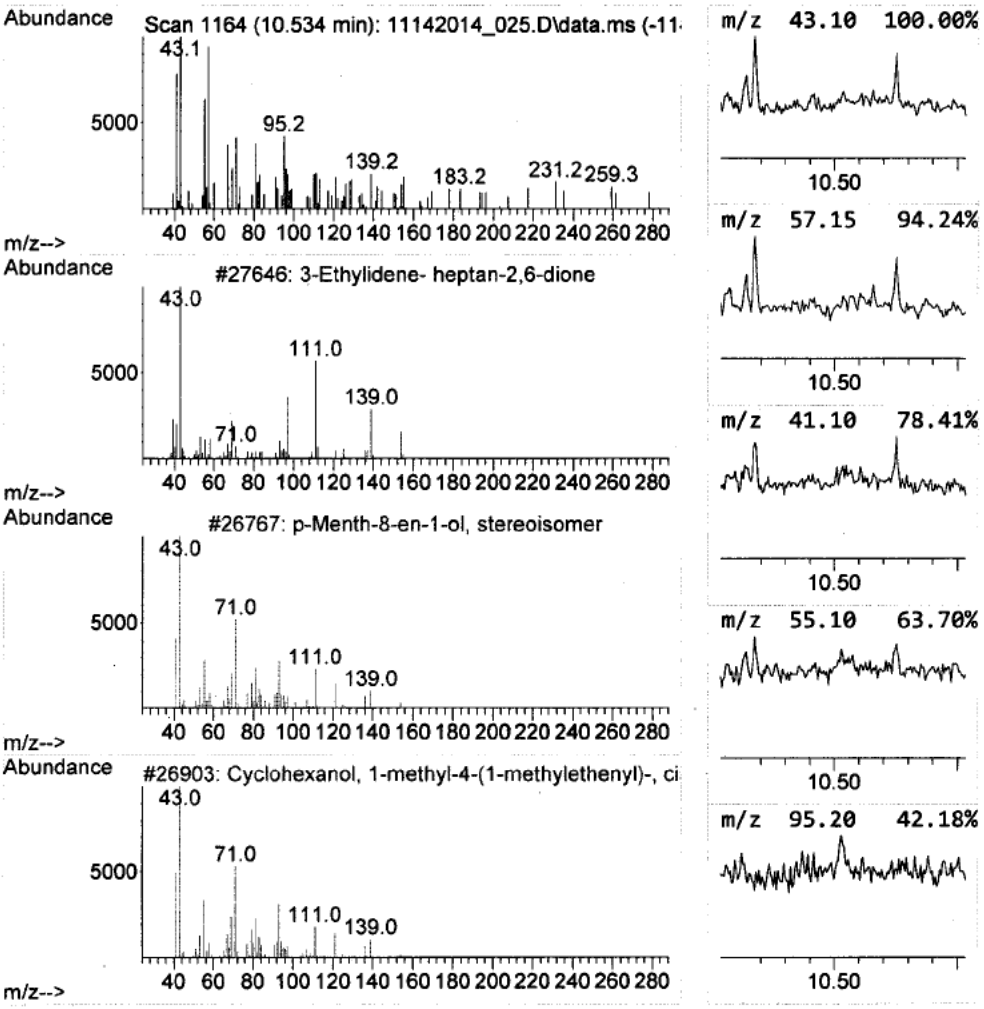
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 10 3-Ethylidene- heptan-2,6-dione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.534	0.69 ug/mL	146978	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylidene- heptan-2,6-dione	154	C9H14O2	1000223-47-9	18
2	p-Menth-8-en-1-ol, stereoisomer	154	C10H18O	007299-40-3	18
3	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	14
4	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	14
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	11



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Operator : [redacted]
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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

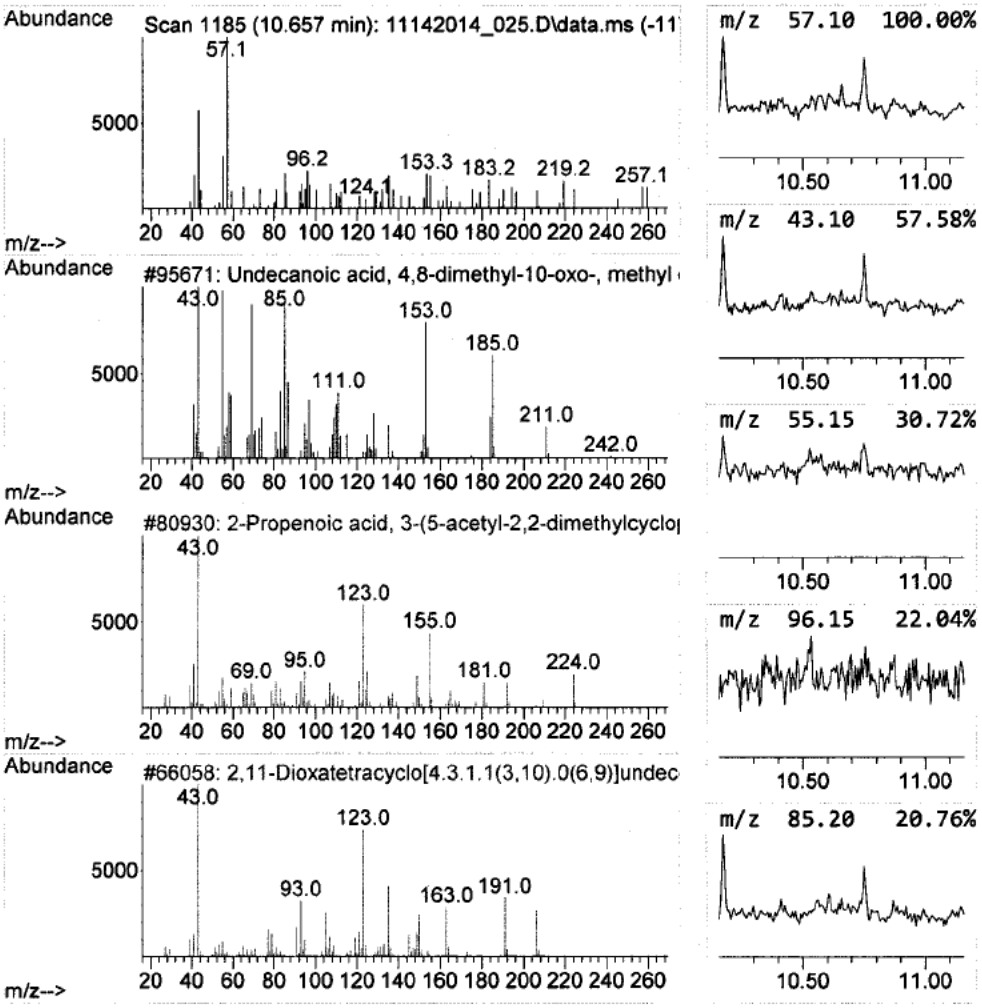
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 11 Undecanoic acid, 4,8-dimeth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	0.55 ug/mL	116160	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid, 4,8-dimethyl-10...	242	C14H26O3	005024-24-8	14
2	2-Propenoic acid, 3-(5-acetyl-2,...	224	C13H20O3	077383-94-9	11
3	2,11-Dioxatetracyclo[4.3.1.1(3,1...	206	C13H18O2	1000194-97-3	11
4	trans-(2-Chlorovinyl)trichlorosi...	194	C2H2Cl4Si	1000139-96-7	10
5	2,3-Dehydro-4-oxo-7,8-dihydro-.b...	206	C13H18O2	083646-60-0	10



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ALS Vial : 24 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

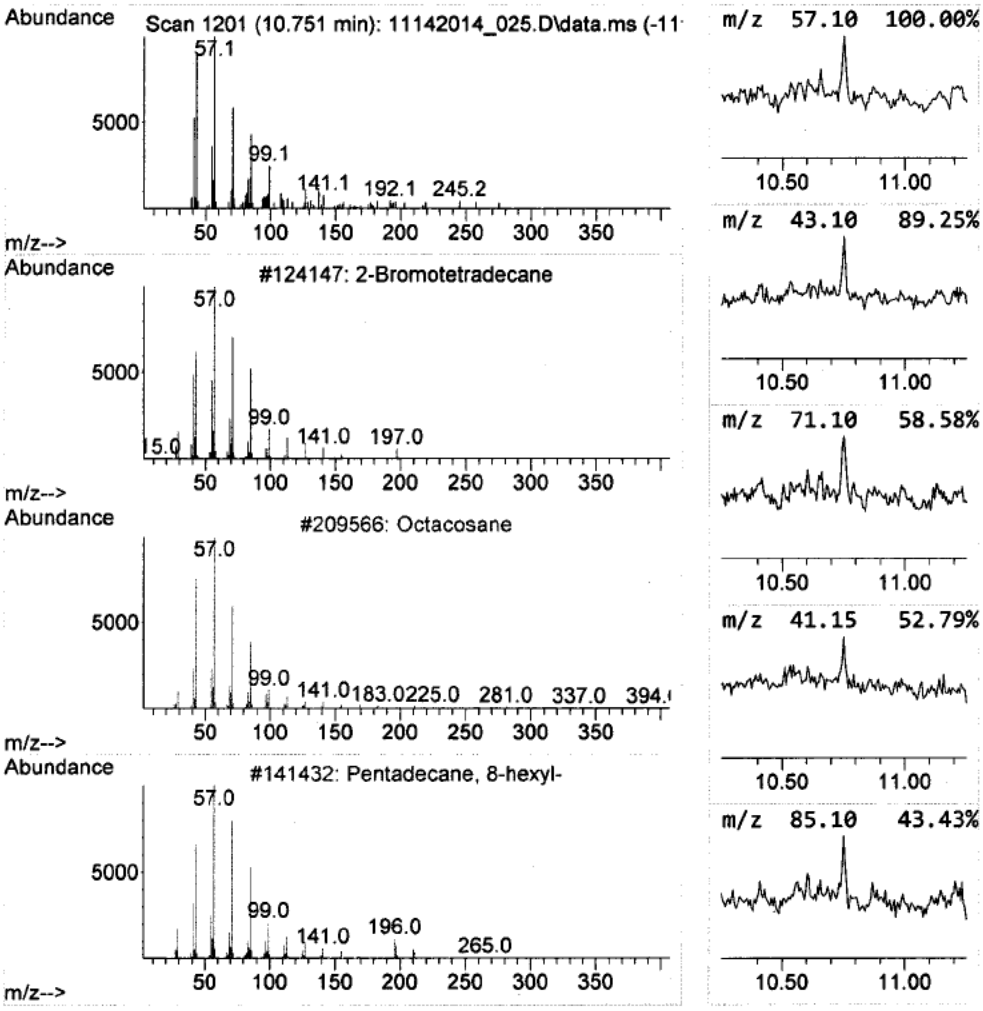
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 12 2-Bromotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.751	0.73 ug/mL	154952	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	52
2	Octacosane	394	C28H58	000630-02-4	50
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	50
4	2-methyloctacosane	408	C29H60	1000376-72-8	50
5	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	47



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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

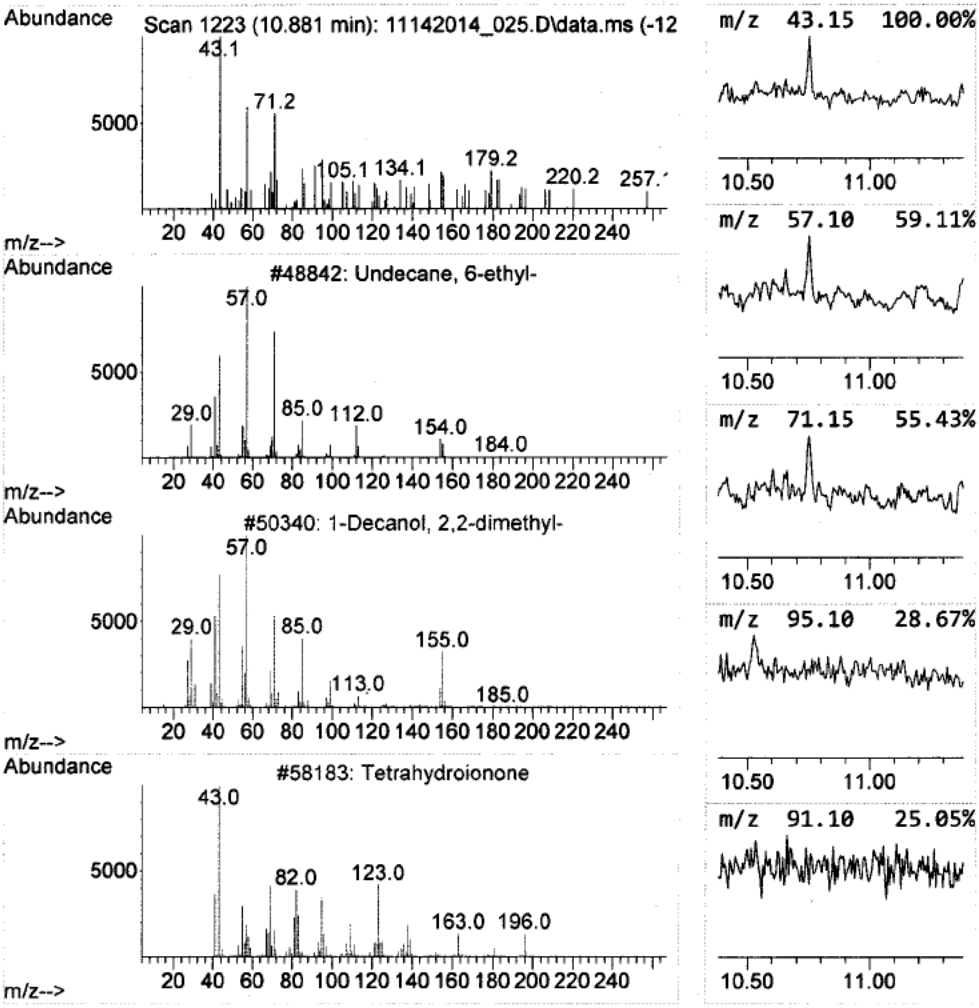
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 13 Undecane, 6-ethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	0.46 ug/mL	98659	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-	184	C13H28	017312-60-6	16
2	1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	14
3	Tetrahydroionone	196	C13H24O	060761-23-1	10
4	6-Tetradecanesulfonic acid, buty...	334	C18H38O3S	1000280-27-4	10
5	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	10



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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

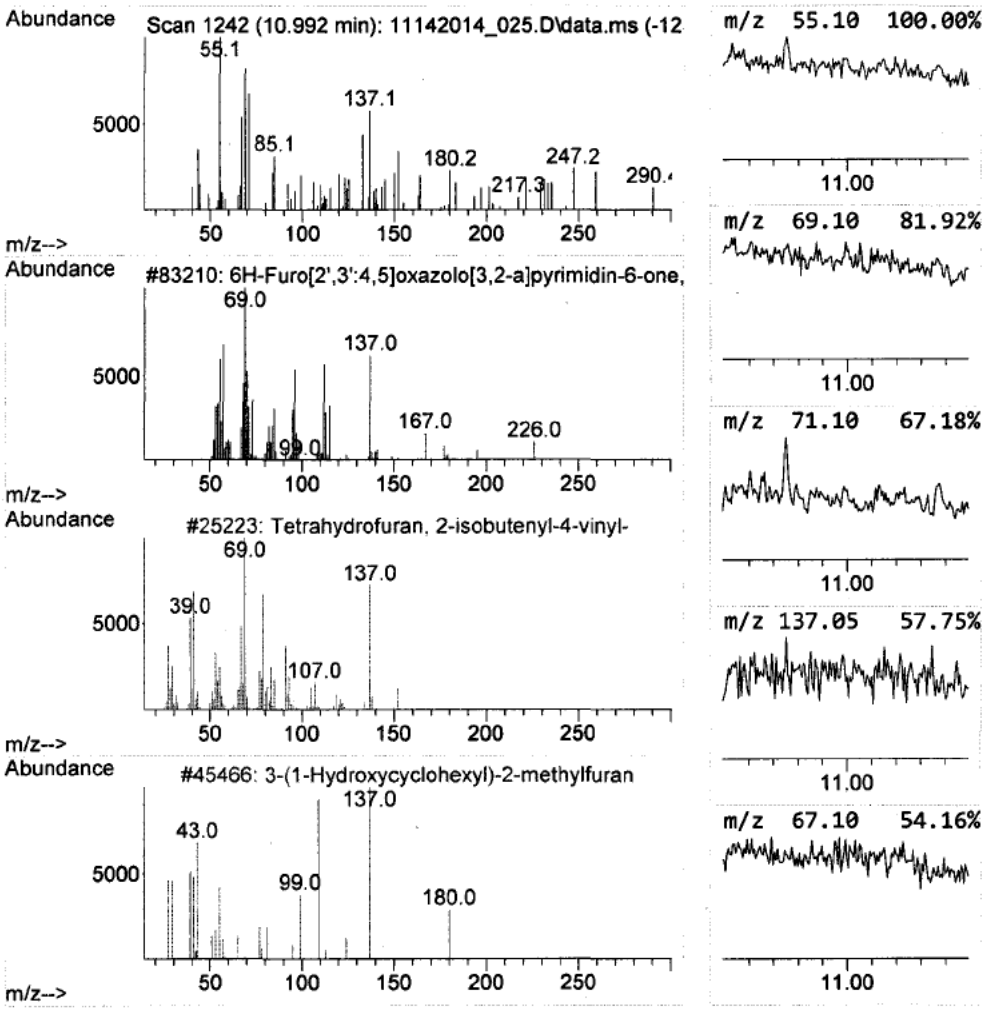
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 14 6H-Furo[2',3':4,5]oxazolo[3... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	0.54 ug/mL	114584	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Furo[2',3':4,5]oxazolo[3,2-a]...	226	C9H10N2O5	003736-77-4	25
2	Tetrahydrofuran, 2-isobutenyl-4-...	152	C10H16O	1000150-01-5	17
3	3-(1-Hydroxycyclohexyl)-2-methyl...	180	C11H16O2	1000281-33-6	11
4	Dodecane, 1,12-dibromo-	326	C12H24Br2	003344-70-5	10
5	Cyclopropanecarboxylic acid, hyd...	208	C12H20N2O	1000264-07-5	10



Library Search Compound Report

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Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

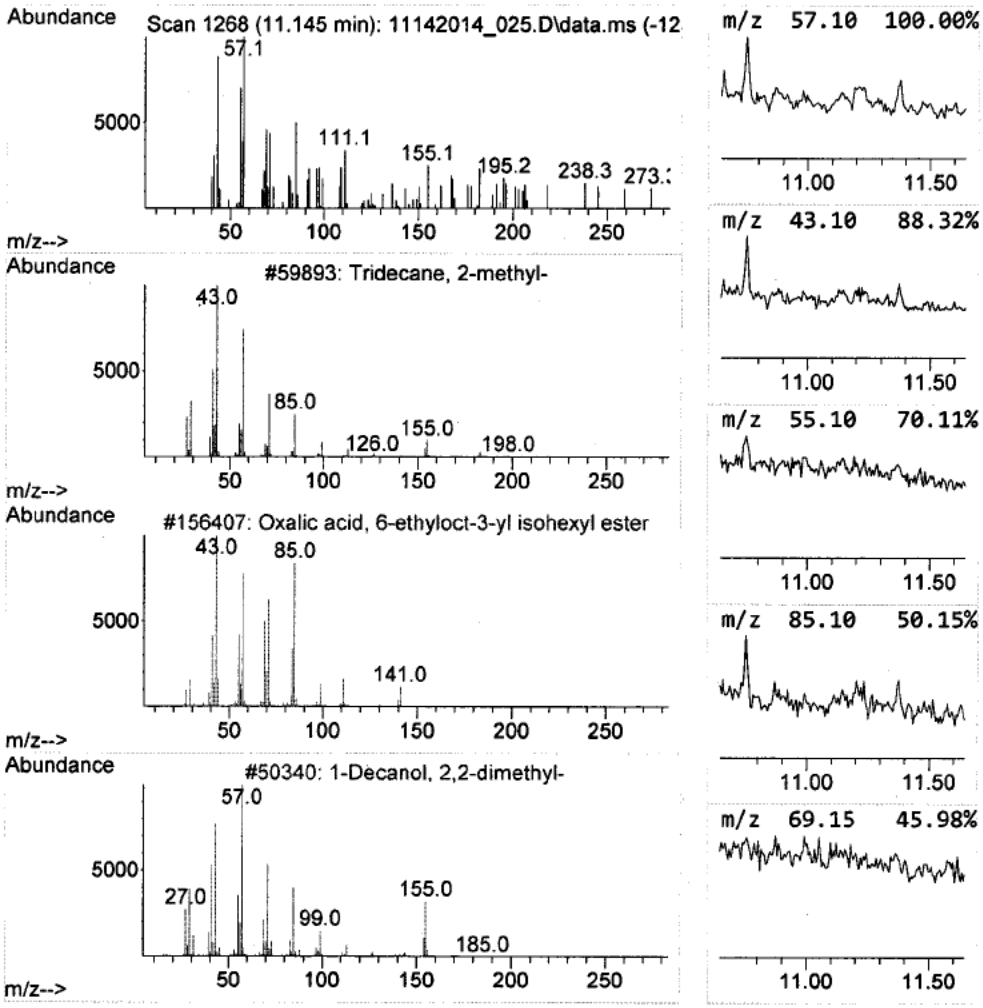
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 15 Tridecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	0.55 ug/mL	116368	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	14
2	Oxalic acid, 6-ethyloct-3-yl iso...	314	C18H3404	1000309-34-3	14
3	1-Decanol, 2,2-dimethyl-	186	C12H260	002370-15-2	14
4	Sulfurous acid, octadecyl 2-prop...	376	C21H4403S	1000309-12-7	14
5	1-Hydroxymethyl-7,7-dimethyl-bic...	182	C10H1403	1000210-65-7	12



Library Search Compound Report

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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

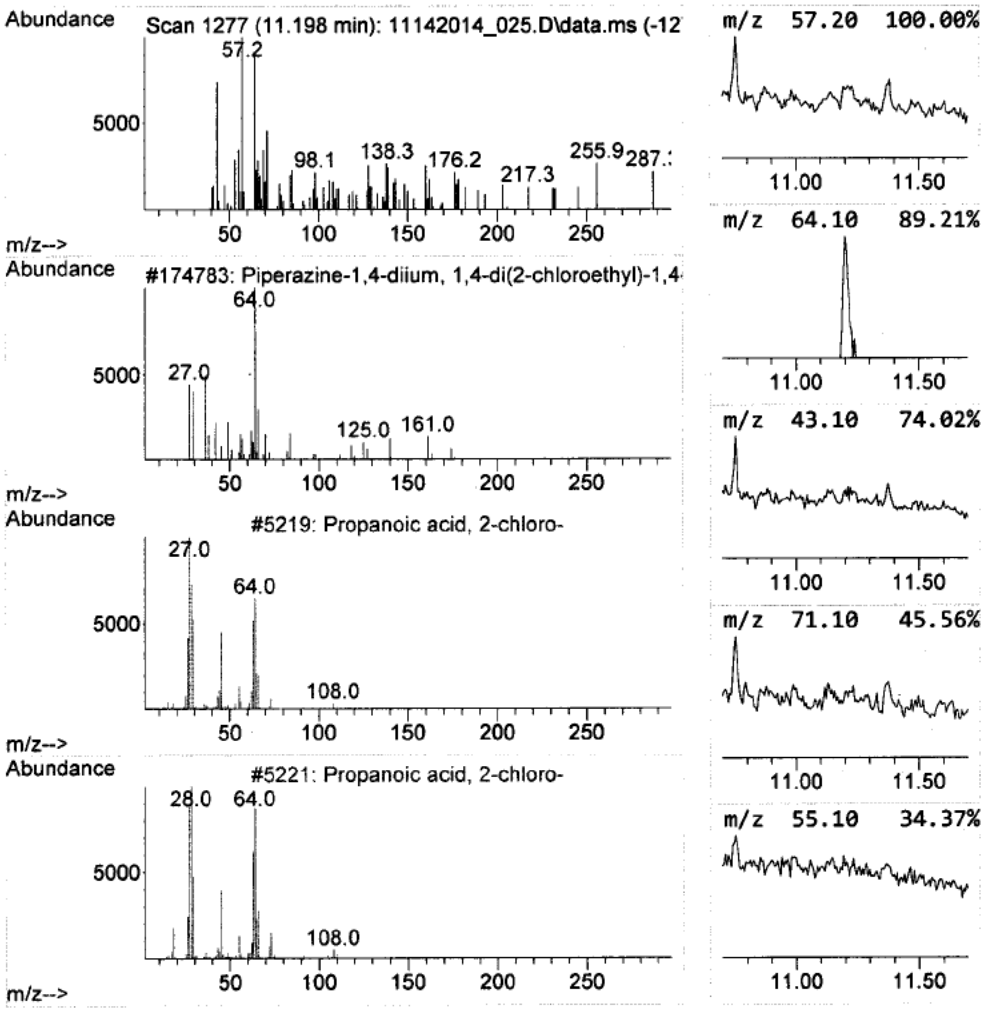
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 16 Piperazine-1,4-diium, 1,4-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.198	0.93 ug/mL	197355	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperazine-1,4-diium, 1,4-di(2-c...	338	C12H26Cl4N2	1000273-25-4	45
2	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	38
3	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	38
4	Butane, 1-(methylsulfinyl)-	120	C5H12OS	002976-98-9	38
5	Thiosulfuric acid, S-[2-(2-hydro...	289	C11H15NO4S2	062209-43-2	28



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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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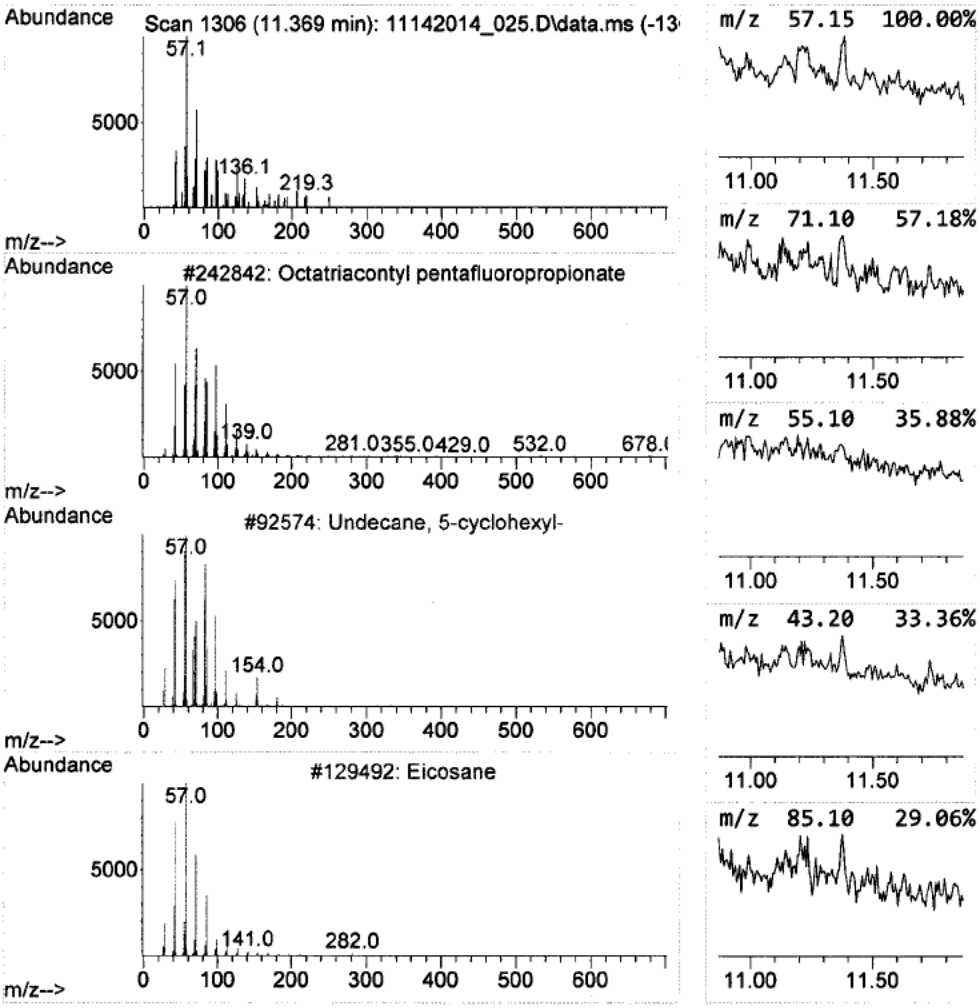
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 17 Octatriacontyl pentafluorop... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.369	0.47 ug/mL	100550	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	37
2	Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	32
3	Eicosane	282	C20H42	000112-95-8	27
4	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	27
5	Docosane	310	C22H46	000629-97-0	27



Library Search Compound Report

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Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

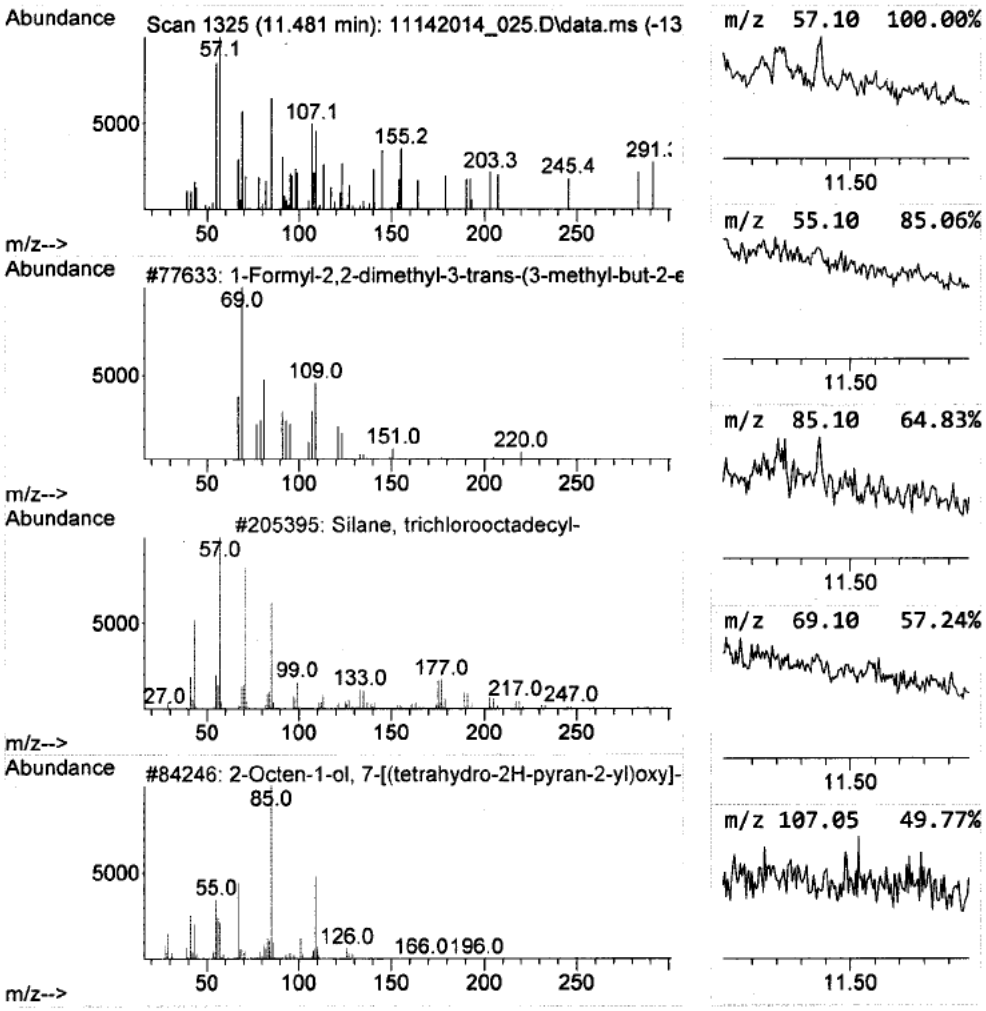
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 18 1-Formyl-2,2-dimethyl-3-tra... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.481	0.41 ug/mL	86767	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	9
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	9
3	2-Octen-1-ol, 7-[(tetrahydro-2H-...	228	C13H24O3	077758-38-4	9
4	Urs-12-en-28-ol	426	C30H50O	010153-88-5	9
5	Pipobroman	354	C10H16Br2N2O2	000054-91-1	9



Library Search Compound Report

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Data File : 11142014_025.D
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Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

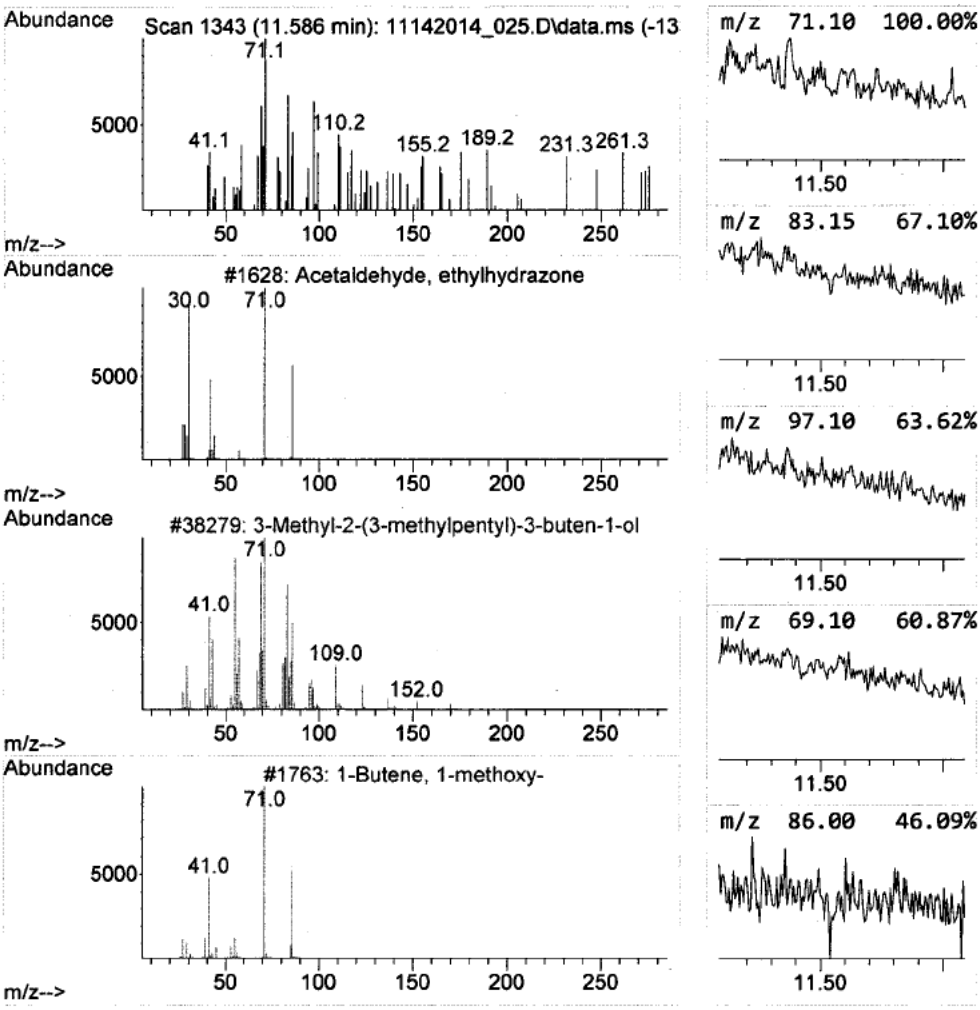
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 19 Acetaldehyde, ethylhydrazone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.586	0.63 ug/mL	132973	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, ethylhydrazone	86	C4H10N2	020487-02-9	14
2	3-Methyl-2-(3-methylpentyl)-3-bu...	170	C11H22O	013066-54-1	12
3	1-Butene, 1-methoxy-	86	C5H10O	029512-02-5	10
4	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	10
5	Meperidine	247	C15H21NO2	000057-42-1	10



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Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

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

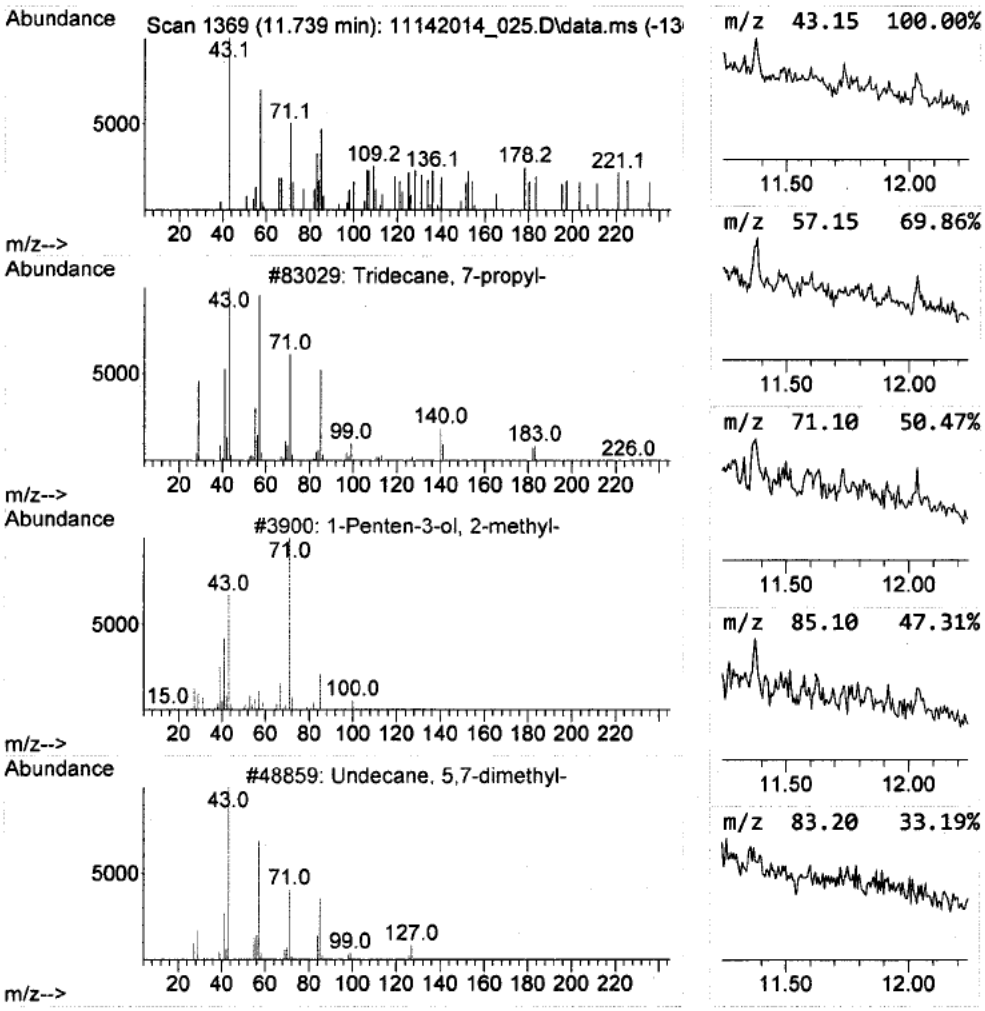
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 20 Tridecane, 7-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	0.60 ug/mL	126607	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-propyl-	226	C16H34	055045-09-5	14
2	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	10
3	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	10
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	10
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	10



Tentatively Identified Compound (LSC) summary

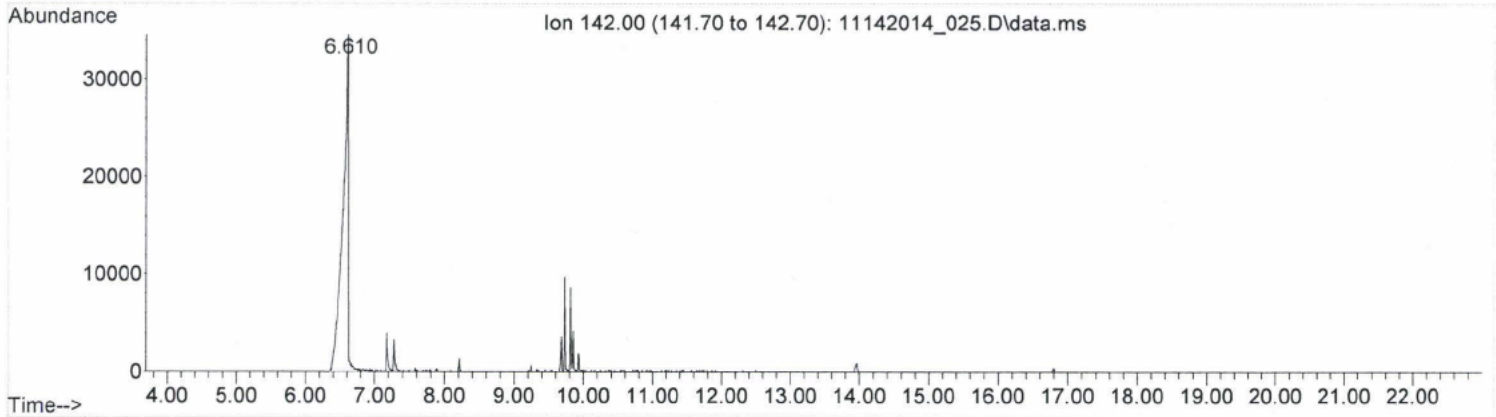
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_025.D
Acq On : 14 Nov 2014 09:36 pm
Operator : [redacted]
Sample : NE36692-C
Misc : Tag # NE36692-C, Lab Rep #3, 1X
ALS Vial : 24 Sample Multiplier: 1

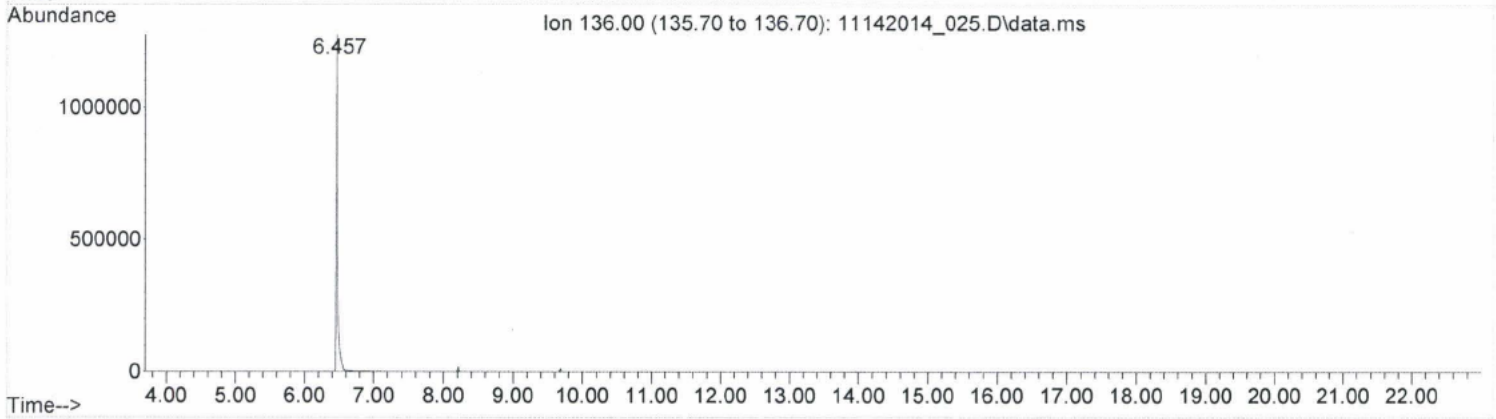
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

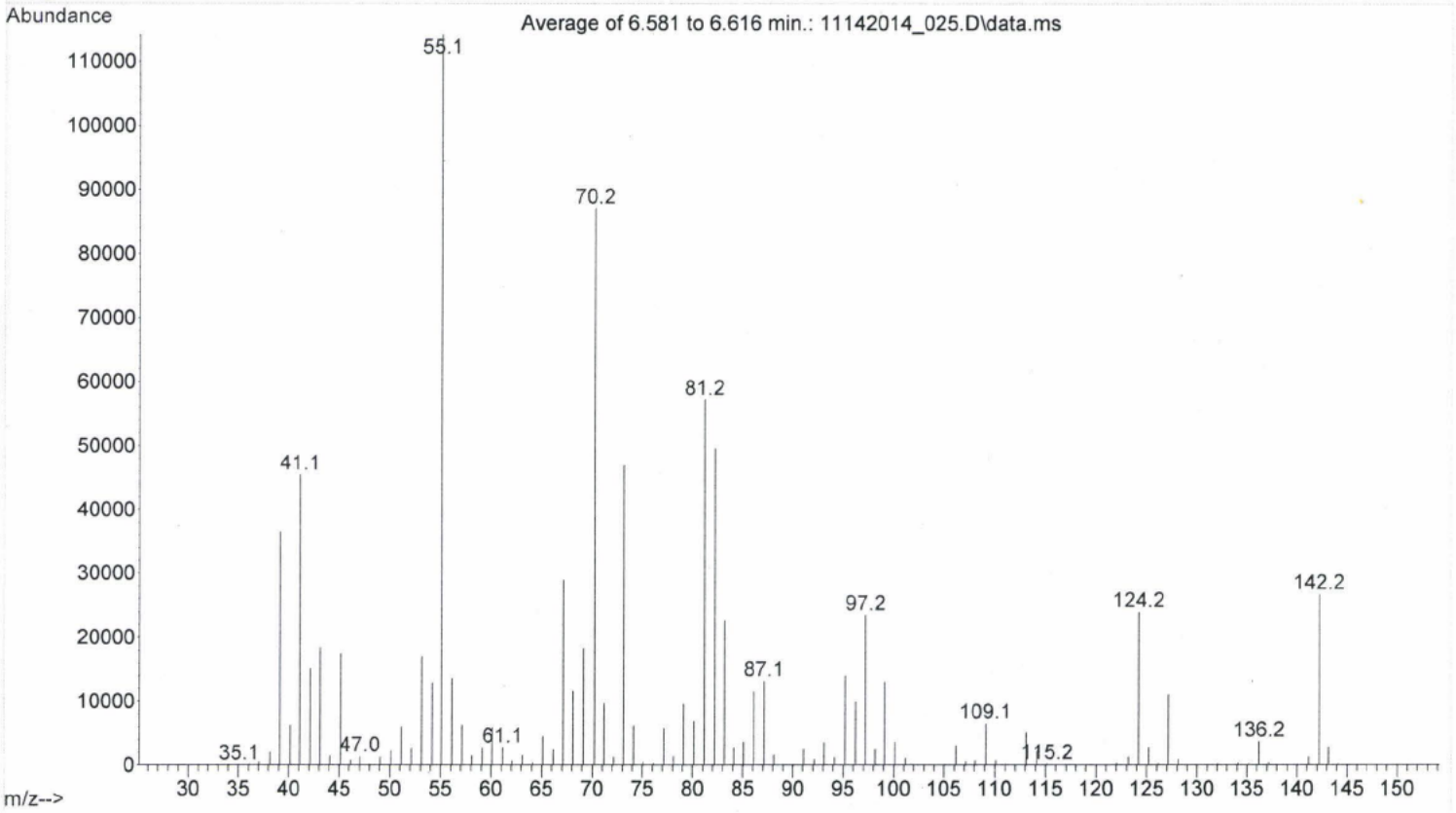
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
p-Xylene	3.787	0.5	ug/mL	75975	1	5.081	3163170	20.0
cis,cis,cis-7,1...	5.405	0.4	ug/mL	64126	1	5.081	3163170	20.0
Cyclohexanemeth...	5.716	0.4	ug/mL	58065	1	5.081	3163170	20.0
Cyclohexanecarb...	6.604	16.8	ug/mL	4904340	2	6.457	5847390	20.0
Acetic acid, ch...	8.593	0.4	ug/mL	91666	3	8.216	4584080	20.0
Hexadecane, 2,6...	9.193	0.3	ug/mL	60457	4	9.681	4251020	20.0
Phenanthrene, 2...	9.534	0.4	ug/mL	81997	4	9.681	4251020	20.0
1H-Pyrazole, 1,...	9.851	5.6	ug/mL	1194170	4	9.681	4251020	20.0
1H-Imidazole,1-...	9.928	2.7	ug/mL	583069	4	9.681	4251020	20.0
3-Ethylidene- h...	10.534	0.7	ug/mL	146978	4	9.681	4251020	20.0
Undecanoic acid...	10.657	0.5	ug/mL	116160	4	9.681	4251020	20.0
2-Bromotetradecane	10.751	0.7	ug/mL	154952	4	9.681	4251020	20.0
Undecane, 6-ethyl-	10.881	0.5	ug/mL	98659	4	9.681	4251020	20.0
6H-Furo[2',3':4...	10.992	0.5	ug/mL	114584	4	9.681	4251020	20.0
Tridecane, 2-me...	11.145	0.5	ug/mL	116368	4	9.681	4251020	20.0
Piperazine-1,4-...	11.198	0.9	ug/mL	197355	4	9.681	4251020	20.0
Octatriacontyl ...	11.369	0.5	ug/mL	100550	4	9.681	4251020	20.0
1-Formyl-2,2-di...	11.481	0.4	ug/mL	86767	4	9.681	4251020	20.0
Acetaldehyde, e...	11.586	0.6	ug/mL	132973	4	9.681	4251020	20.0
Tridecane, 7-pr...	11.739	0.6	ug/mL	126607	4	9.681	4251020	20.0

File :D:[redacted]\RP1616\11142014_Run\11142014_025.D
Operator : [redacted]
Acquired : 14 Nov 2014 09:36 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36692-C
Misc Info : Tag # NE36692-C, Lab Rep #3, 1X
Vial Number: 24







[redacted] RP1616 12/17/14

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Nov 17 11:05:46 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	399956	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1763247	20.00 ug/mL	# 0.00
5) Acenaphthene-d10	8.216	164	994942	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.681	188	1497465	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	913916	20.00 ug/mL	0.00
12) Perylene-d12	16.798	264	521847	20.00 ug/mL	0.00
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	556729	9.11 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery =	~~72.88%~~	
Target Compounds					Qvalue
2) MCHM	5.540	55	54447m	1.53 ug/mL	
4) PPH	6.863	94	11055m	0.58 ug/mL	
6) 1,4-CHDM	0.000		0	N.D. d	
8) DM-1,4-CHDC	0.000		0	N.D. d	
9) di-PPH	8.539	59	47526m	1.72 ug/mL	

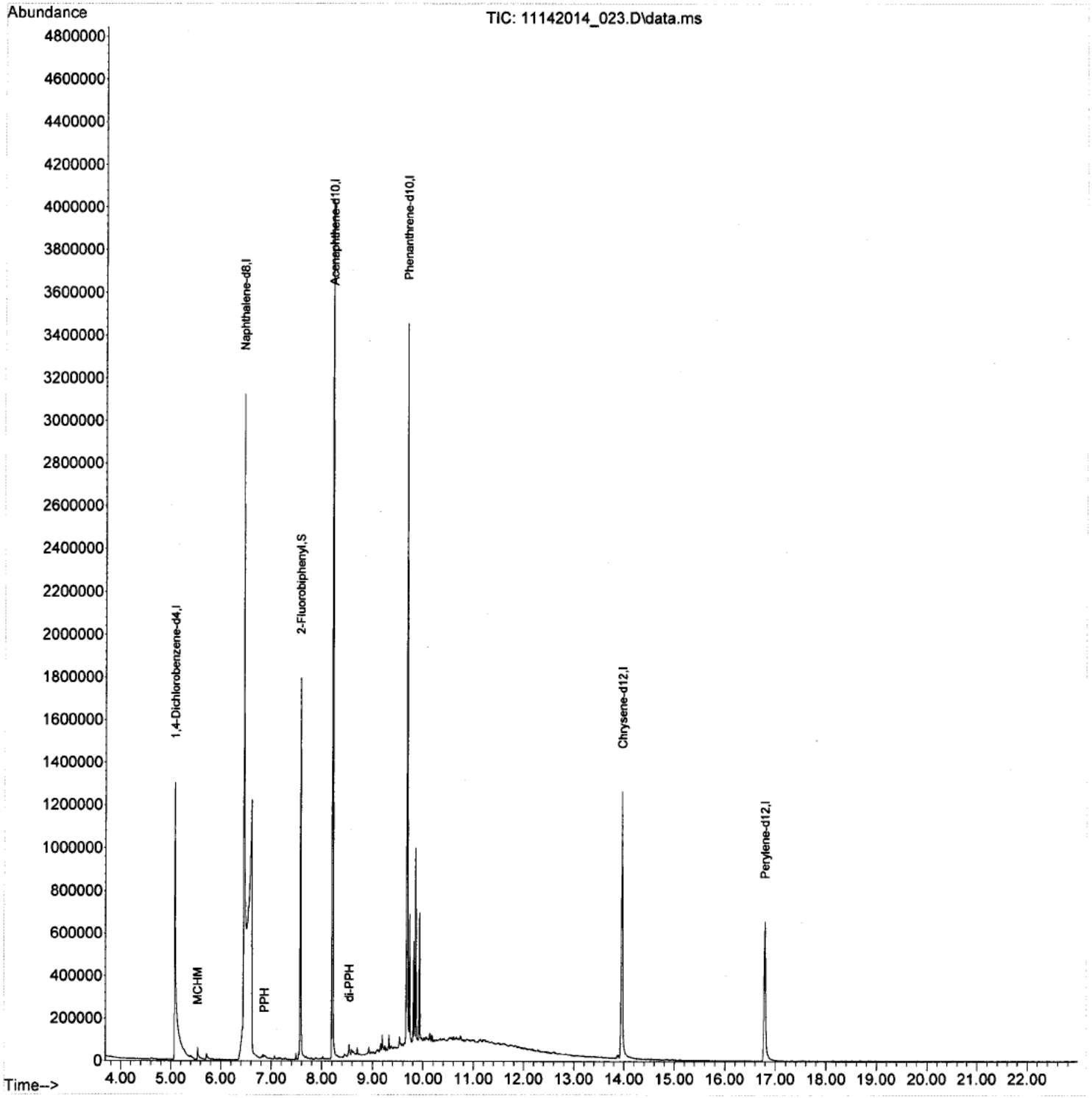
see Analyst Narrative, Surrogate Recovery

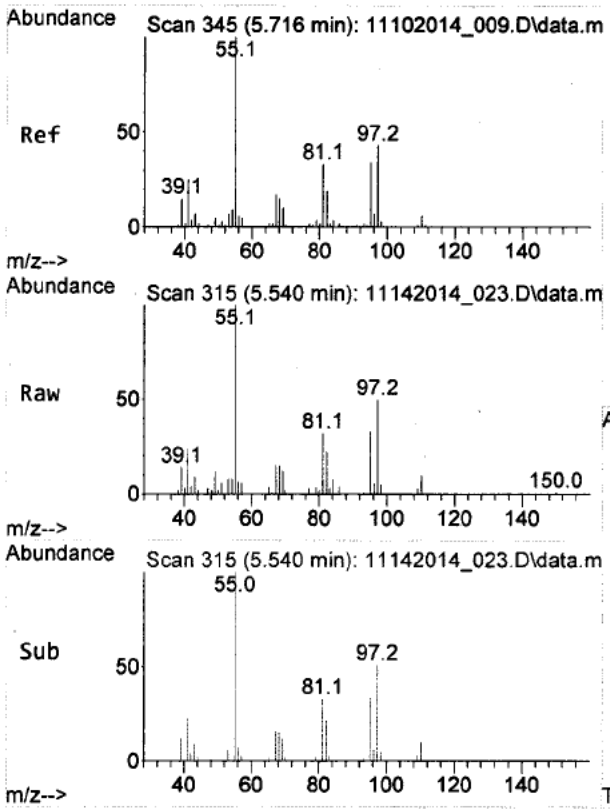
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Nov 17 11:05:46 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

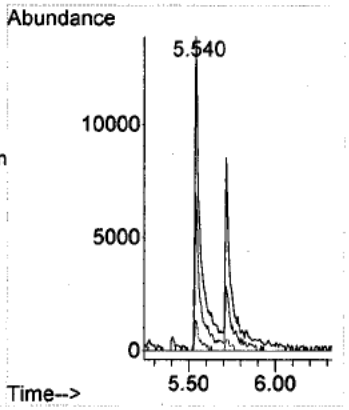


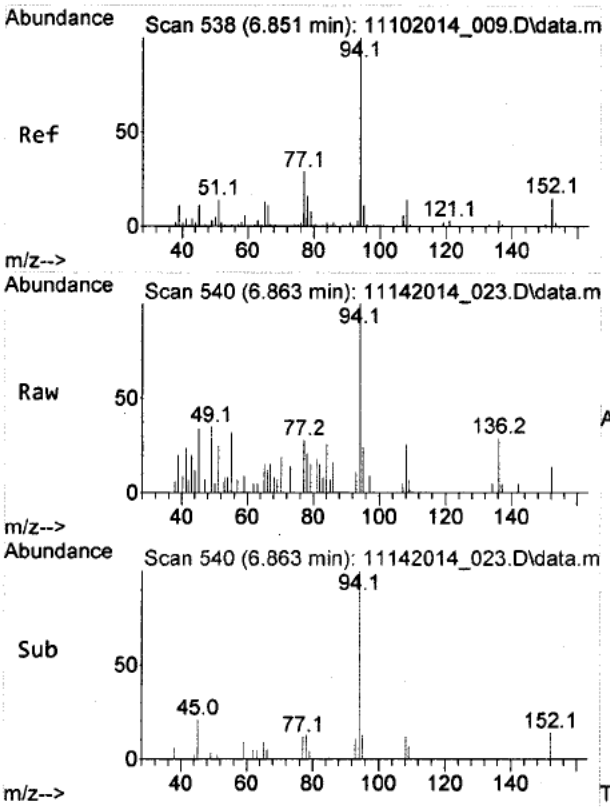


#2
MCHM
Concen: 1.53 ug/mL m
RT: 5.540 min Scan# 315
Delta R.T. -0.176 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 55 Resp: 54447

Ion	Ratio	Lower	Upper
55	100		
97	25.6	34.6	51.8#
110	3.8	4.8	7.2#

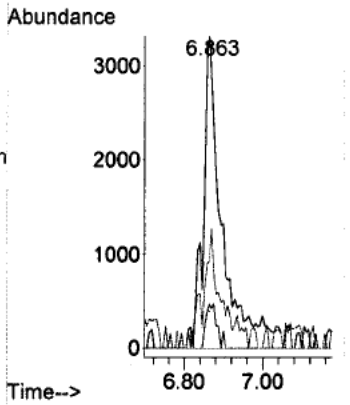


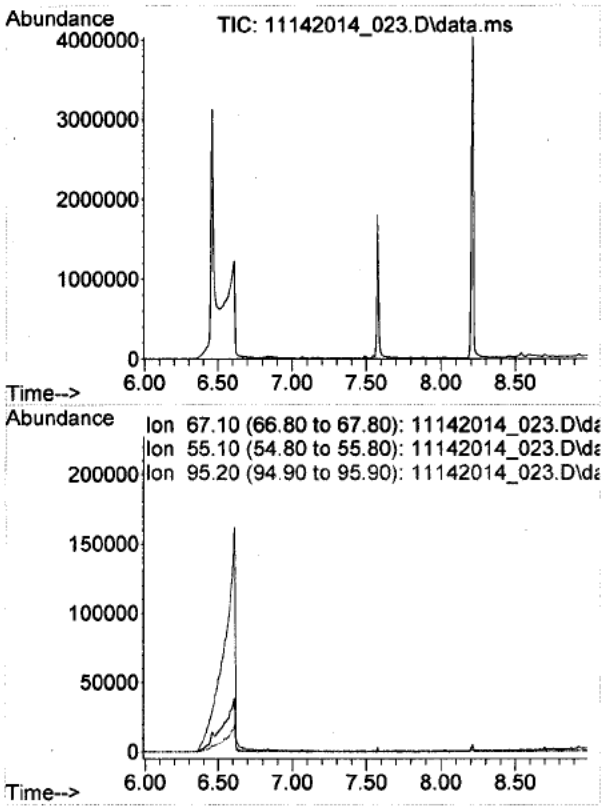


#4
PPH
Concen: 0.58 ug/mL m
RT: 6.863 min Scan# 540
Delta R.T. 0.006 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 94 Resp: 11055

Ion	Ratio	Lower	Upper
94	100		
152	8.4	13.4	20.0#
77	19.7	21.2	31.8#



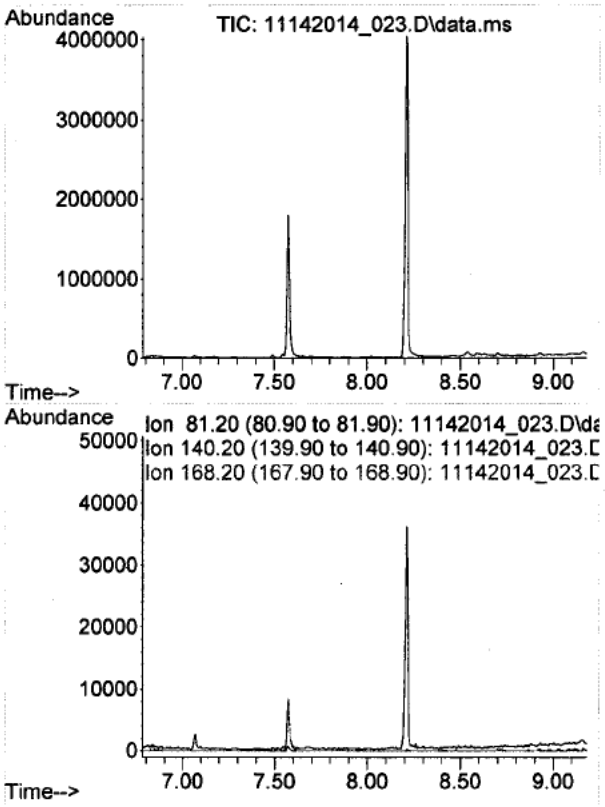


#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8

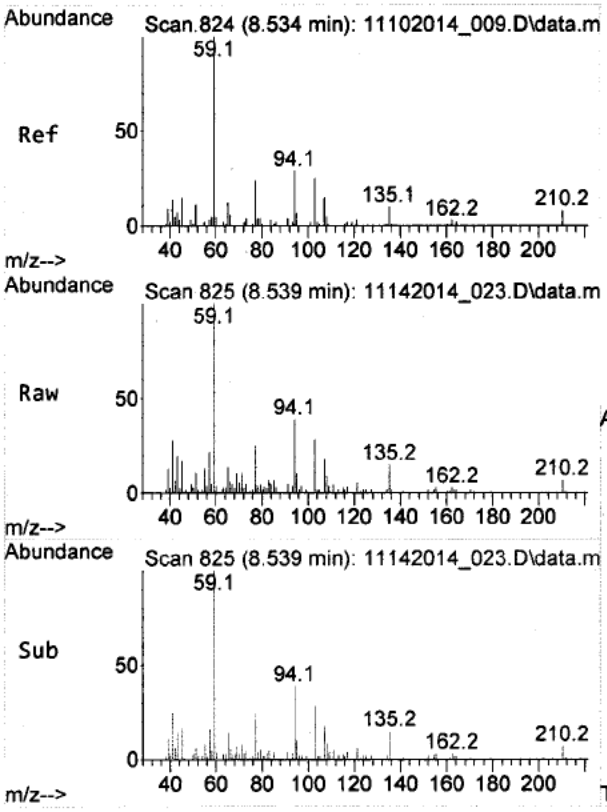


#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 81

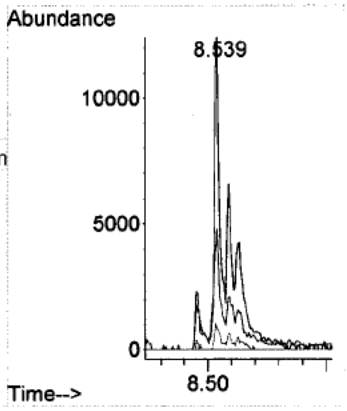
Sig	Exp Ratio
81	100
140	61.8
168	17.7



#9
di-PPH
Concen: 1.72 ug/mL m
RT: 8.539 min Scan# 825
Delta R.T. -0.001 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 59 Resp: 47526

Ion	Ratio	Lower	Upper
59	100		
94	18.4	23.0	34.6#
210	3.3	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Dec 01 12:30:24 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	685394	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1763247	20.00 ug/mL	# 0.00
24) Acenaphthene-d10	8.216	164	994942	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.681	188	1497465	20.00 ug/mL	0.00
49) Chrysene-d12	13.963	240	915856	20.00 ug/mL	-0.01
58) Perylene-d12	16.798	264	523590	20.00 ug/mL	-0.01
Target Compounds					Qvalue
2) Bis(2-chloroethyl) ether	0.000		0	N.D.	
3) n-Decane	0.000		0	N.D. d	
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.	
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...	6.610	55	858712	69.89 ug/mL	94
14) n-Dodecane	0.000		0	N.D. d	
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	0.000		0	N.D. d	
19) Hexachlorobutadiene	0.000		0	N.D.	
20) 2-Methylnapthalene	7.175	142	3332	0.04 ug/mL	87
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	0.000		0	N.D. d	
23) n-Tetradecane	7.698	57	2574	0.05 ug/mL#	93
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	0.000		0	N.D. d	
30) 2,4-Dinitrotoluene	0.000		0	N.D. d	
31) n-Hexadecane	8.698	57	4220	0.08 ug/mL#	95
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. d	
39) Hexachlorobenzene	0.000		0	N.D.	
40) n-Octadecane	9.645	57	7917	0.15 ug/mL#	60
41) Phenanthrene	0.000		0	N.D. d	
42) Anthracene	0.000		0	N.D. d	
43) Carbazole	0.000		0	N.D. d	
44) Dibutyl Phthalate	0.000		0	N.D. d	
45) n-Eicosane	10.745	57	5348	0.10 ug/mL#	88

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Dec 01 12:30:24 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

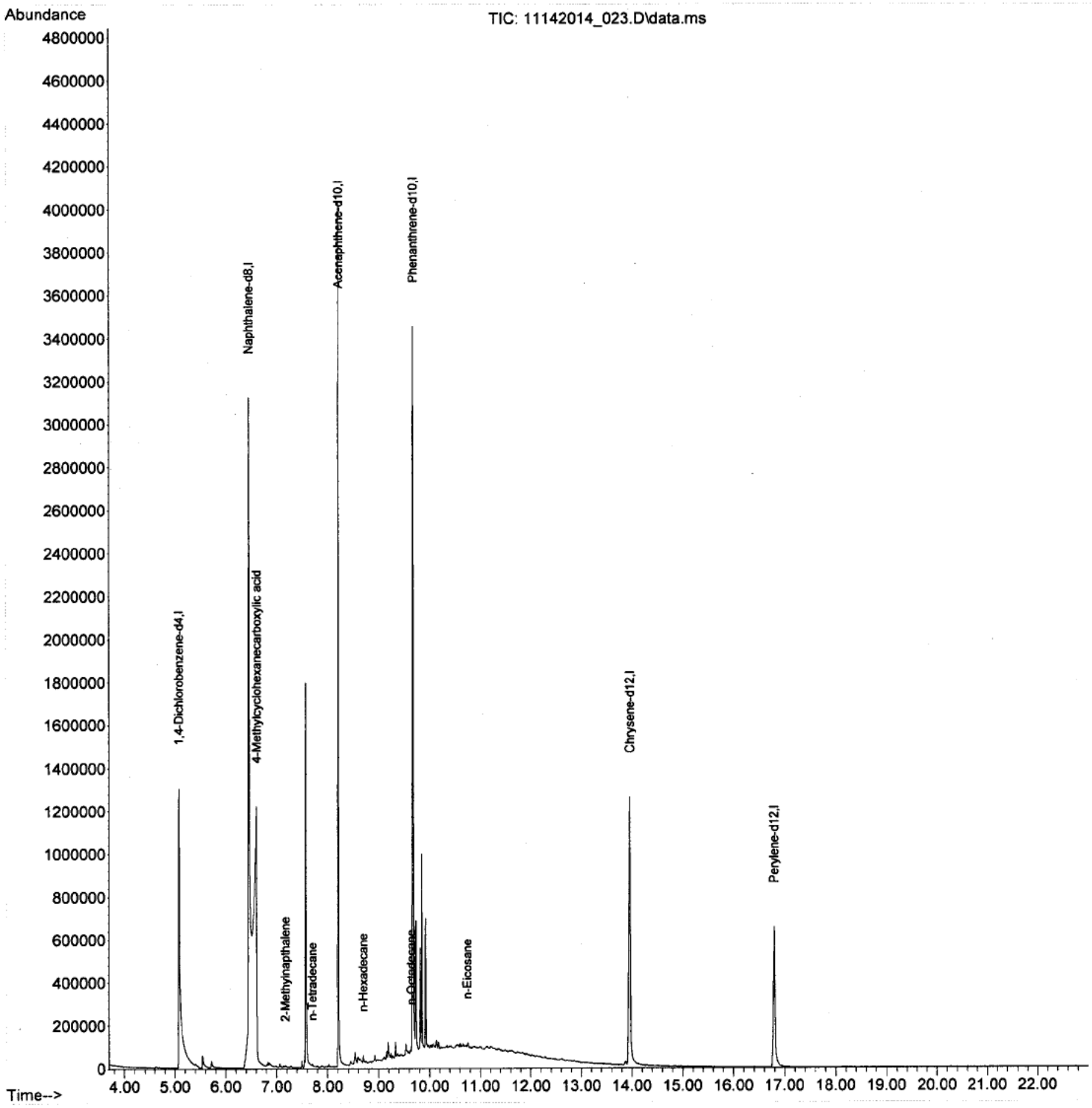
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	0.000		0	N.D.	d
47) Pyrene	0.000		0	N.D.	d
48) n-Docosane	0.000		0	N.D.	d
50) Benzyl Butyl Phthalate	0.000		0	N.D.	d
51) n-Tetracosane	0.000		0	N.D.	d
52) n-Hexacosane	0.000		0	N.D.	d
53) n-Octacosane	0.000		0	N.D.	d
54) Benz[a]anthracene	0.000		0	N.D.	d
55) Chrysene	0.000		0	N.D.	d
56) Bis(2-ethylhexyl) Phth...	0.000		0	N.D.	d
57) Di-n-octyl Phthalate	0.000		0	N.D.	d
59) Benzo[b]fluoranthene	0.000		0	N.D.	
60) Benzo(k)fluoranthene	0.000		0	N.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.	

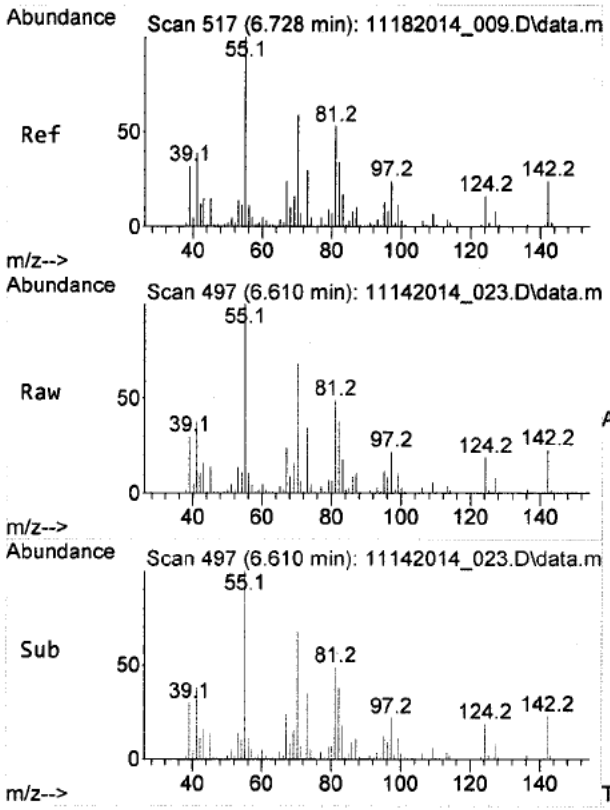
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Dec 01 12:30:24 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

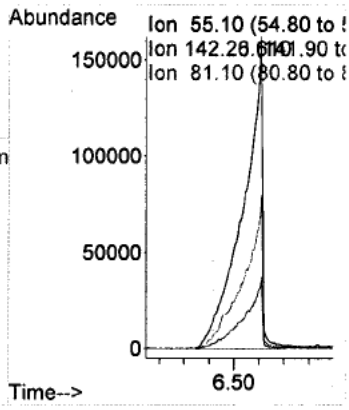


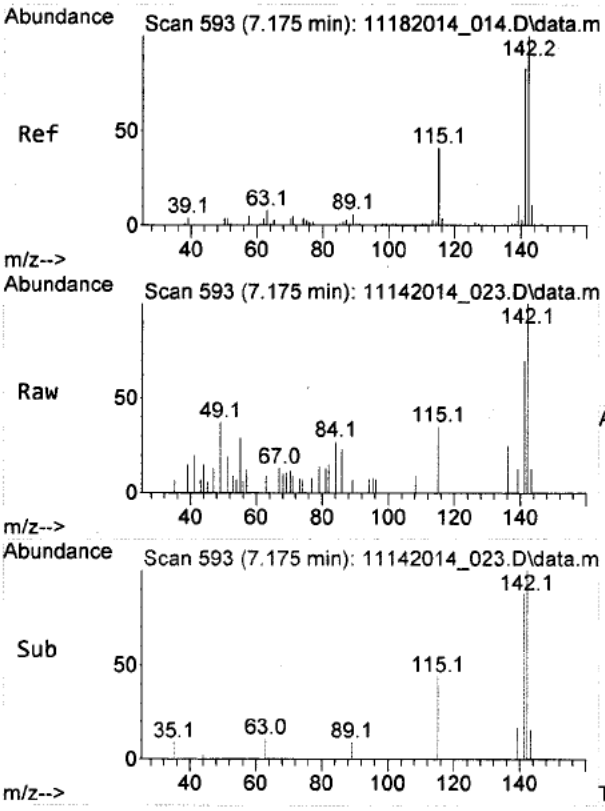


#12
4-Methylcyclohexanecarboxylic acid
Concen: 69.89 ug/mL
RT: 6.610 min Scan# 497
Delta R.T. -0.118 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 55 Resp: 858712

Ion	Ratio	Lower	Upper
55	100		
142	21.5	19.1	28.7
81	48.4	42.3	63.5

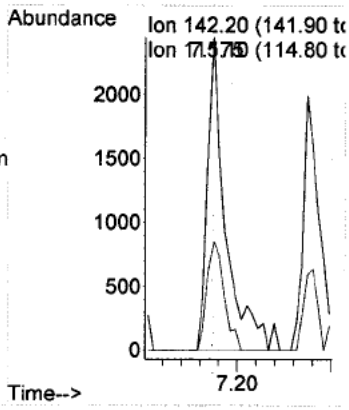


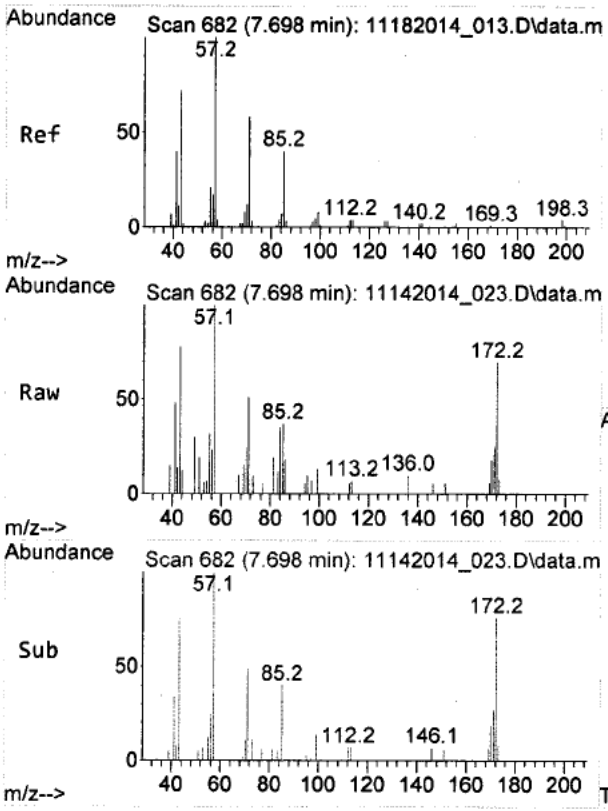


#20
2-Methylnapthalene
Concen: 0.04 ug/mL
RT: 7.175 min Scan# 593
Delta R.T. -0.000 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion:142 Resp: 3332

Ion	Ratio	Lower	Upper
142	100		
115	33.1	33.0	49.4

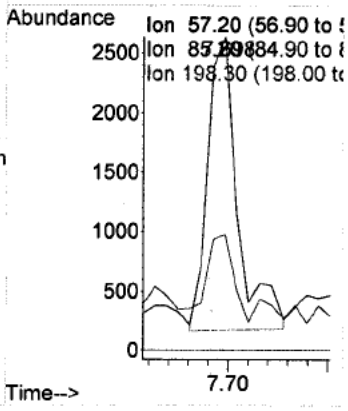


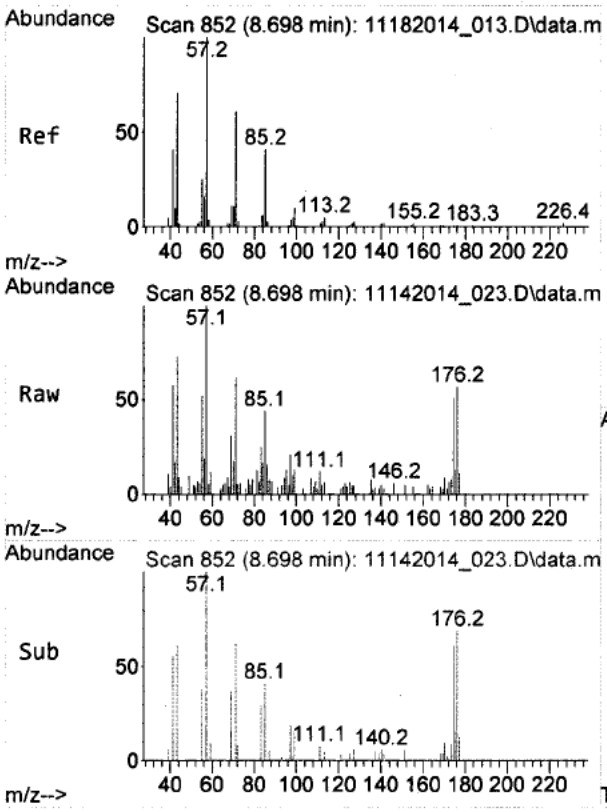


#23
n-Tetradecane
Concen: 0.05 ug/mL
RT: 7.698 min Scan# 682
Delta R.T. 0.000 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 57 Resp: 2574

Ion	Ratio	Lower	Upper
57	100		
85	35.7	31.6	47.4
198	0.0	3.1	4.7#

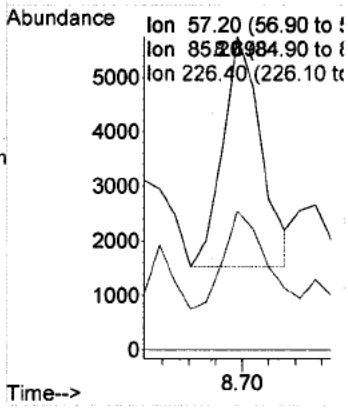


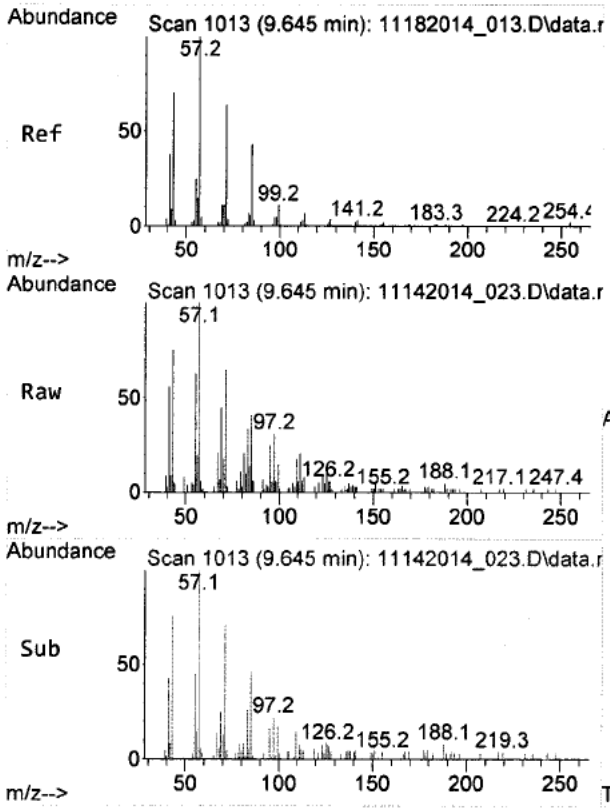


#31
n-Hexadecane
Concen: 0.08 ug/mL
RT: 8.698 min Scan# 852
Delta R.T. 0.000 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 57 Resp: 4220

Ion	Ratio	Lower	Upper
57	100		
85	46.4	35.1	52.7
226	0.0	3.1	4.7#

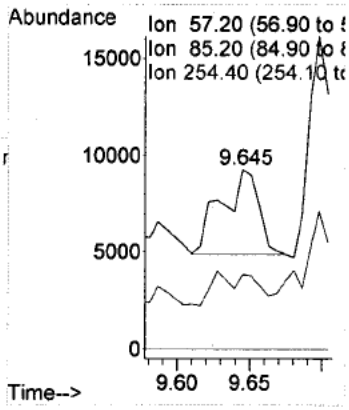


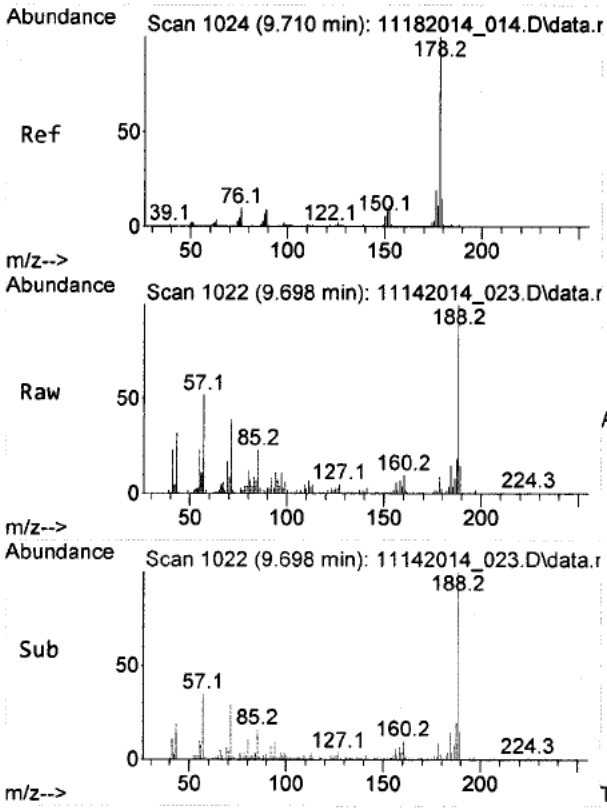


#40
n-Octadecane
Concen: 0.15 ug/mL
RT: 9.645 min Scan# 1013
Delta R.T. 0.000 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 57 Resp: 7917

Ion	Ratio	Lower	Upper
57	100		
85	16.2	34.5	51.7#
254	0.0	1.4	2.2#

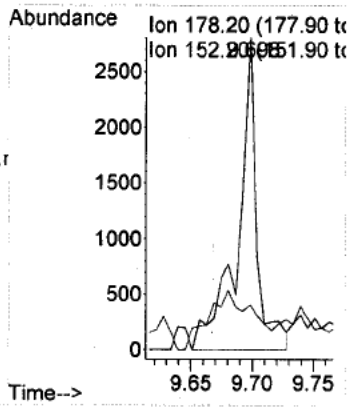


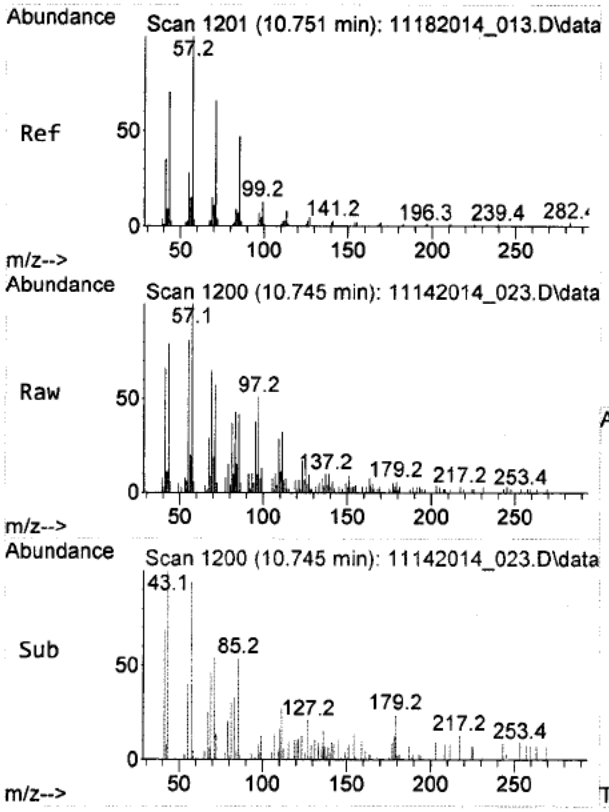


#41
Phenanthrene
Concen: 0.03 ug/mL
RT: 9.698 min Scan# 1022
Delta R.T. -0.012 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion:178 Resp: 3047

Ion	Ratio	Lower	Upper
178	100		
152	44.4	8.5	12.7#

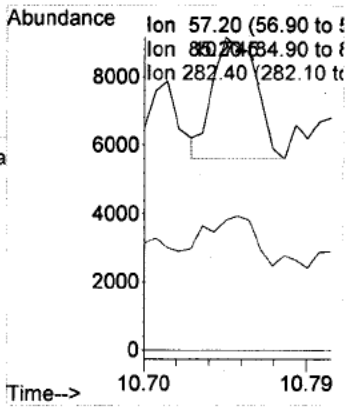




#45
n-Eicosane
Concen: 0.10 ug/mL
RT: 10.745 min Scan# 1200
Delta R.T. -0.006 min
Lab File: 11142014_023.D
Acq: 14 Nov 2014 08:37 pm

Tgt Ion: 57 Resp: 5348

Ion	Ratio	Lower	Upper
57	100		
85	55.4	37.8	56.8
282	0.0	1.4	2.2#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 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_023.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.769	13	14	42	rVB5	7648	44754	0.47%	0.122%
2	5.081	233	237	289	rBV	1299764	2987496	31.33%	8.172%
3	5.404	289	292	305	rVB9	18125	57525	0.60%	0.157%
4	5.540	312	315	342	rBV	56512	120478	1.26%	0.330%
5	5.716	342	345	362	rVV	30032	61232	0.64%	0.167%
6	6.457	451	471	495	rBV	3122353	9536868	100.00%	26.088%
7	6.610	495	497	500	rVB	1160695	1019843	10.69%	2.790%
8	7.575	658	661	679	rVB	1782908	1628462	17.08%	4.455%
9	8.210	764	769	772	rBV	4026291	4183964	43.87%	11.445%
10	8.539	818	825	831	rVV3	56508	100274	1.05%	0.274%
11	8.586	831	833	838	rVV3	34432	63409	0.66%	0.173%
12	8.628	838	840	849	rVV6	23832	56564	0.59%	0.155%
13	8.698	849	852	878	rVV3	36009	73259	0.77%	0.200%
14	9.104	914	921	927	rBV6	17241	48564	0.51%	0.133%
15	9.192	933	936	942	rVV	74720	77537	0.81%	0.212%
16	9.328	956	959	964	rBV	70541	61800	0.65%	0.169%
17	9.375	964	967	991	rVV	12458	42039	0.44%	0.115%
18	9.533	991	994	1001	rBV2	51738	81991	0.86%	0.224%
19	9.681	1013	1019	1022	rBV	3363433	3858737	40.46%	10.556%
20	9.733	1024	1028	1038	rVV	600413	610733	6.40%	1.671%
21	9.816	1038	1042	1045	rVV	472226	417833	4.38%	1.143%
22	9.851	1045	1048	1057	rVV	911035	836506	8.77%	2.288%
23	9.928	1057	1061	1093	rVV	611101	766049	8.03%	2.096%
24	10.133	1093	1096	1100	rVV2	46352	72305	0.76%	0.198%
25	10.175	1100	1103	1174	rVV2	38394	546610	5.73%	1.495%
26	10.604	1174	1176	1198	rVV2	39837	253699	2.66%	0.694%
27	10.745	1198	1200	1556	rVB2	87899	4776015	50.08%	13.065%
28	12.851	1556	1558	1586	rVB2	13121	60815	0.64%	0.166%
29	13.963	1737	1747	1773	rBV	1250655	2597443	27.24%	7.105%
30	16.798	2218	2229	2270	rVV	655864	1513732	15.87%	4.141%

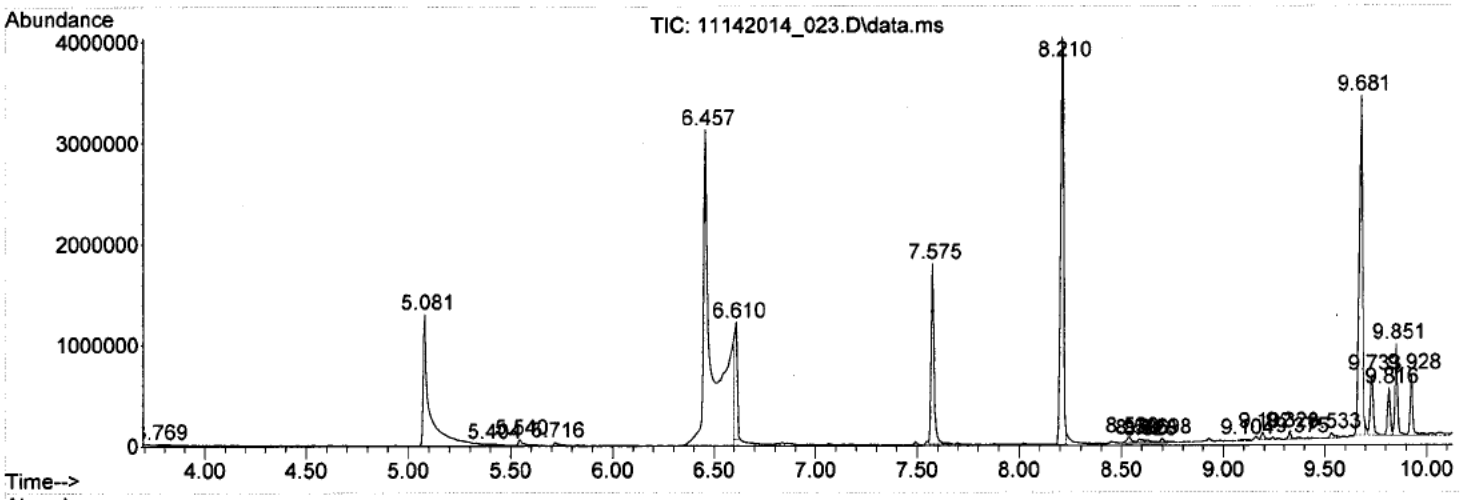
Sum of corrected areas: 36556536

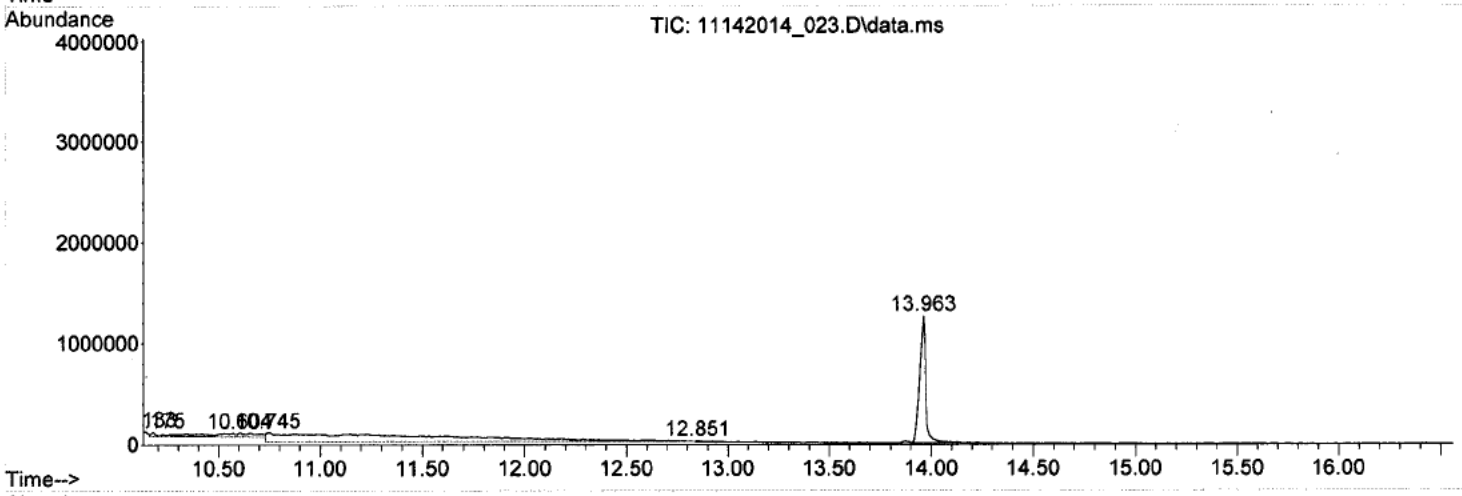
LSC Report - Integrated Chromatogram

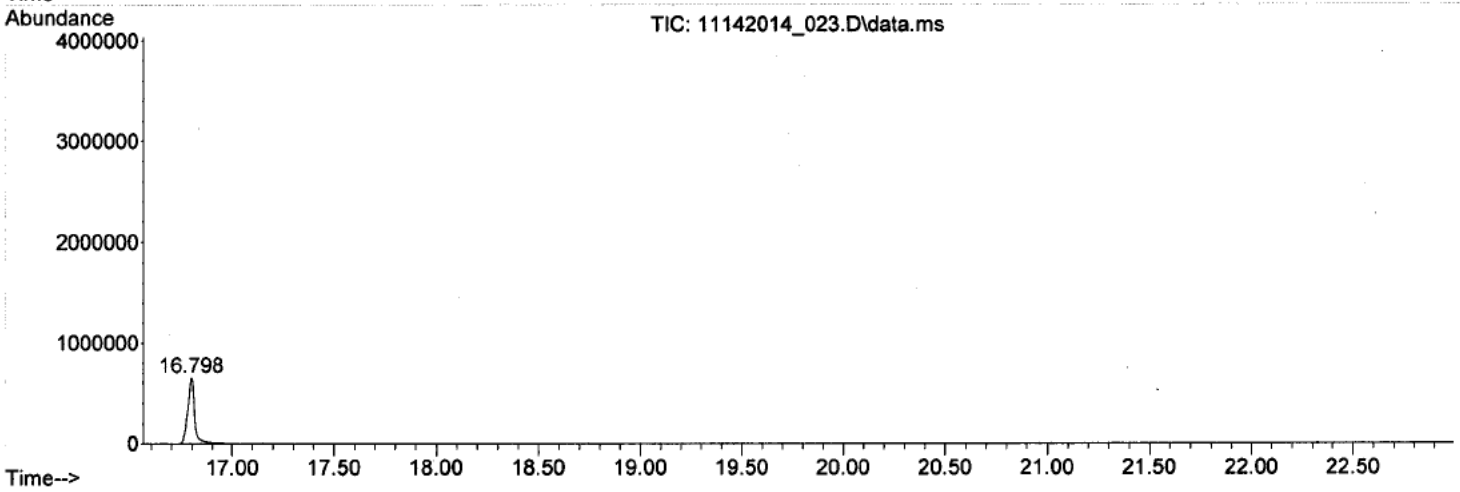
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

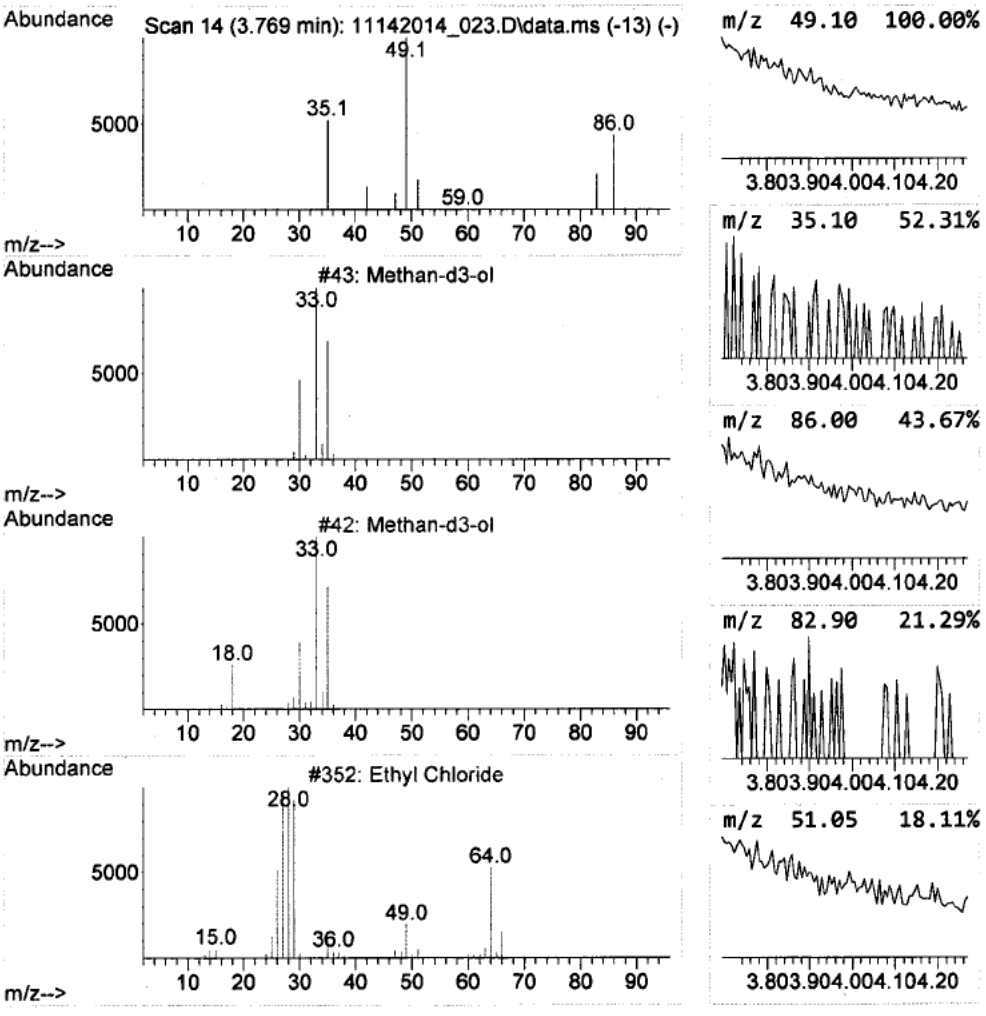
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 1 Methan-d3-ol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.769	0.30 ug/mL	44754	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methan-d3-ol	35	CHD3O	001849-29-2	3
2	Methan-d3-ol	35	CHD3O	001849-29-2	3
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	2
4	Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	2
5	Acetic acid, chloro-, ethyl ester	122	C4H7ClO2	000105-39-5	1



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

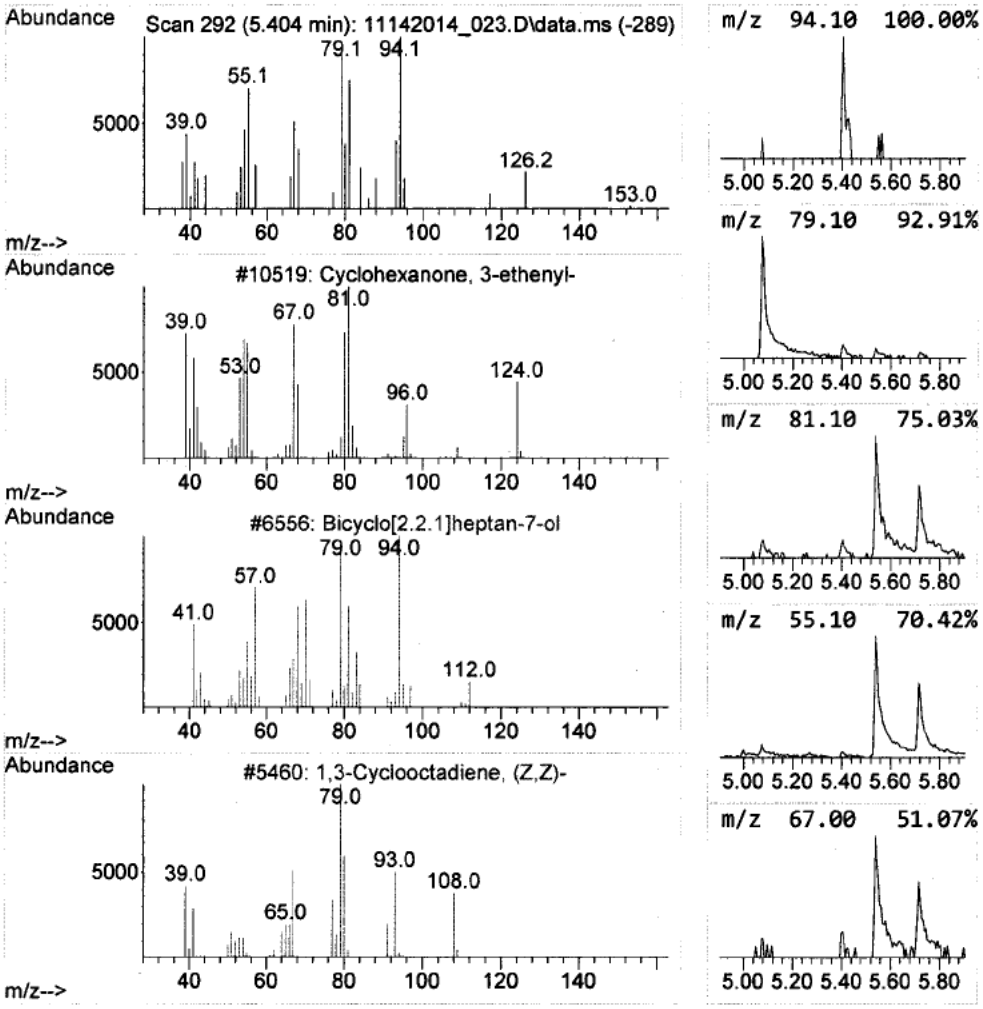
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 2 Cyclohexanone, 3-ethenyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.404	0.39 ug/mL	57525	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-ethenyl-	124	C8H12O	001740-63-2	35
2	Bicyclo[2.2.1]heptan-7-ol	112	C7H12O	002566-48-5	35
3	1,3-Cyclooctadiene, (Z,Z)-	108	C8H12	003806-59-5	27
4	Tricyclo[4.1.1.0(2,5)]octane	108	C8H12	070970-60-4	25
5	1,3-Cyclooctadiene	108	C8H12	001700-10-3	22



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

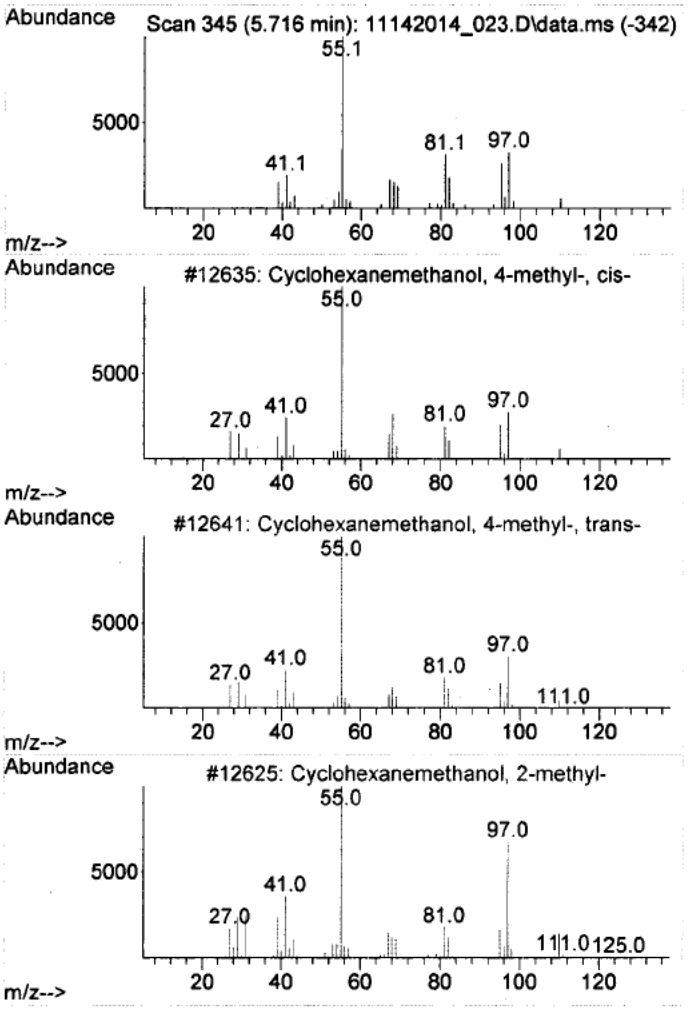
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

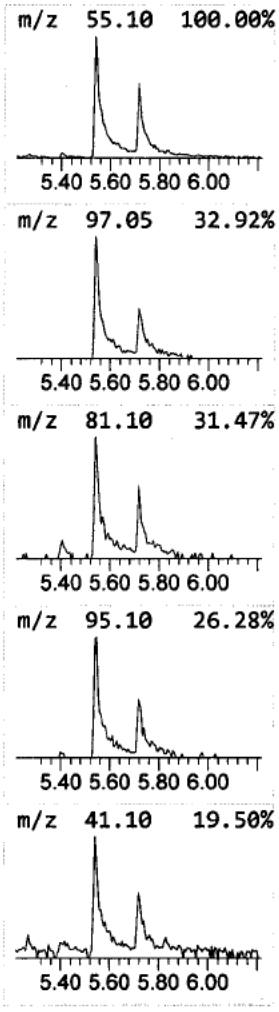
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 3 Cyclohexanemethanol, 4-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	0.41 ug/mL	61232	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	72
2	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	72
3	Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	56
4	Cycloheptanemethanol	128	C8H16O	004448-75-3	53
5	Cycloheptanemethanol	128	C8H16O	004448-75-3	53





Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

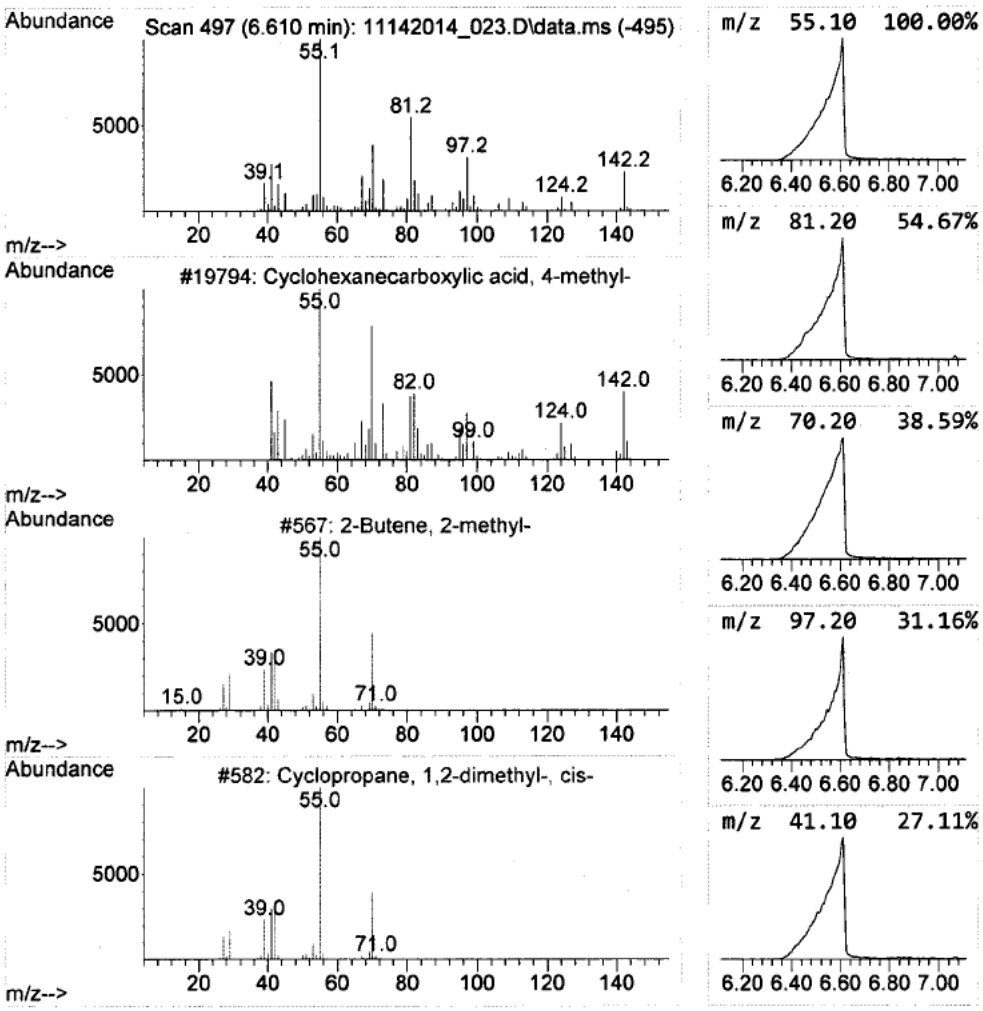
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 4 Cyclohexanecarboxylic acid,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	2.14 ug/mL	1019840	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	64
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	30
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	27
4	2-Methyl-1-butene	70	C5H10	000563-46-2	27
5	Dichloroacetic acid, 1-cyclopent...	224	C9H14Cl2O2	1000282-56-3	27



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

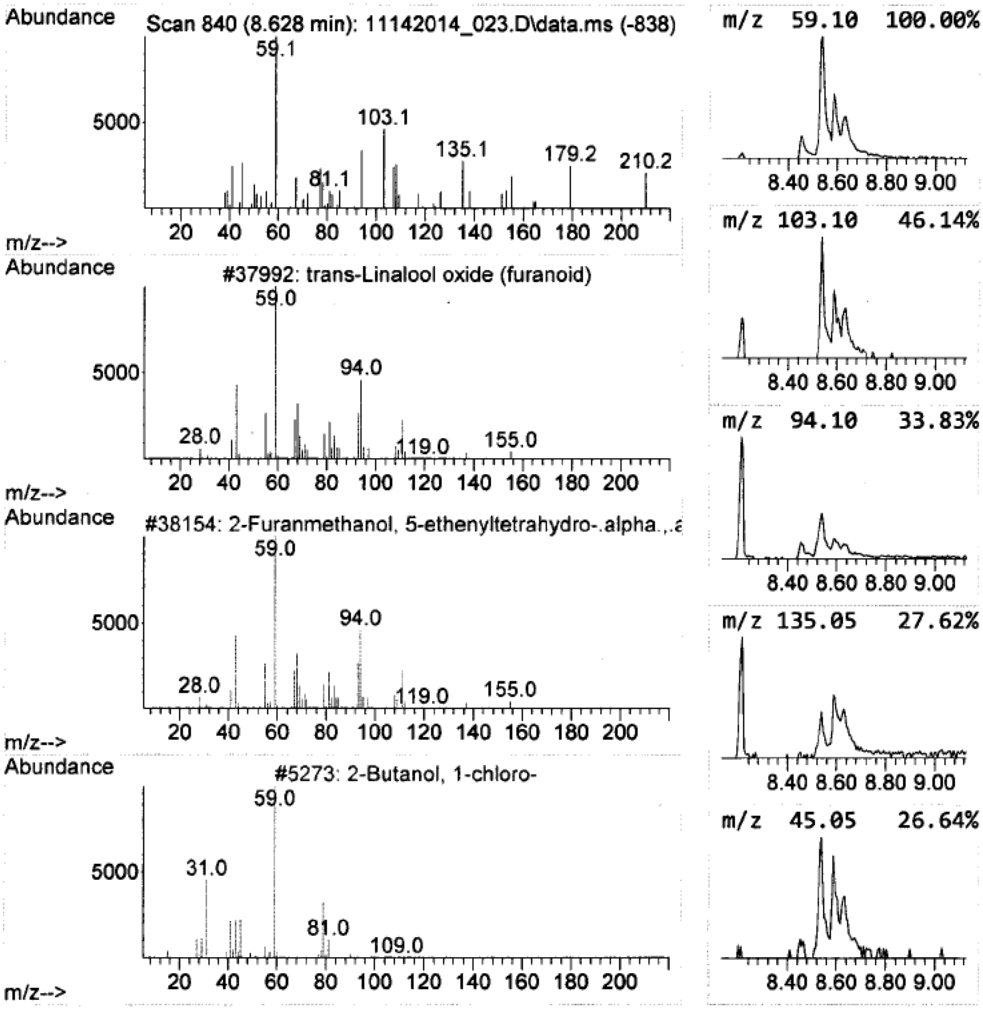
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 5 trans-Linalool oxide (furan... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	0.27 ug/mL	56564	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Linalool oxide (furanoid)	170	C10H18O2	034995-77-2	16
2	2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	16
3	2-Butanol, 1-chloro-	108	C4H9ClO	001873-25-2	14
4	2-Hydroxymethyl-5-(1-hydroxy-1-i...	184	C10H16O3	097762-06-6	12
5	2,3-Dimercaptopropan-1-ol	124	C3H8OS2	000059-52-9	10



Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

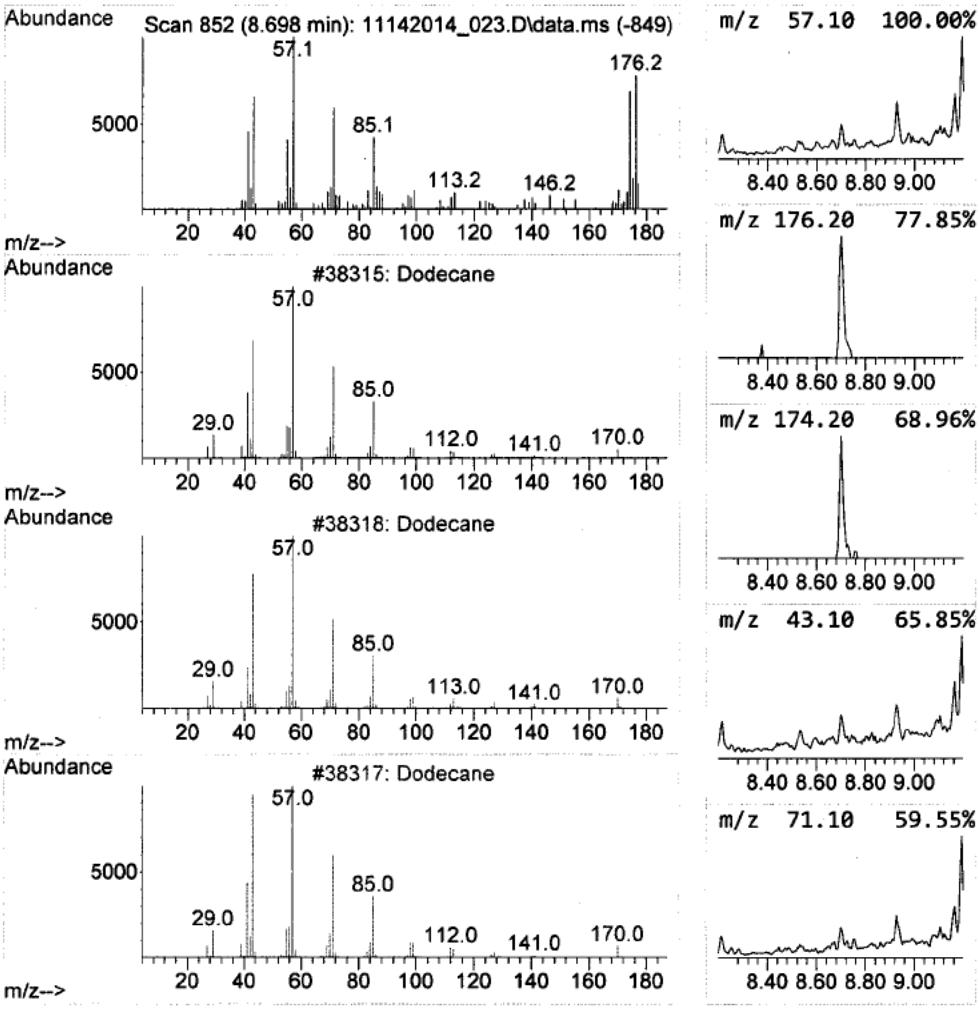
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 6 Dodecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.698	0.35 ug/mL	73259	Acenaphthene-d10	8.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	49
2	Dodecane	170	C12H26	000112-40-3	42
3	Dodecane	170	C12H26	000112-40-3	30
4	Heptacosane	380	C27H56	000593-49-7	25
5	Tetracosane	338	C24H50	000646-31-1	25



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

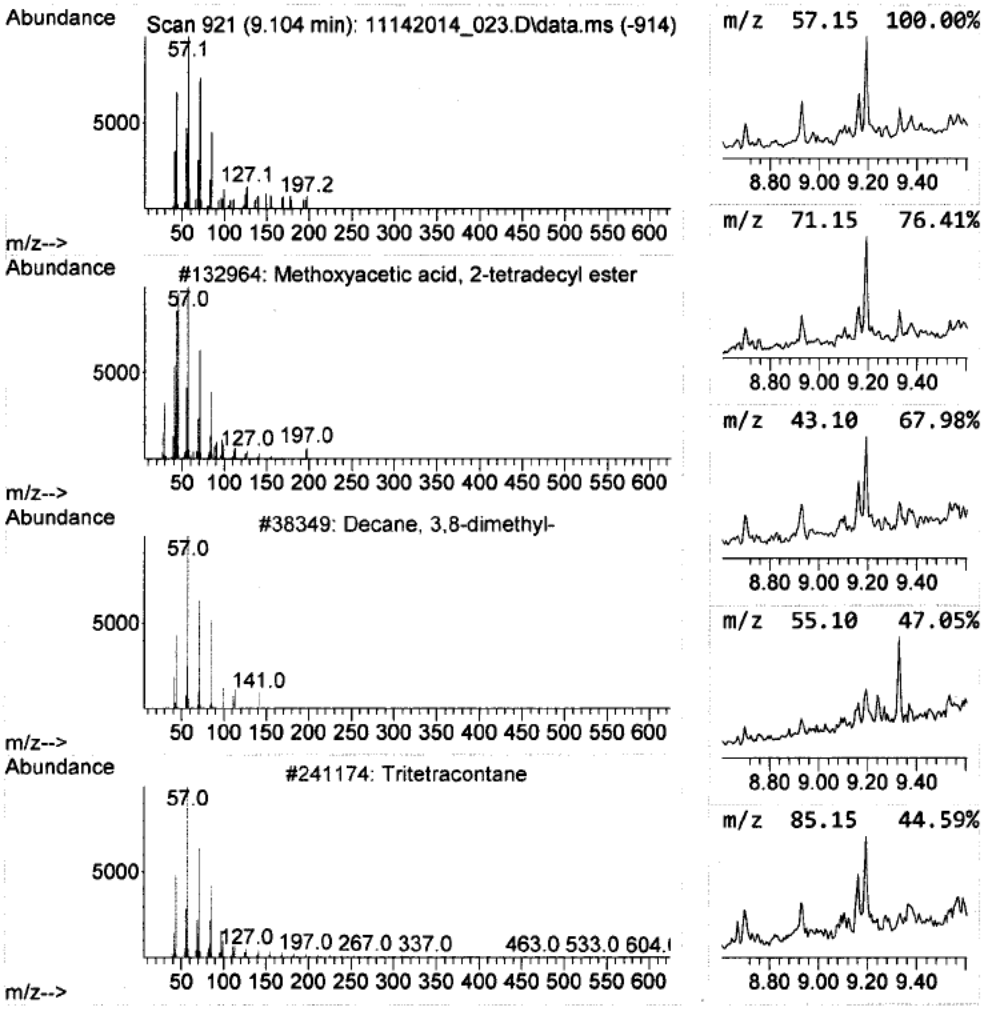
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 7 Methoxyacetic acid, 2-tetra... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.104	0.25 ug/mL	48564	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-tetradecyl...	286	C17H3403	1000282-04-8	86
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
3	Tritetracontane	605	C43H88	007098-21-7	64
4	Tetradecane	198	C14H30	000629-59-4	64
5	Tridecane	184	C13H28	000629-50-5	64



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

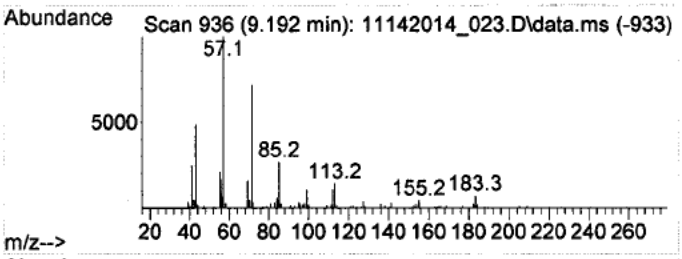
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

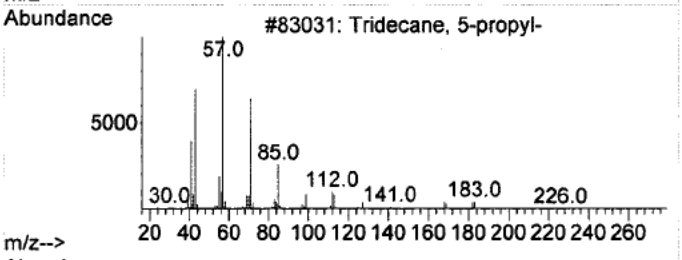
****

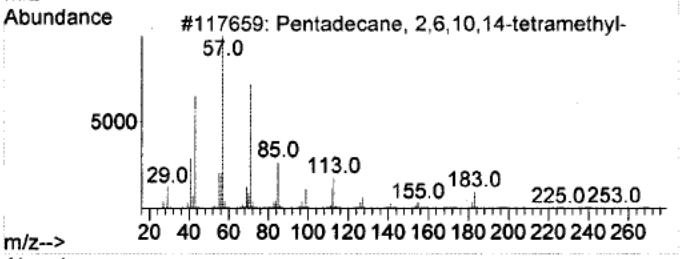
Peak Number 8 Tridecane, 5-propyl- Concentration Rank 12

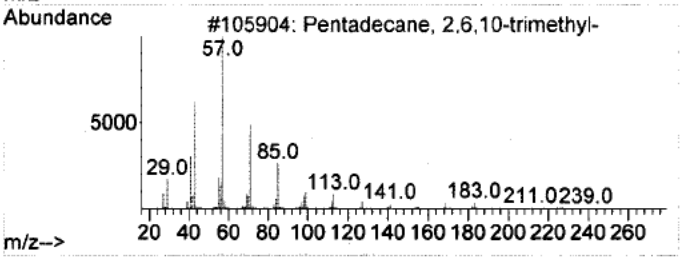
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.192	0.40 ug/mL	77537	Phenanthrene-d10	9.681

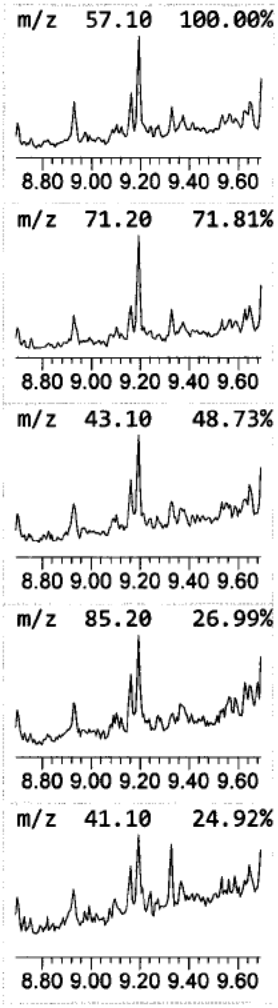
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	83
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	78
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	78
5	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

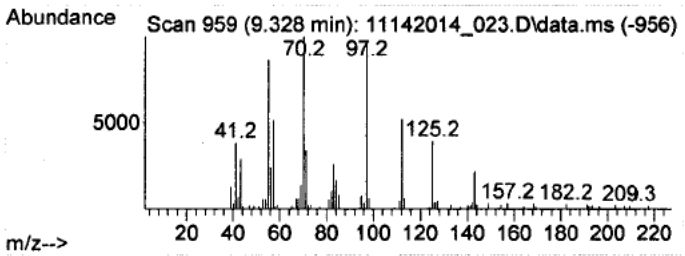
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

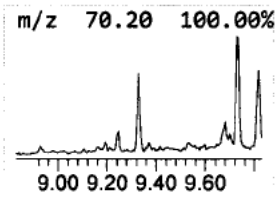
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

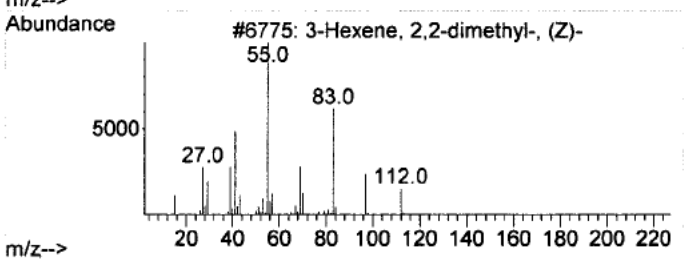
****
Peak Number 9 3-Hexene, 2,2-dimethyl-, (Z)- Concentration Rank 16

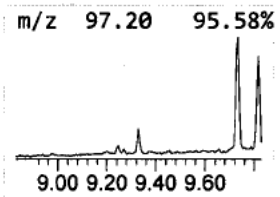
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	0.32 ug/mL	61800	Phenanthrene-d10	9.681

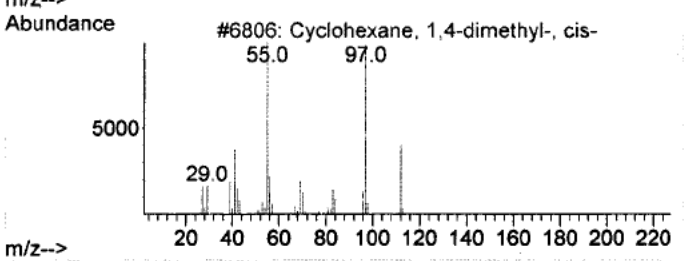
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexene, 2,2-dimethyl-, (Z)-	112	C8H16	000690-92-6	46
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	38
3	6-Methyl-cyclohex-2-en-1-ol	112	C7H12O	1000144-17-3	35
4	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	35
5	Heptane, 3-methylene-	112	C8H16	001632-16-2	35

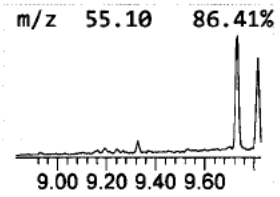


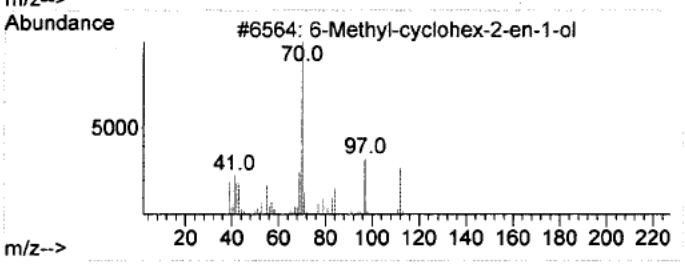


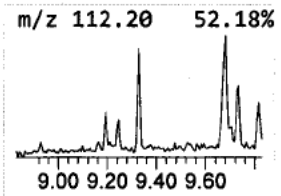


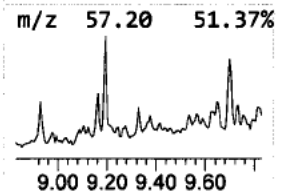












Library Search Compound Report

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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

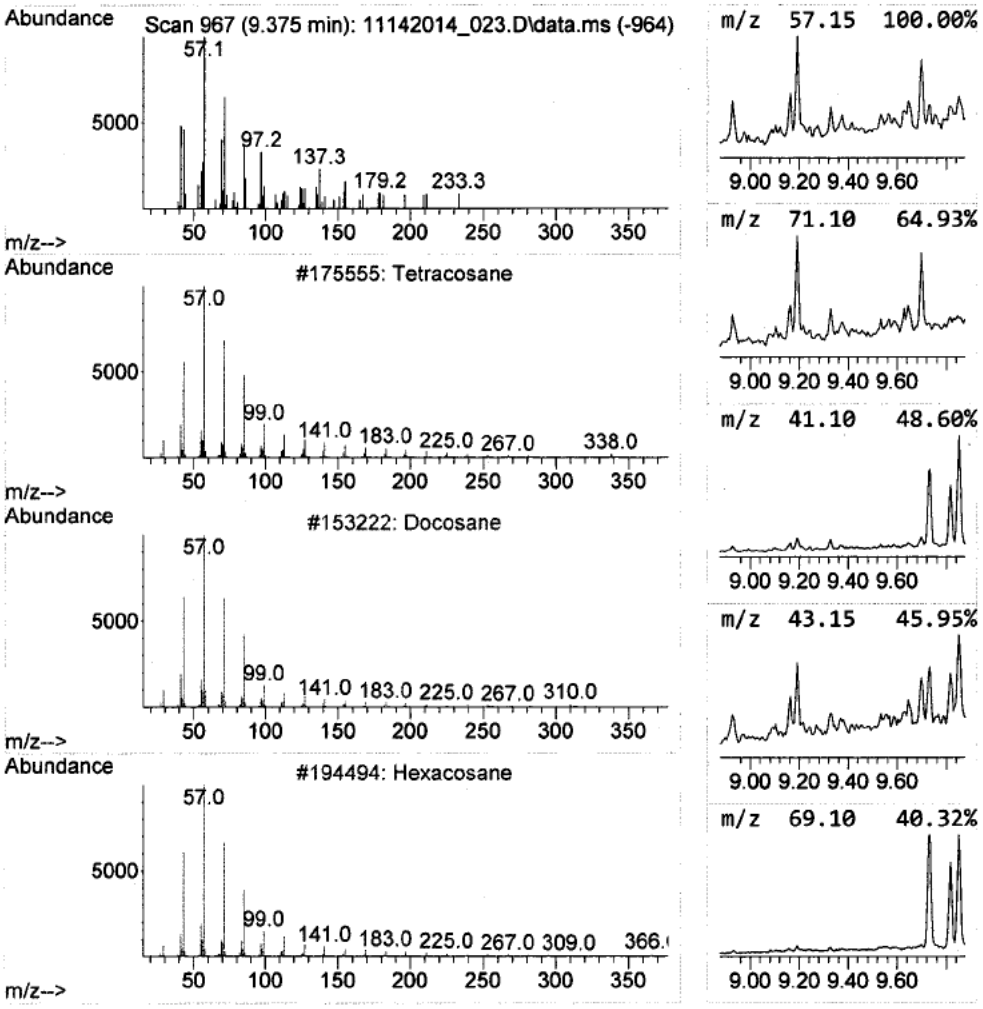
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 10 Tetracosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.375	0.22 ug/mL	42039	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	35
2	Docosane	310	C22H46	000629-97-0	35
3	Hexacosane	366	C26H54	000630-01-3	35
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	35
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	35



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

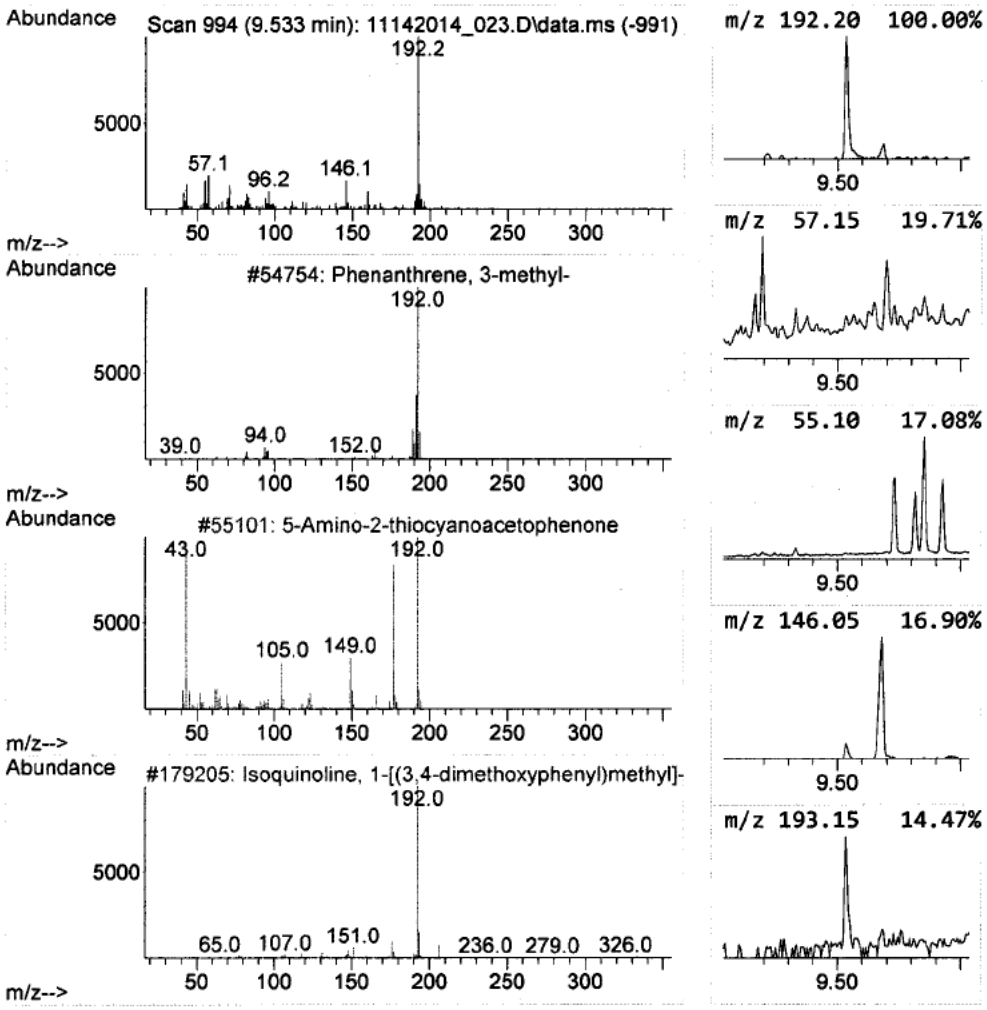
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 11 Phenanthrene, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	0.42 ug/mL	81991	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	53
2	5-Amino-2-thiocyanoacetophenone	192	C9H8N2OS	014428-51-4	53
3	Isoquinoline, 1-[(3,4-dimethoxyp...	343	C20H25NO4	013074-31-2	53
4	2,4-Diamino-6-(hydroxymethyl)pte...	192	C7H8N6O	000945-24-4	53
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53



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Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

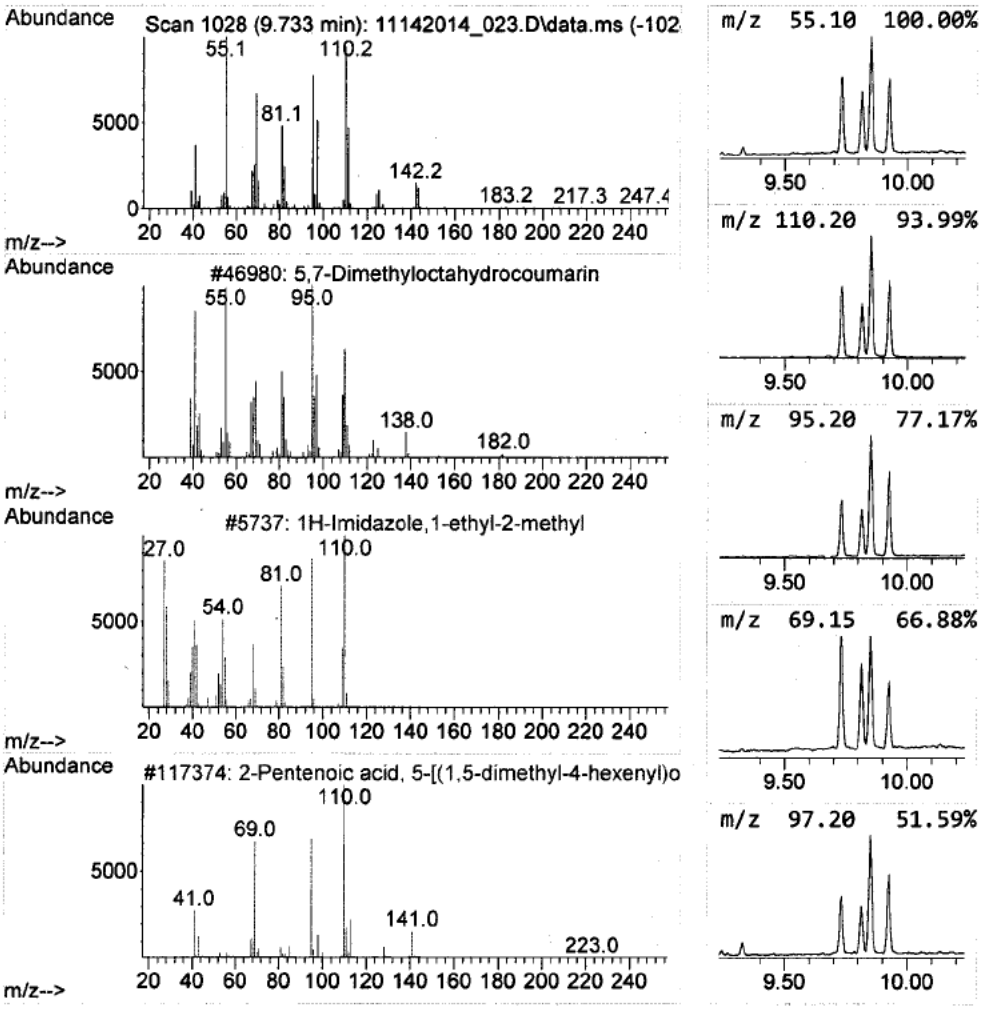
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 12 5,7-Dimethyloctahydrocoumarin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	3.17 ug/mL	610733	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Dimethyloctahydrocoumarin	182	C11H18O2	1000109-81-5	43
2	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	38
3	2-Pentenoic acid, 5-[(1,5-dimeth...	268	C16H28O3	053311-39-0	37
4	Cyclopentanecarboxylic acid, 2-e...	224	C14H24O2	1000282-59-1	35
5	Cyclohexanone, 4-methylidene-	110	C7H10O	029648-66-6	27



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

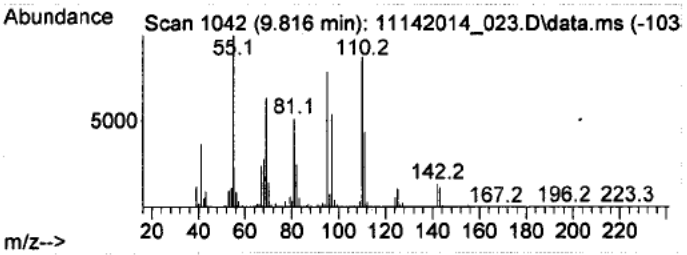
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

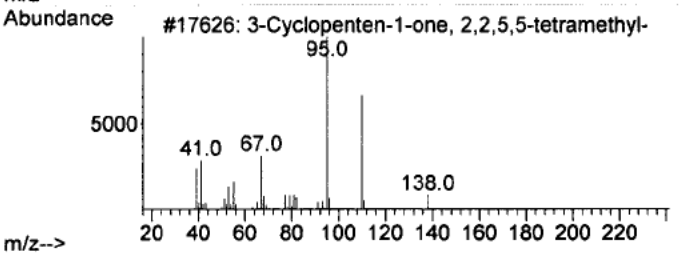
****

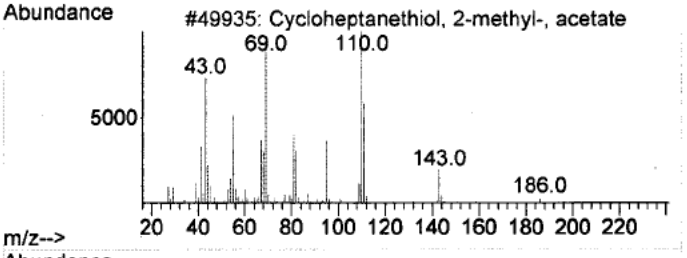
Peak Number 13 3-Cyclopenten-1-one, 2,2,5,... Concentration Rank 6

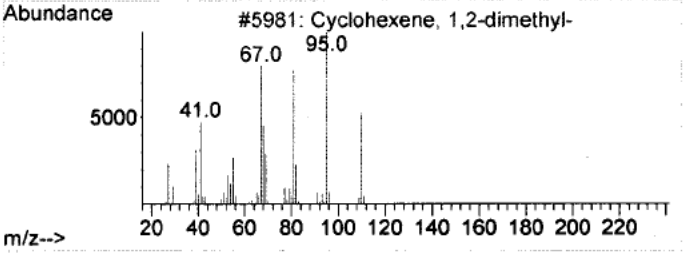
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	2.17 ug/mL	417833	Phenanthrene-d10	9.681

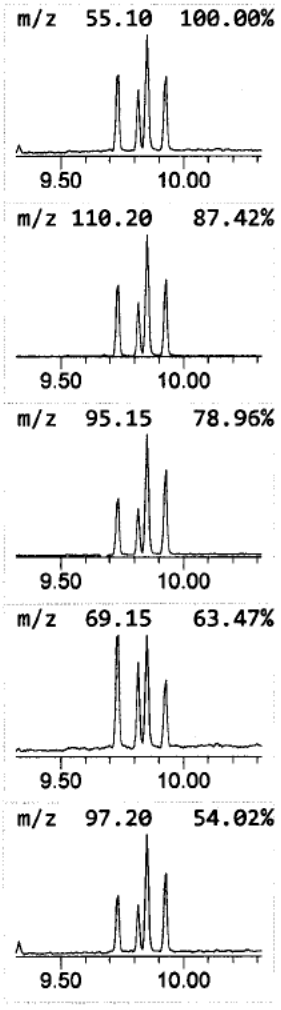
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	43
2	Cycloheptanethiol, 2-methyl-, ac...	186	C10H18OS	1000141-66-2	43
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	38
4	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	38
5	Cyclohexanethiol, 2-ethyl-, acetate	186	C10H18OS	1000141-66-7	35











Library Search Compound Report

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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

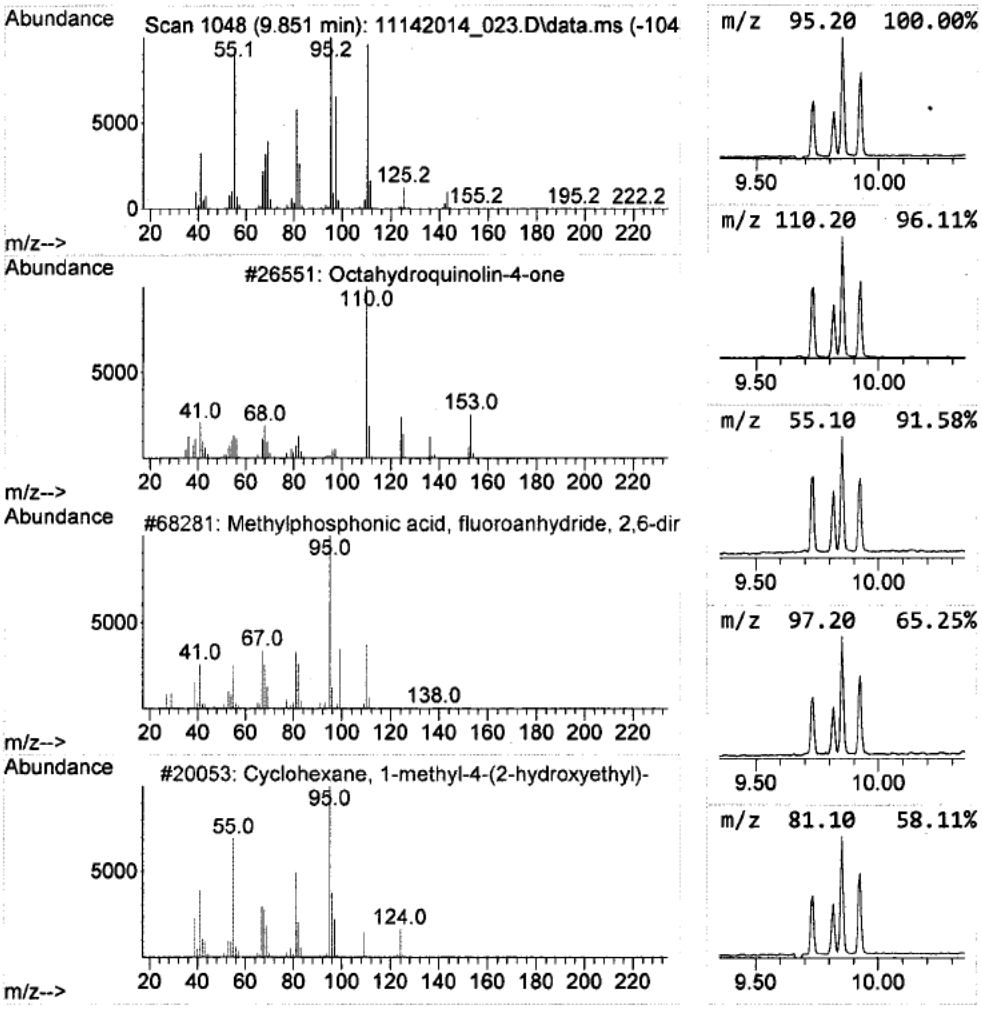
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 14 Octahydroquinolin-4-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	4.34 ug/mL	836506	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octahydroquinolin-4-one	153	C9H15NO	1000302-88-0	38
2	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	37
3	Cyclohexane, 1-methyl-4-(2-hydro...	142	C9H18O	004916-87-4	32
4	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	32
5	Imidazole-5-carboxylic amide, N-...	125	C5H7N3O	053525-55-6	30



Library Search Compound Report

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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

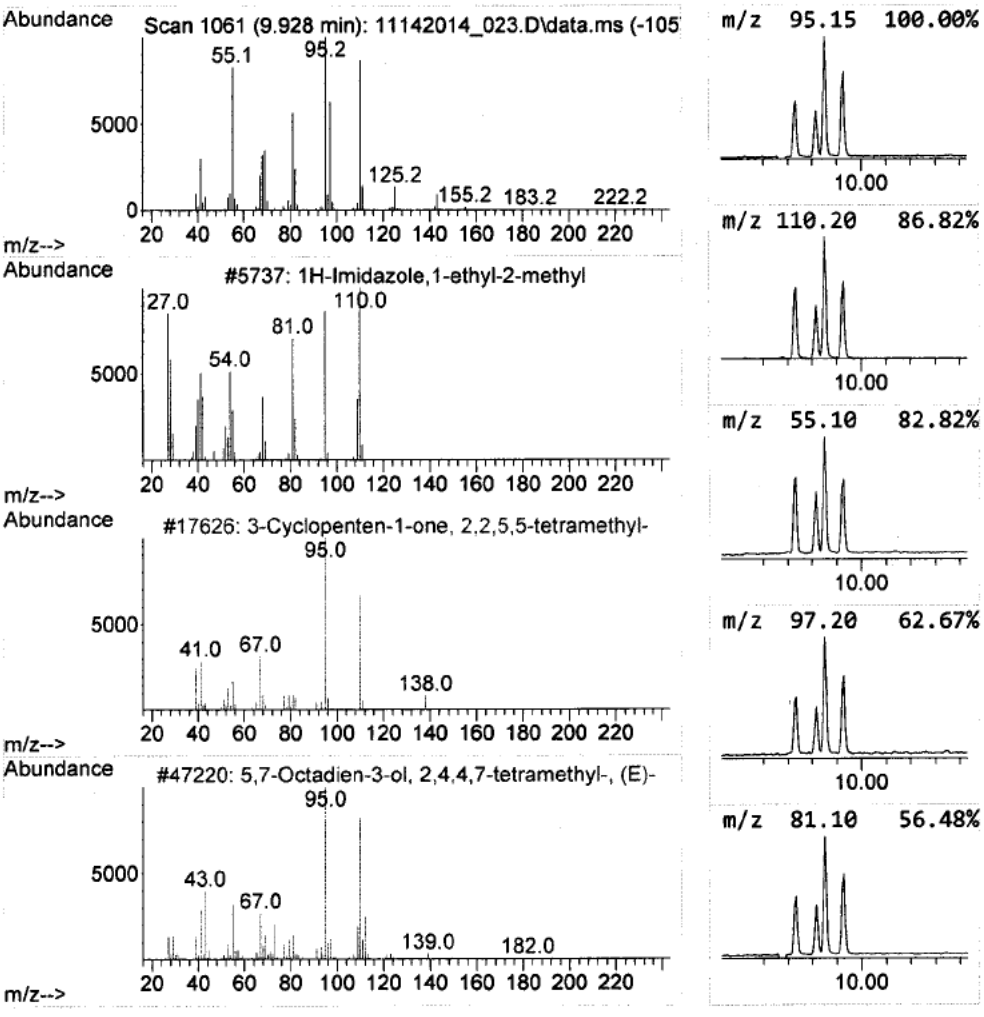
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 15 1H-Imidazole,1-ethyl-2-methyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	3.97 ug/mL	766049	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	58
2	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	50
3	5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	40
4	Imidazole-5-carboxylic amide, N-...	125	C5H7N3O	053525-55-6	38
5	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	38



Library Search Compound Report

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Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

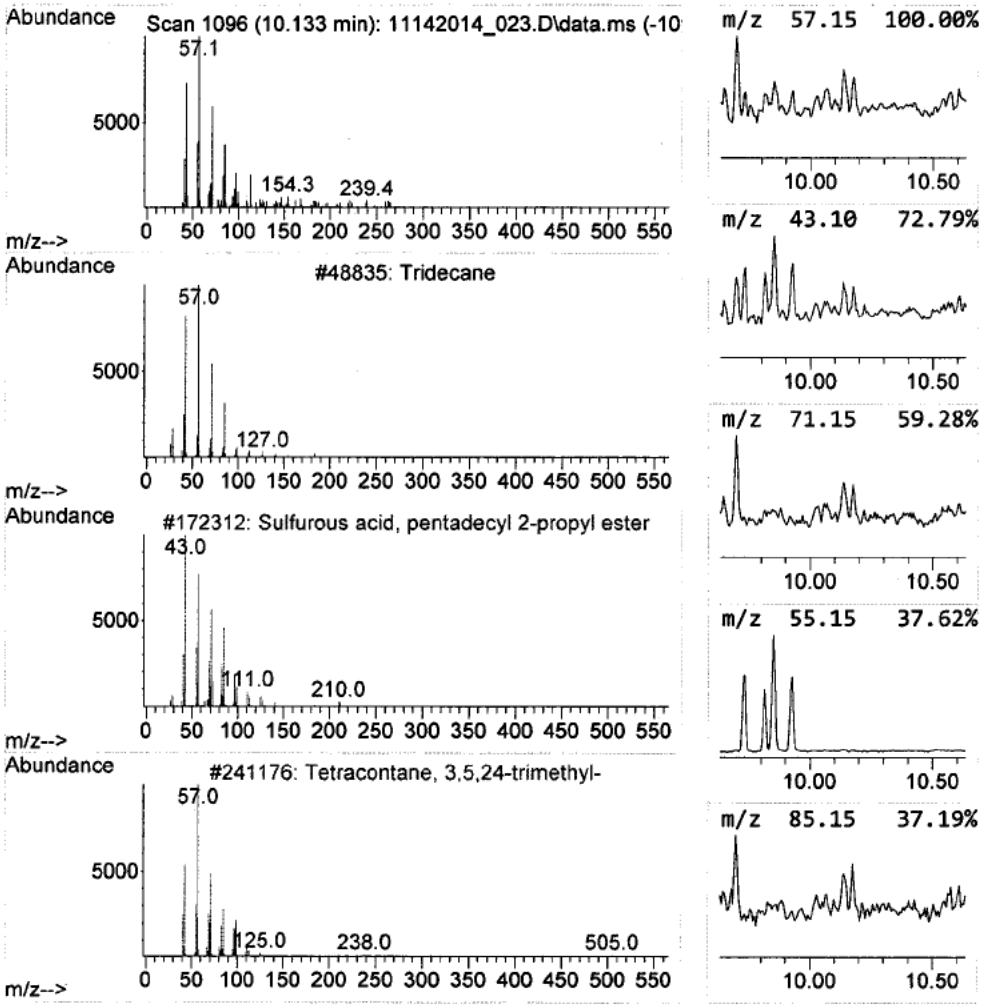
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 16 Tridecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	0.37 ug/mL	72305	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	64
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	58
3	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	53
4	Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	52
5	Tridecane	184	C13H28	000629-50-5	52



Library Search Compound Report

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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

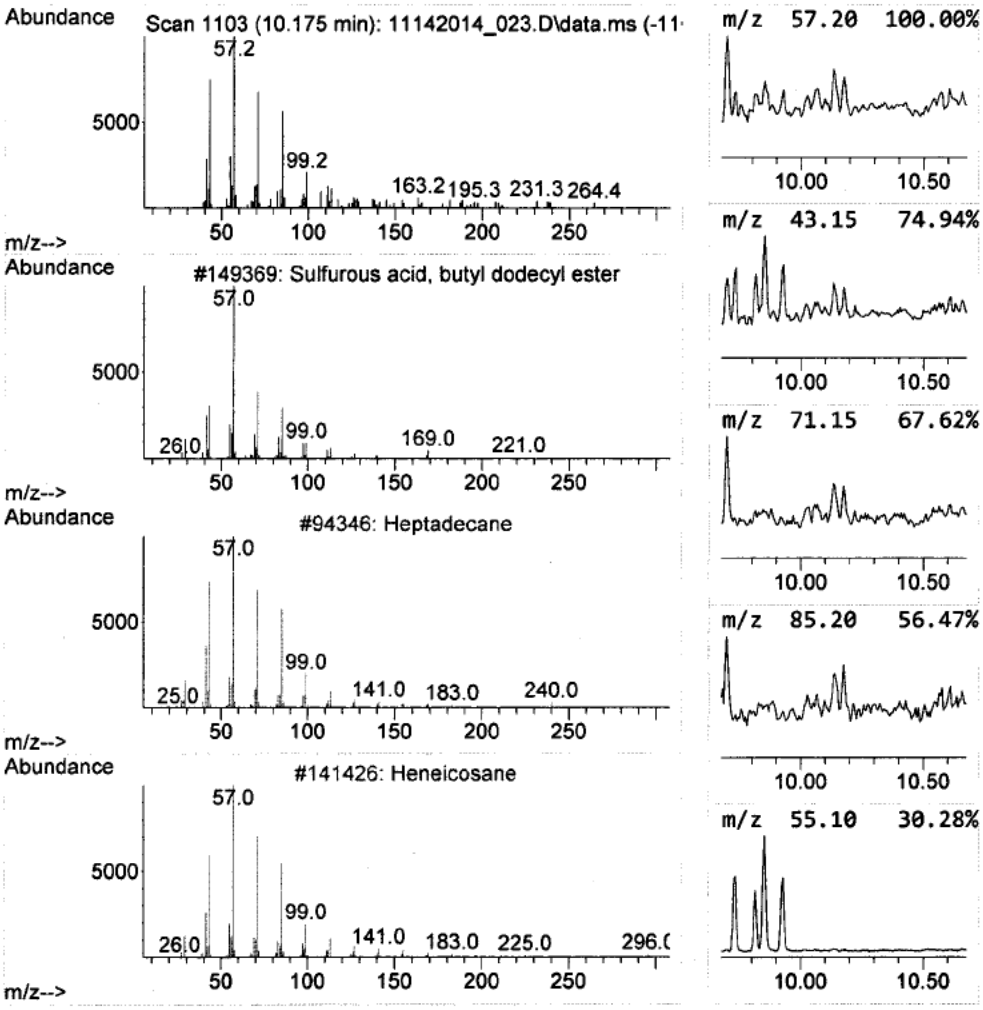
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 17 Sulfurous acid, butyl dodec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.175	2.83 ug/mL	546610	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72
2	Heptadecane	240	C17H36	000629-78-7	70
3	Heneicosane	296	C21H44	000629-94-7	68
4	Hexacosane	366	C26H54	000630-01-3	58
5	Hexadecane	226	C16H34	000544-76-3	58



Library Search Compound Report

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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

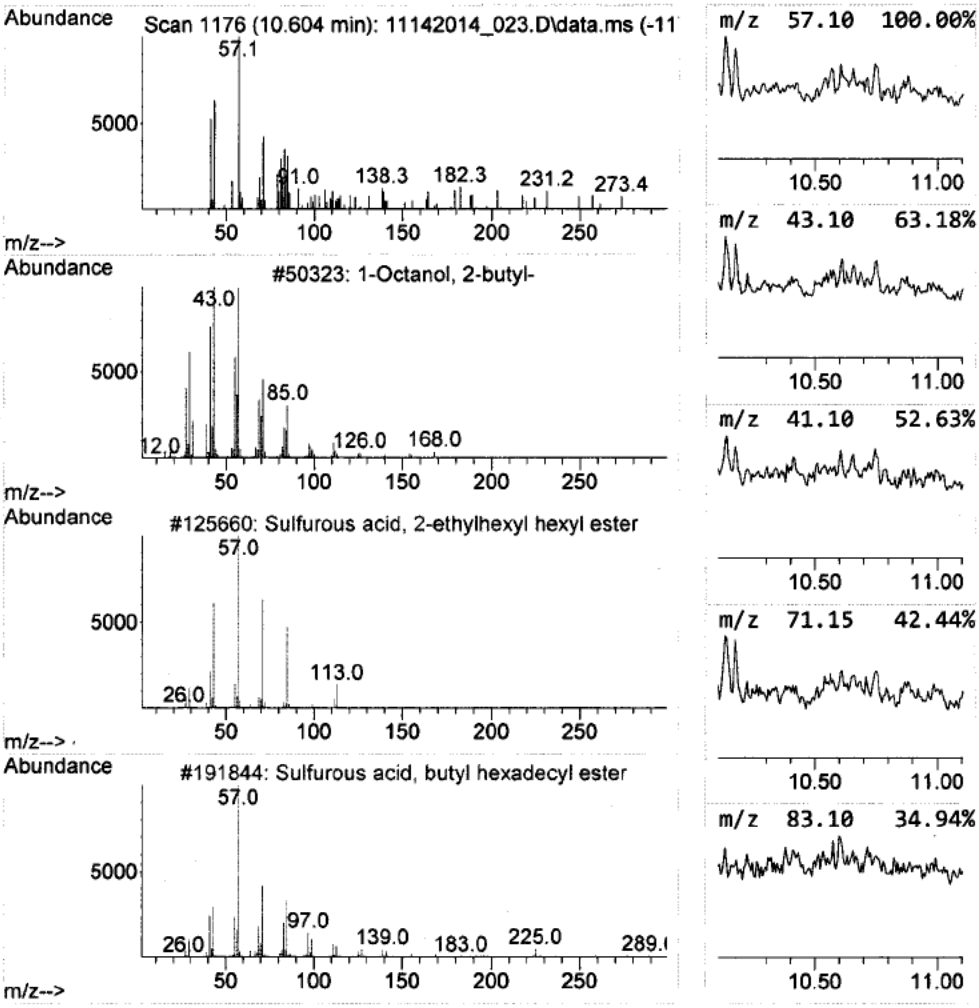
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 18 1-Octanol, 2-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	1.31 ug/mL	253699	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	38
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	38
3	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	38
4	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	38
5	1-Bromo-4-bromomethyldecane	312	C11H22Br2	061639-11-0	38



Library Search Compound Report

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Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

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

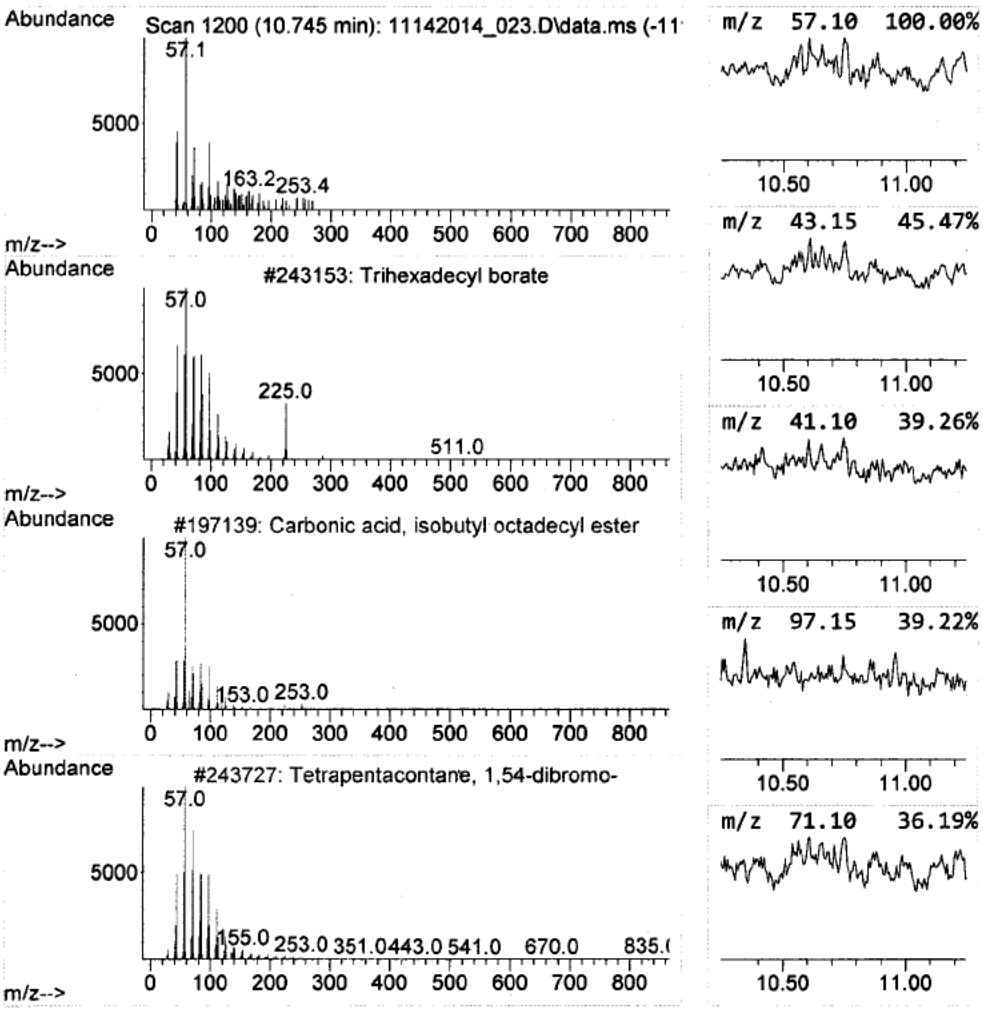
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 19 Trihexadecyl borate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	24.75 ug/mL	4776020	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trihexadecyl borate	735	C48H99BO3	002665-11-4	32
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	27
3	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	23
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	20
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	13



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Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

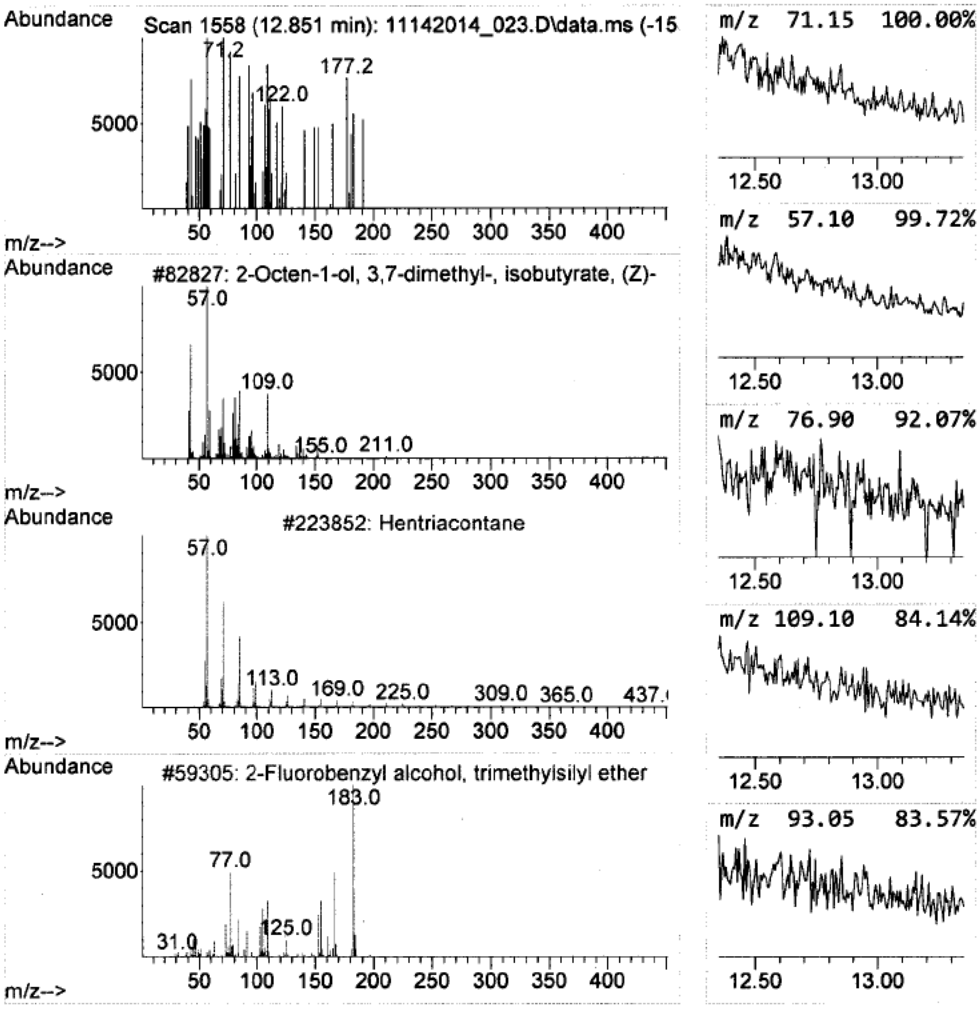
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 20 2-Octen-1-ol, 3,7-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	0.47 ug/mL	60815	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octen-1-ol, 3,7-dimethyl-, iso...	226	C14H26O2	1000132-45-6	10
2	Hentriacontane	437	C31H64	000630-04-6	9
3	2-Fluorobenzyl alcohol, trimethy...	198	C10H15FOSi	1227612-35-2	9
4	Acetamide, 2-chloro-N-(2-cyanoet...	146	C5H7ClN2O	017756-81-9	9
5	Chloroacetic acid, propyl ester	136	C5H9ClO2	005396-24-7	9



Tentatively Identified Compound (LSC) summary

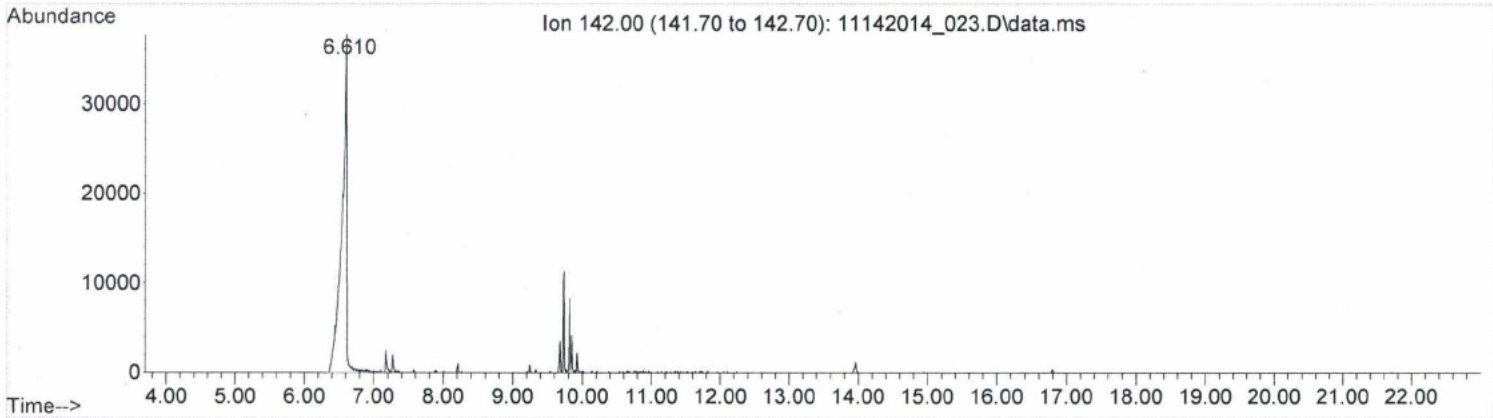
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_023.D
Acq On : 14 Nov 2014 08:37 pm
Operator : [redacted]
Sample : NE36692-B
Misc : Tag # NE36692-B, Lab Rep #2, 1X
ALS Vial : 22 Sample Multiplier: 1

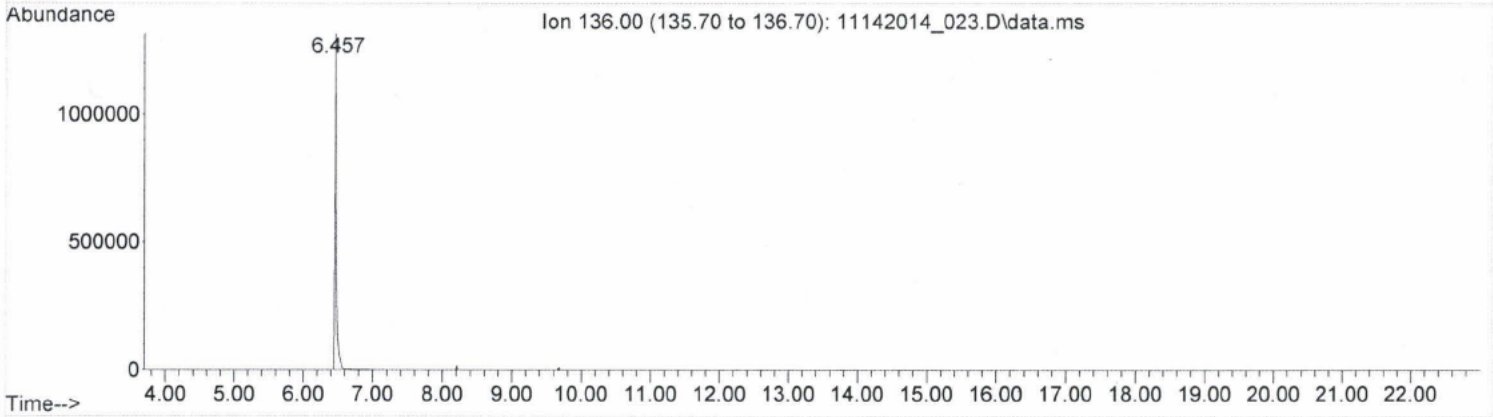
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

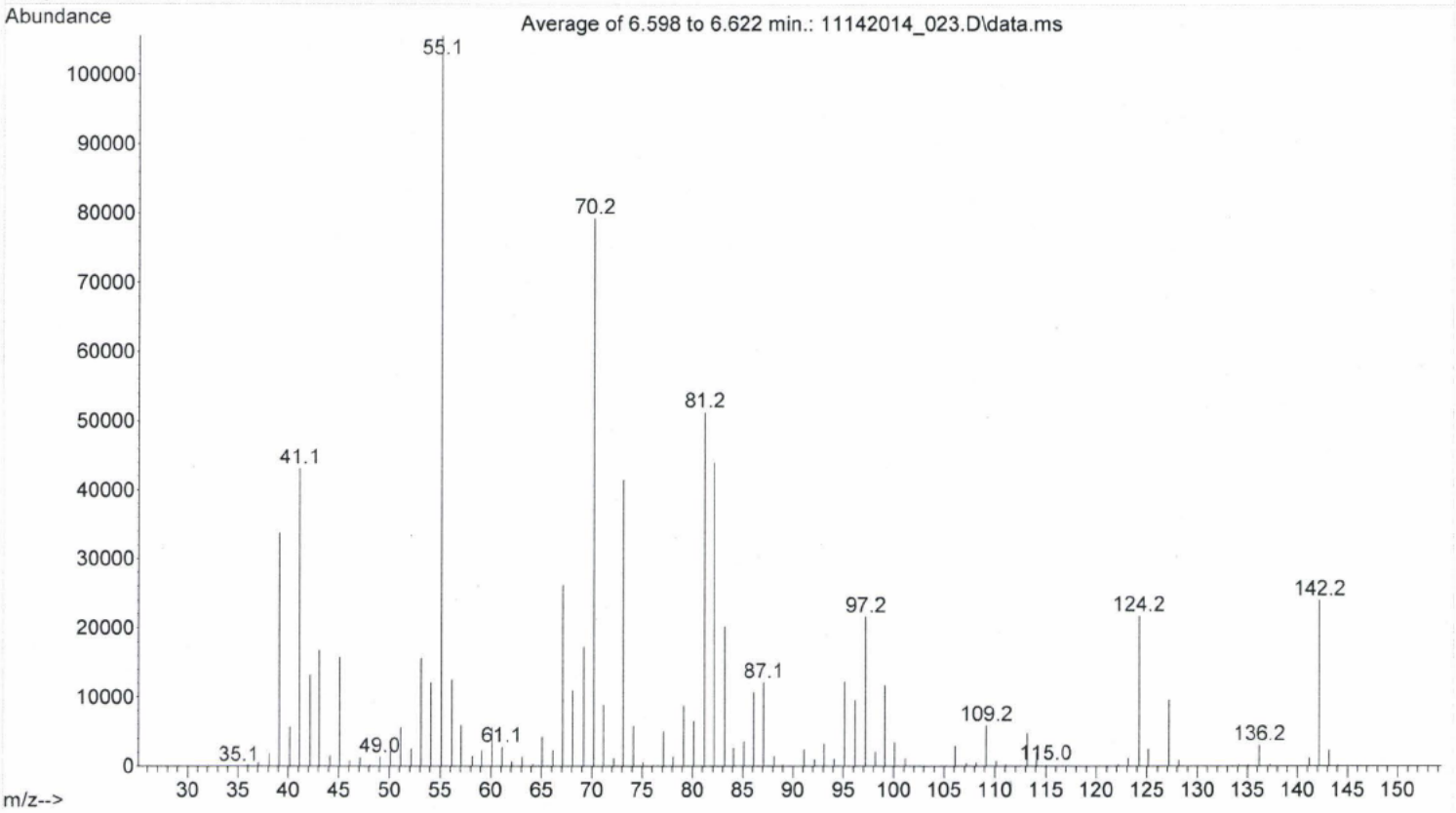
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Methan-d3-ol	3.769	0.3	ug/mL	44754	1	5.081	2987500	20.0
Cyclohexanone, ...	5.404	0.4	ug/mL	57525	1	5.081	2987500	20.0
Cyclohexanemeth...	5.716	0.4	ug/mL	61232	1	5.081	2987500	20.0
Cyclohexanecarb...	6.610	2.1	ug/mL	1019840	2	6.457	9536870	20.0
trans-Linalool ...	8.628	0.3	ug/mL	56564	3	8.216	4183960	20.0
Dodecane	8.698	0.4	ug/mL	73259	3	8.216	4183960	20.0
Methoxyacetic a...	9.104	0.3	ug/mL	48564	4	9.681	3858740	20.0
Tridecane, 5-pr...	9.192	0.4	ug/mL	77537	4	9.681	3858740	20.0
3-Hexene, 2,2-d...	9.328	0.3	ug/mL	61800	4	9.681	3858740	20.0
Tetracosane	9.375	0.2	ug/mL	42039	4	9.681	3858740	20.0
Phenanthrene, 3...	9.533	0.4	ug/mL	81991	4	9.681	3858740	20.0
5,7-Dimethyloct...	9.733	3.2	ug/mL	610733	4	9.681	3858740	20.0
3-Cyclopenten-1...	9.816	2.2	ug/mL	417833	4	9.681	3858740	20.0
Octahydroquinol...	9.851	4.3	ug/mL	836506	4	9.681	3858740	20.0
1H-Imidazole,1-...	9.928	4.0	ug/mL	766049	4	9.681	3858740	20.0
Tridecane	10.133	0.4	ug/mL	72305	4	9.681	3858740	20.0
Sulfurous acid,...	10.175	2.8	ug/mL	546610	4	9.681	3858740	20.0
1-Octanol, 2-bu...	10.604	1.3	ug/mL	253699	4	9.681	3858740	20.0
Trihexadecyl bo...	10.745	24.8	ug/mL	4776020	4	9.681	3858740	20.0
2-Octen-1-ol, 3...	12.851	0.5	ug/mL	60815	5	13.963	2597440	20.0

File :D:[redacted]\RP1616\11142014_Run\11142014_023.D
Operator : [redacted]
Acquired : 14 Nov 2014 08:37 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36692-B
Misc Info : Tag # NE36692-B, Lab Rep #2, 1X
Vial Number: 22







[redacted] RP1616 12/15/14

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

Quant Time: Nov 17 10:49:21 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

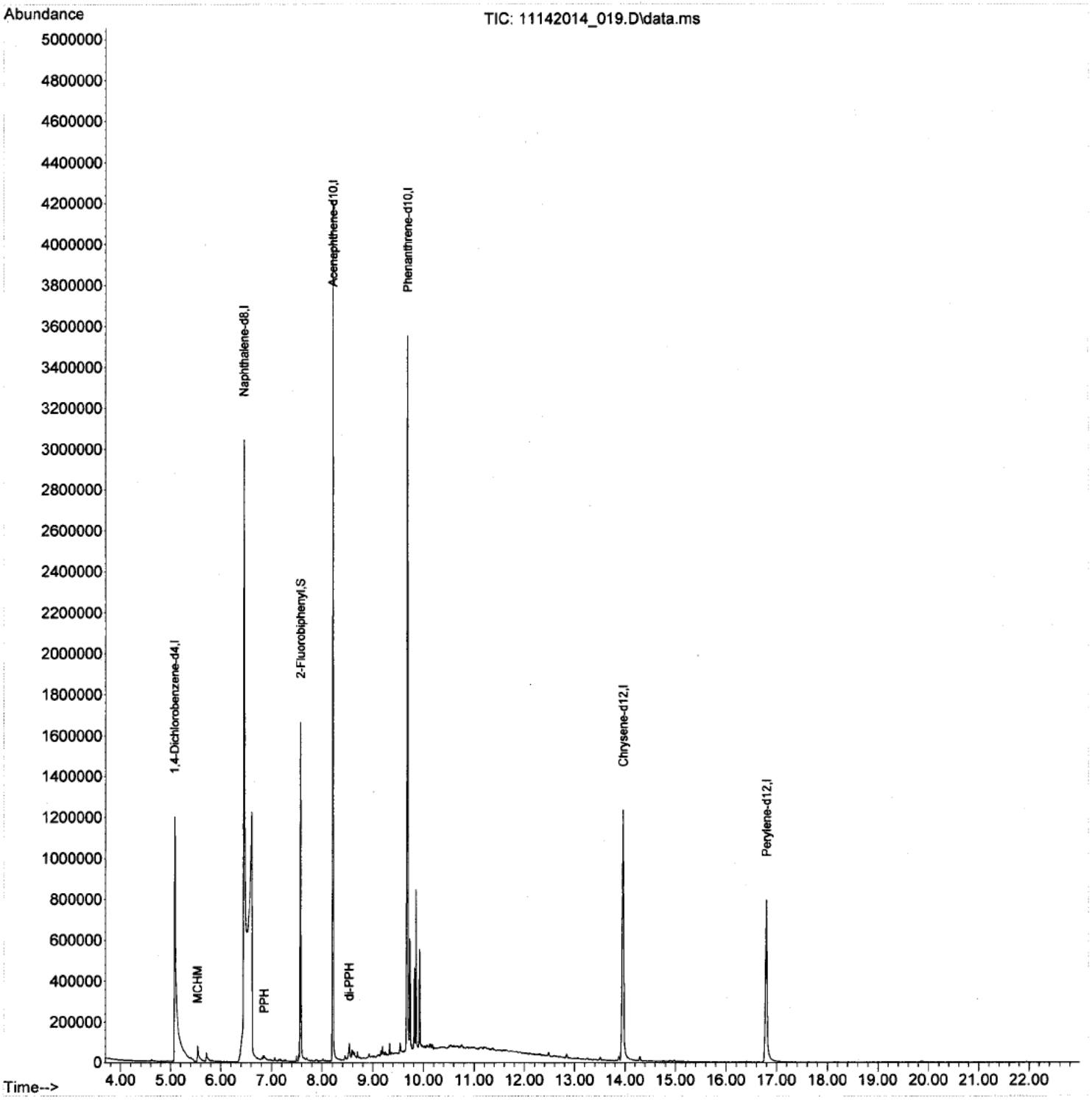
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
Internal Standards					
1) 1,4-Dichlorobenzene-d4	5.075	152	417610	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1850408	20.00 ug/mL	# 0.00
5) Acenaphthene-d10	8.210	164	1034788	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.680	188	1538988	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	890197	20.00 ug/mL	0.00
12) Perylene-d12	16.804	264	622667	20.00 ug/mL	0.01
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	518432	8.15 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery = ~~65.20%~~ see Analyst Narrative, Surrogate Recovery		
Target Compounds					Qvalue
2) MCHM	5.540	55	77124m	2.00 ug/mL	[redacted] 1/7/15
4) PPH	6.857	94	13153m	0.61 ug/mL	
6) 1,4-CHDM	0.000		0	N.D. d	
8) DM-1,4-CHDC	0.000		0	N.D. d	
9) di-PPH	8.534	59	65456m	2.10 ug/mL	

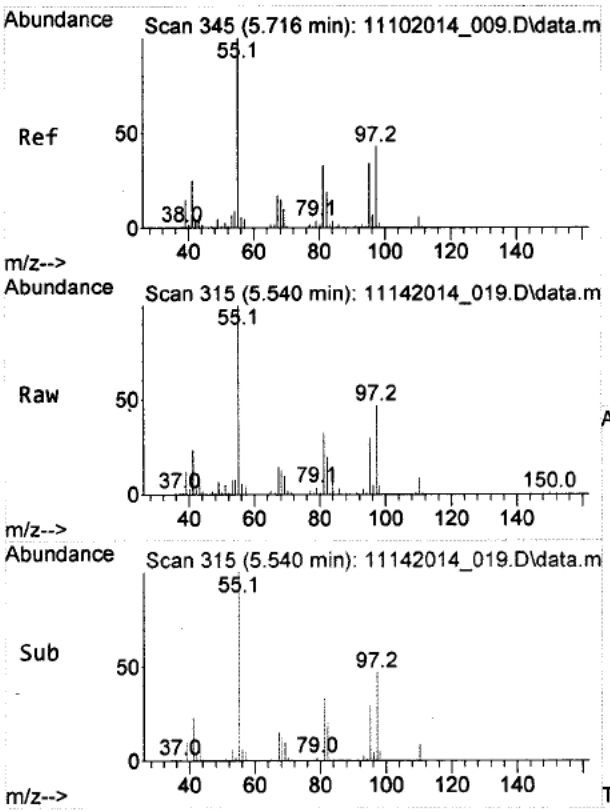
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

Quant Time: Nov 17 10:49:21 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

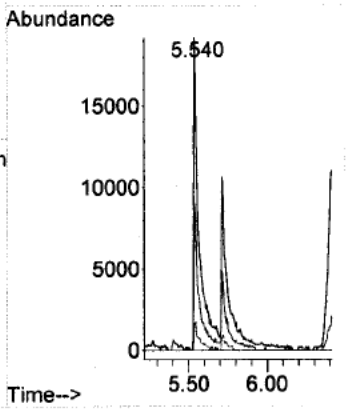


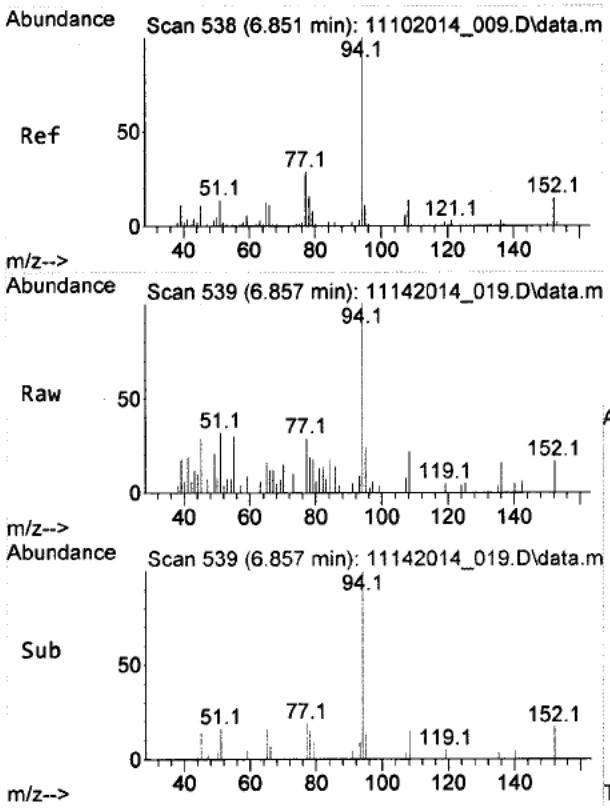


#2
MCHM
Concen: 2.00 ug/mL m
RT: 5.540 min Scan# 315
Delta R.T. -0.176 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 55 Resp: 77124

Ion	Ratio	Lower	Upper
55	100		
97	9.4	34.6	51.8#
110	2.1	4.8	7.2#

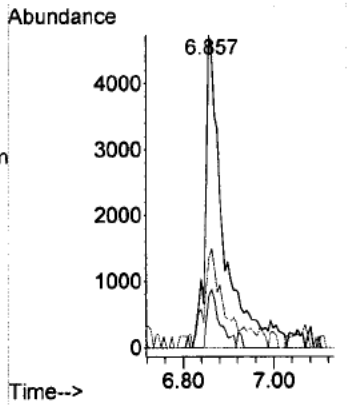


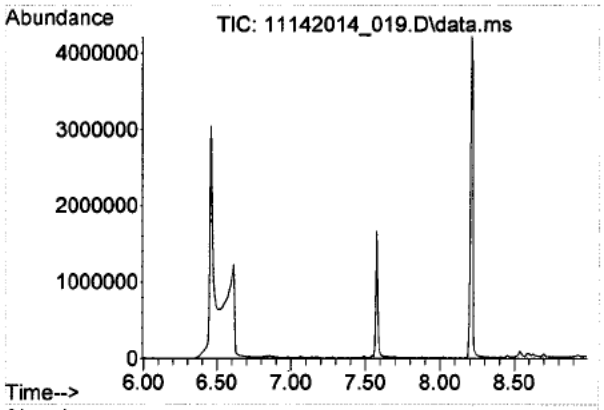


#4
PPH
Concen: 0.61 ug/mL m
RT: 6.857 min Scan# 539
Delta R.T. 0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 94 Resp: 13153

Ion	Ratio	Lower	Upper
94	100		
152	12.5	13.4	20.0#
77	31.7	21.2	31.8



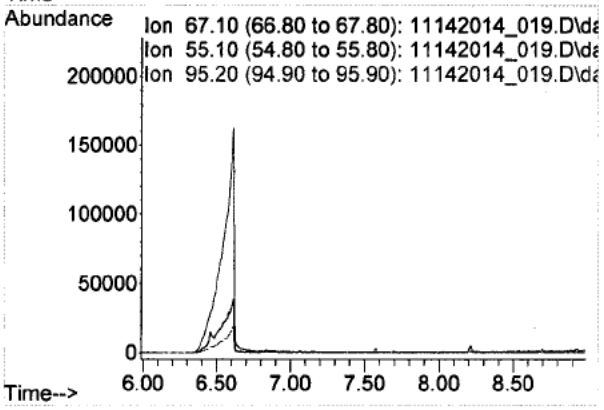


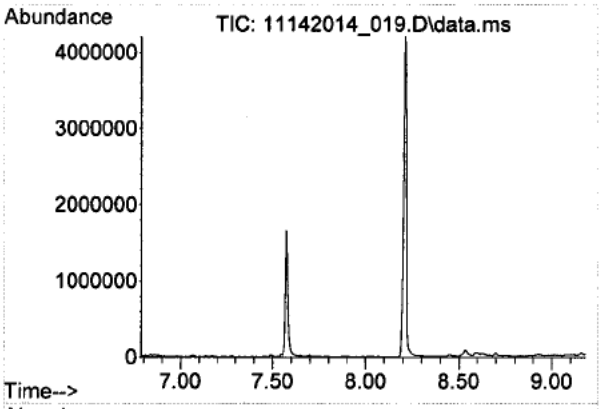
#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8



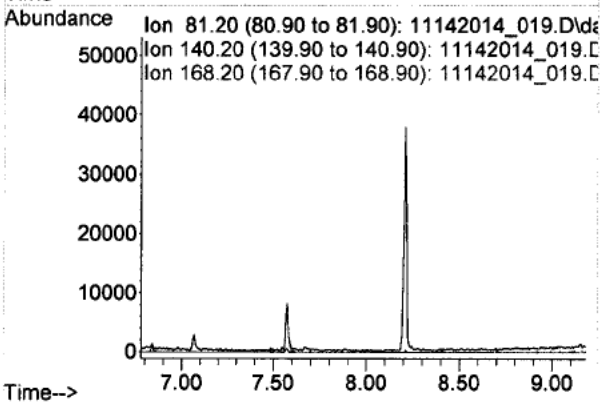


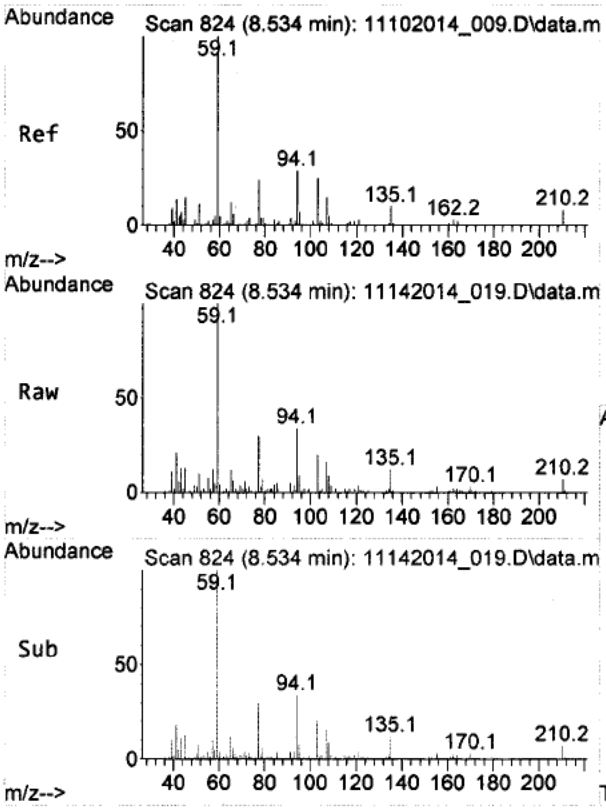
#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 81

Sig	Exp Ratio
81	100
140	61.8
168	17.7

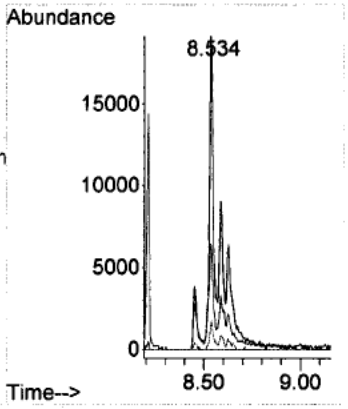




#9
di-PPH
Concen: 2.10 ug/mL m
RT: 8.534 min Scan# 824
Delta R.T. -0.006 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 59 Resp: 65456

Ion	Ratio	Lower	Upper
59	100		
94	17.8	23.0	34.6#
210	3.9	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

Quant Time: Dec 01 11:45:02 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	5.075	150	731128	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1851381	20.00 ug/mL	# 0.00
24) Acenaphthene-d10	8.210	164	1034788	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.680	188	1538988	20.00 ug/mL	0.00
49) Chrysene-d12	13.963	240	891670	20.00 ug/mL	-0.01
58) Perylene-d12	16.804	264	624905	20.00 ug/mL	0.00
Target Compounds					Qvalue
2) Bis(2-chloroethyl) ether	0.000		0	N.D.	
3) n-Decane	0.000		0	N.D. d	
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...	6.616	55	895643	68.34 ug/mL	94
14) n-Dodecane	0.000		0	N.D. d	
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	0.000		0	N.D. d	
19) Hexachlorobutadiene	0.000		0	N.D.	
20) 2-Methylnapthalene	7.175	142	3716	0.04 ug/mL	92
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	7.628	162	89	0.00 ug/mL#	54
23) n-Tetradecane	7.698	57	2566	0.05 ug/mL#	83
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	0.000		0	N.D. d	
30) 2,4-Dinitrotoluene	0.000		0	N.D. d	
31) n-Hexadecane	8.698	57	4514	0.08 ug/mL#	94
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	6820	0.12 ug/mL#	93
41) Phenanthrene	9.698	178	3031	0.03 ug/mL	99
42) Anthracene	0.000		0	N.D. d	
43) Carbazole	0.000		0	N.D. d	
44) Dibutyl Phthalate	0.000		0	N.D. d	
45) n-Eicosane	10.751	57	3656	0.07 ug/mL#	89

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

Quant Time: Dec 01 11:45:02 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

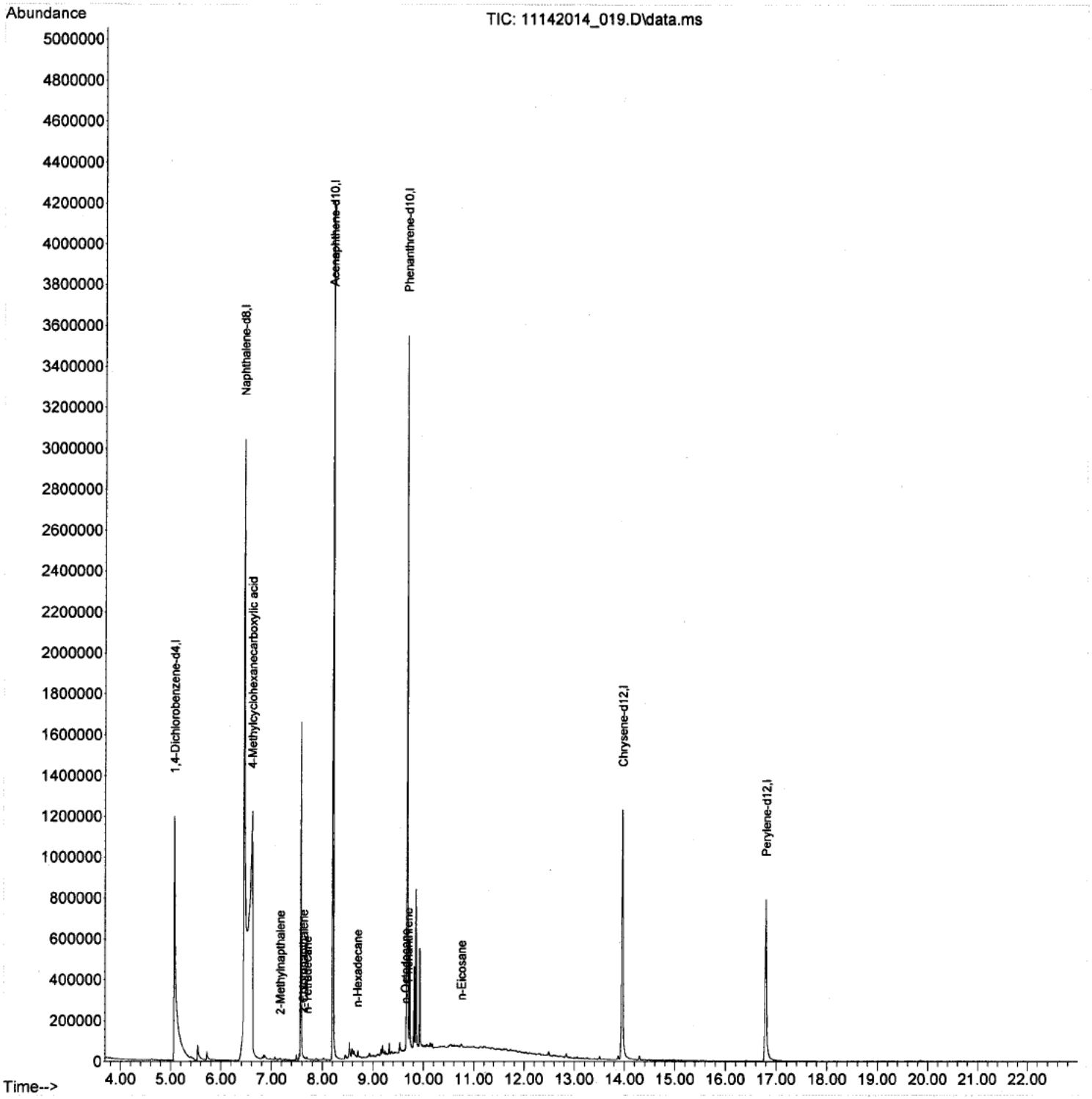
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	0.000		0	N.D. d	
47) Pyrene	0.000		0	N.D. d	
48) n-Docosane	0.000		0	N.D. d	
50) Benzyl Butyl Phthalate	0.000		0	N.D. d	
51) n-Tetracosane	0.000		0	N.D. d	
52) n-Hexacosane	0.000		0	N.D. d	
53) n-Octacosane	0.000		0	N.D. d	
54) Benz[a]anthracene	0.000		0	N.D. d	
55) Chrysene	0.000		0	N.D. d	
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.	
60) Benzo(k)fluoranthene	0.000		0	N.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.	

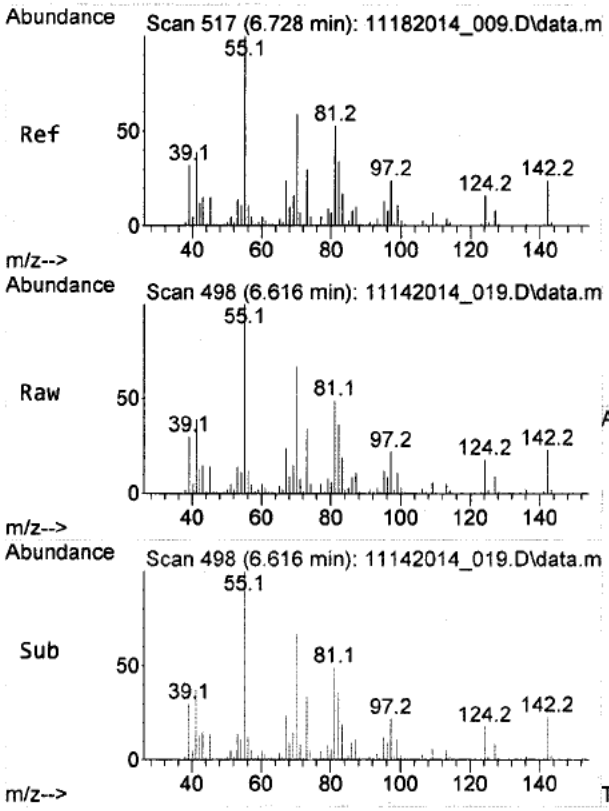
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

Quant Time: Dec 01 11:45:02 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

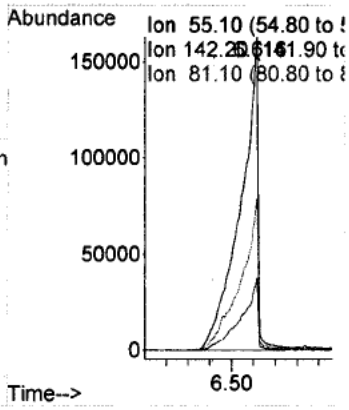


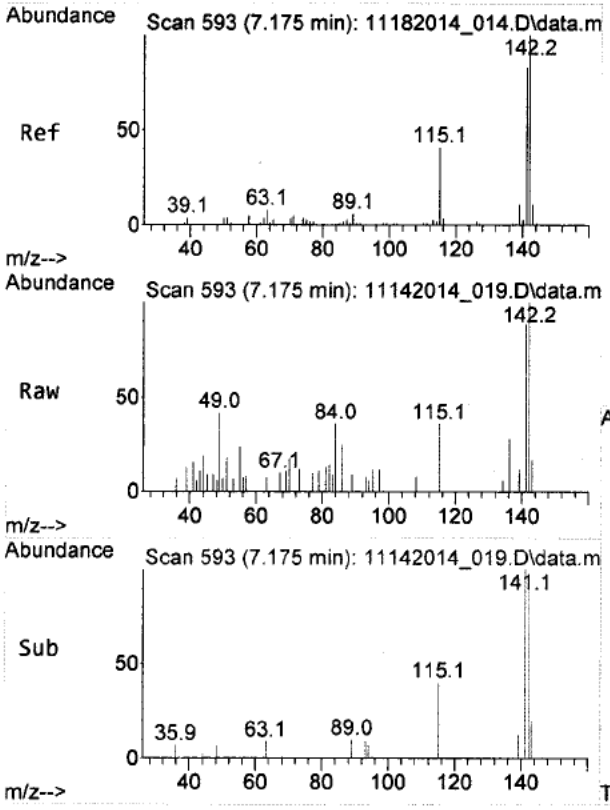


#12
4-Methylcyclohexanecarboxylic acid
Concen: 68.34 ug/mL
RT: 6.616 min Scan# 498
Delta R.T. -0.112 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 55 Resp: 895643

Ion	Ratio	Lower	Upper
55	100		
142	21.7	19.1	28.7
81	48.0	42.3	63.5

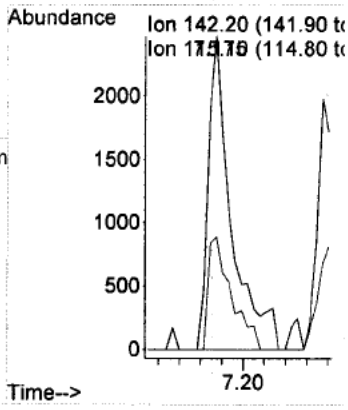


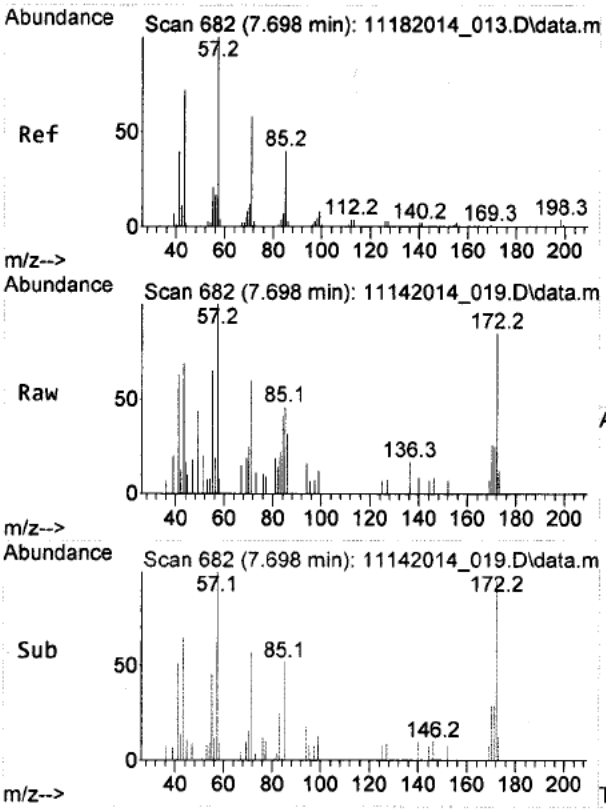


#20
2-Methylnapthalene
Concen: 0.04 ug/mL
RT: 7.175 min Scan# 593
Delta R.T. -0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion:142 Resp: 3716

Ion	Ratio	Lower	Upper
142	100		
115	36.0	33.0	49.4

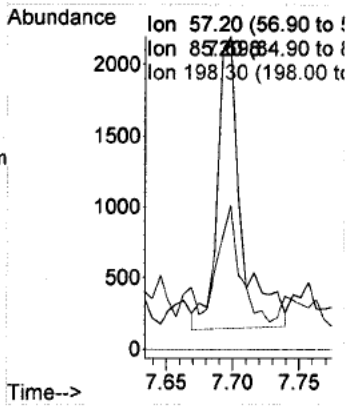


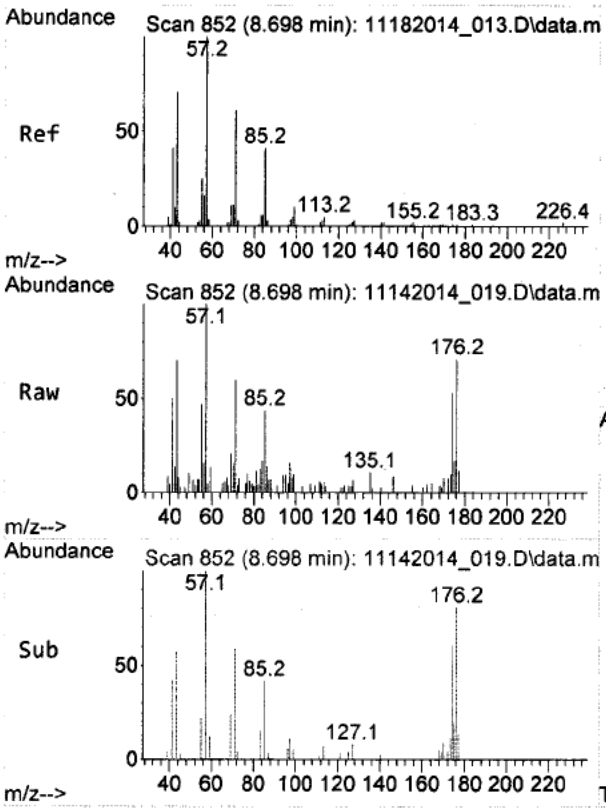


#23
n-Tetradecane
Concen: 0.05 ug/mL
RT: 7.698 min Scan# 682
Delta R.T. 0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 57 Resp: 2566

Ion	Ratio	Lower	Upper
57	100		
85	50.0	31.6	47.4#
198	0.0	3.1	4.7#

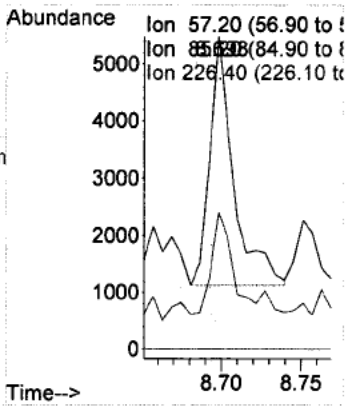


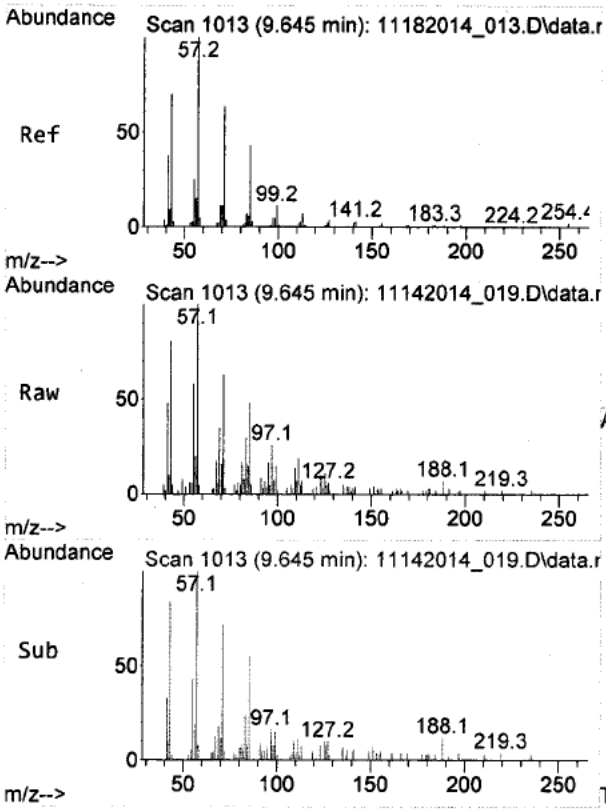


#31
n-Hexadecane
Concen: 0.08 ug/mL
RT: 8.698 min Scan# 852
Delta R.T. 0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 57 Resp: 4514

Ion	Ratio	Lower	Upper
57	100		
85	40.3	35.1	52.7
226	0.0	3.1	4.7#

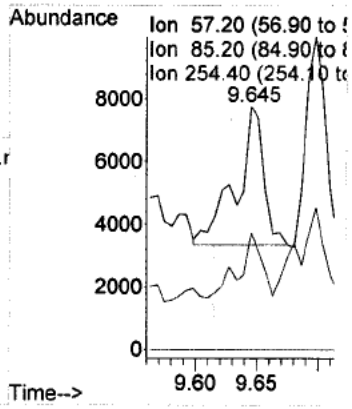


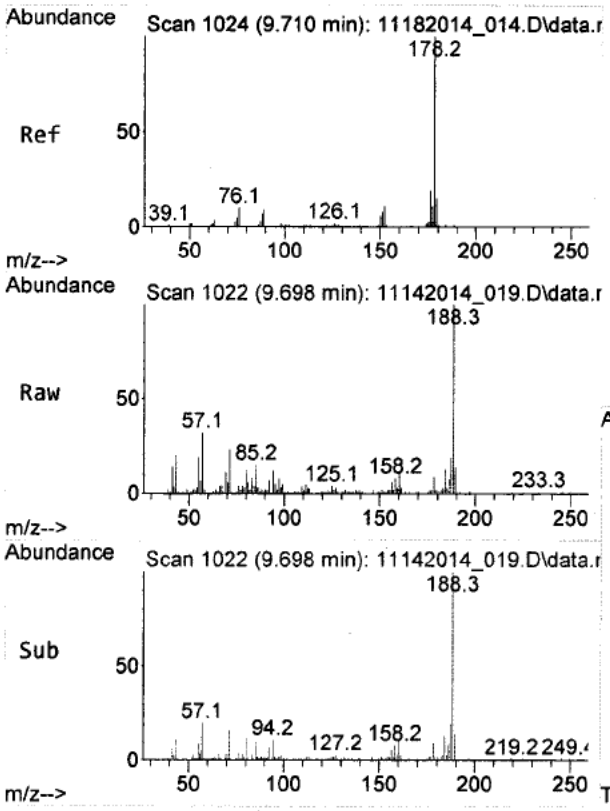


#40
n-Octadecane
Concen: 0.12 ug/mL
RT: 9.645 min Scan# 1013
Delta R.T. 0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 57 Resp: 6820

Ion	Ratio	Lower	Upper
57	100		
85	38.5	34.5	51.7
254	0.0	1.4	2.2#

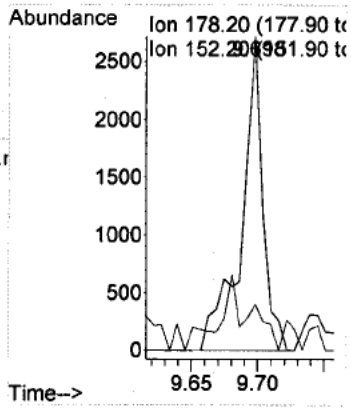


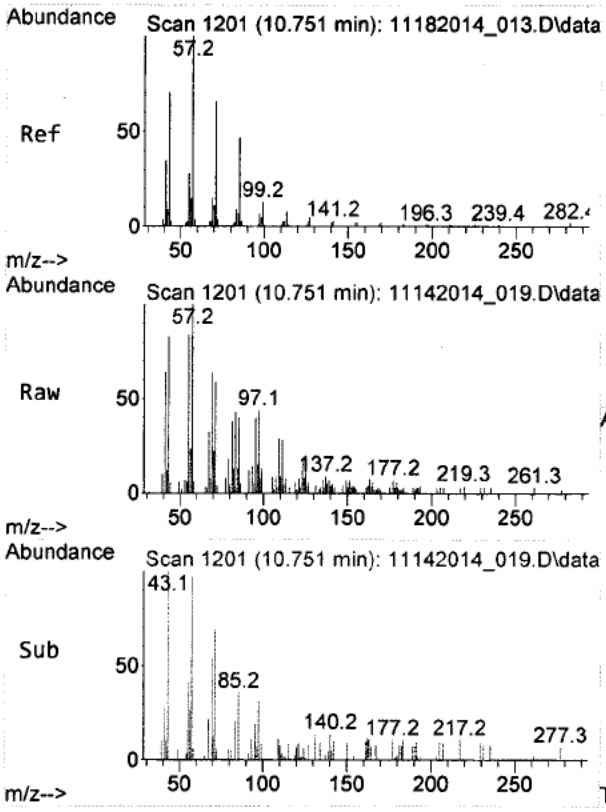


#41
Phenanthrene
Concen: 0.03 ug/mL
RT: 9.698 min Scan# 1022
Delta R.T. -0.012 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion:178 Resp: 3031

Ion	Ratio	Lower	Upper
178	100		
152	10.2	8.5	12.7

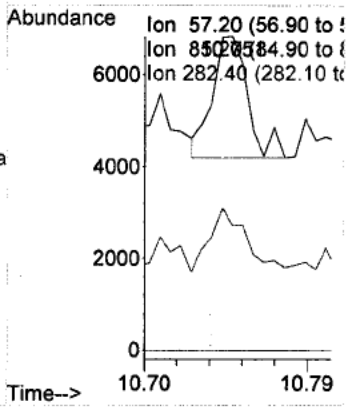




#45
n-Eicosane
Concen: 0.07 ug/mL
RT: 10.751 min Scan# 1201
Delta R.T. 0.000 min
Lab File: 11142014_019.D
Acq: 14 Nov 2014 06:41 pm

Tgt Ion: 57 Resp: 3656

Ion	Ratio	Lower	Upper
57	100		
85	54.8	37.8	56.8
282	0.0	1.4	2.2#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 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_019.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	225	236	289	rBV	1194925	3121308	50.25%	7.741%
2	6.457	447	471	483	rBV	3042529	6211783	100.00%	15.405%
3	6.616	483	498	527	rVV	1216737	5011522	80.68%	12.428%
4	7.575	651	661	677	rBV	1657862	1601009	25.77%	3.970%
5	8.210	761	769	797	rVV	4206278	4542431	73.13%	11.265%
6	8.586	831	833	849	rVV3	55433	213131	3.43%	0.529%
7	9.533	987	994	1003	rVV	89421	289744	4.66%	0.719%
8	9.680	1007	1019	1025	rVV	3547657	4449102	71.62%	11.033%
9	9.728	1025	1027	1035	rVV	600674	734180	11.82%	1.821%
10	9.851	1035	1048	1055	rVV2	841039	1523969	24.53%	3.779%
11	9.922	1055	1060	1075	rVV	550176	981174	15.80%	2.433%
12	10.063	1081	1084	1091	rVV8	79669	260052	4.19%	0.645%
13	10.133	1091	1096	1101	rVV6	87432	261516	4.21%	0.649%
14	10.216	1107	1110	1121	rVV6	66983	319709	5.15%	0.793%
15	10.416	1129	1144	1151	rVV6	72070	532249	8.57%	1.320%
16	10.539	1151	1165	1181	rVV6	80736	770906	12.41%	1.912%
17	10.657	1181	1185	1197	rVV6	76842	407490	6.56%	1.011%
18	10.751	1197	1201	1217	rVV9	83133	496549	7.99%	1.231%
19	10.998	1233	1243	1259	rVV9	71828	600163	9.66%	1.488%
20	11.145	1259	1268	1273	rVV9	70213	330060	5.31%	0.819%
21	11.192	1273	1276	1301	rVV9	71320	634044	10.21%	1.572%
22	11.369	1301	1306	1319	rVV9	65538	375035	6.04%	0.930%
23	11.486	1319	1326	1339	rVV9	58318	392064	6.31%	0.972%
24	11.639	1339	1352	1363	rVV9	57728	454476	7.32%	1.127%
25	11.727	1363	1367	1383	rVV9	54131	352141	5.67%	0.873%
26	11.916	1393	1399	1417	rVV9	48131	354444	5.71%	0.879%
27	12.110	1425	1432	1459	rVV9	39986	420098	6.76%	1.042%
28	12.586	1509	1513	1533	rVV9	29226	212082	3.41%	0.526%
29	13.963	1737	1747	1783	rVV	1231835	2663424	42.88%	6.605%
30	16.804	2215	2230	2269	rVV	794853	1808390	29.11%	4.485%

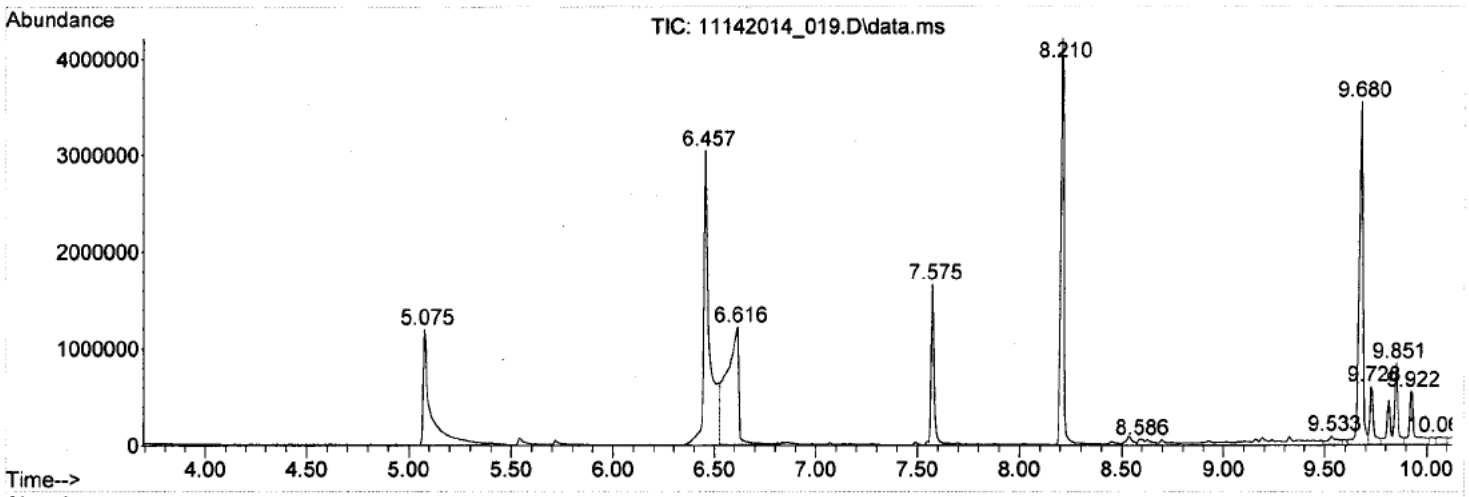
Sum of corrected areas: 40324245

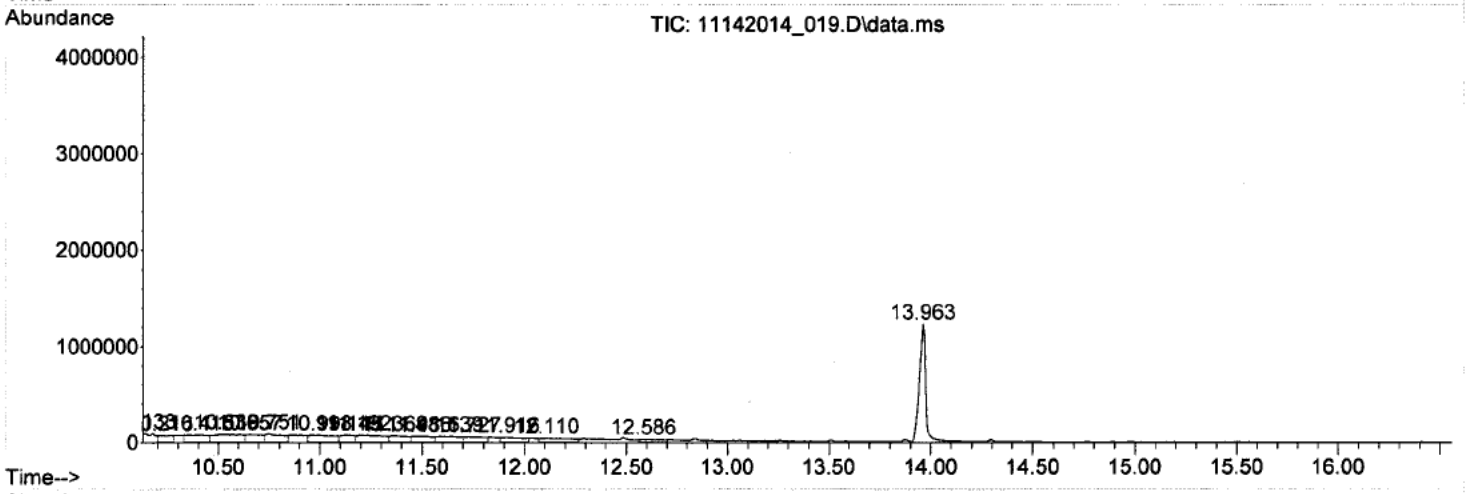
LSC Report - Integrated Chromatogram

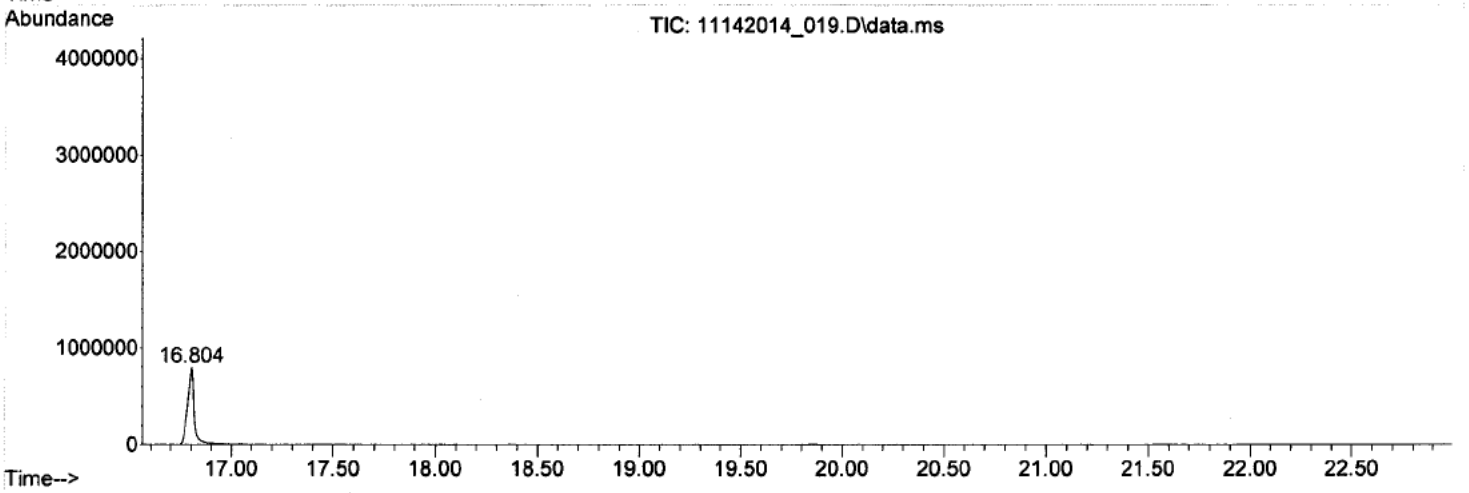
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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

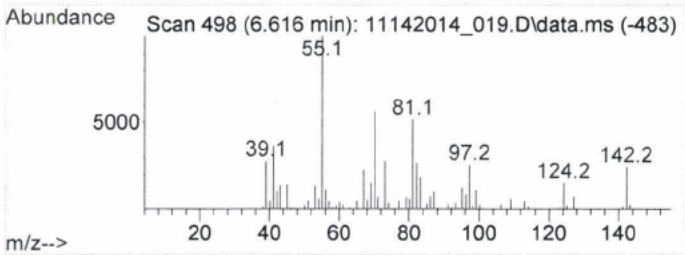
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

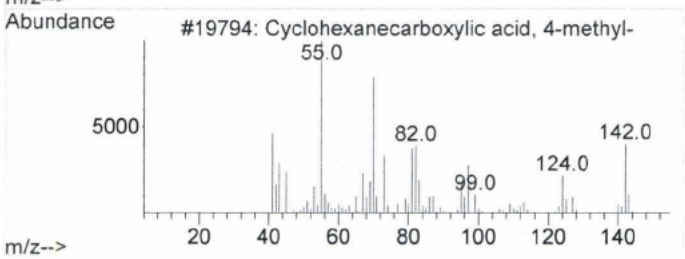
****

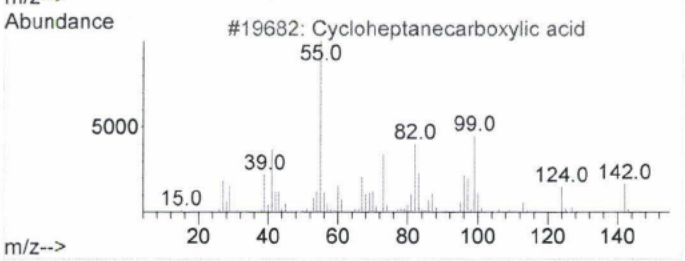
Peak Number 1 Cyclohexanecarboxylic acid,... Concentration Rank 1

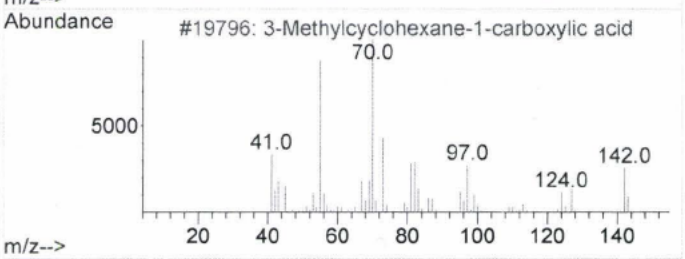
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.616	16.14 ug/mL	5011520	Naphthalene-d8	6.457

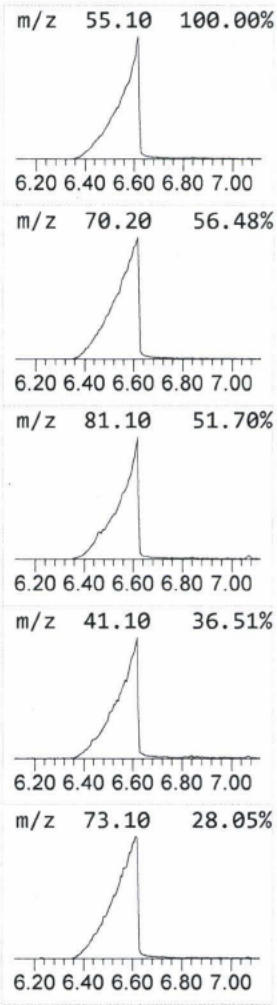
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	91
2	Cycloheptanecarboxylic acid	142	C8H14O2	001460-16-8	60
3	3-Methylcyclohexane-1-carboxylic...	142	C8H14O2	1000132-15-7	43
4	Cyclohexanecarboxylic acid, 2-me...	142	C8H14O2	056586-13-1	38
5	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	20











Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

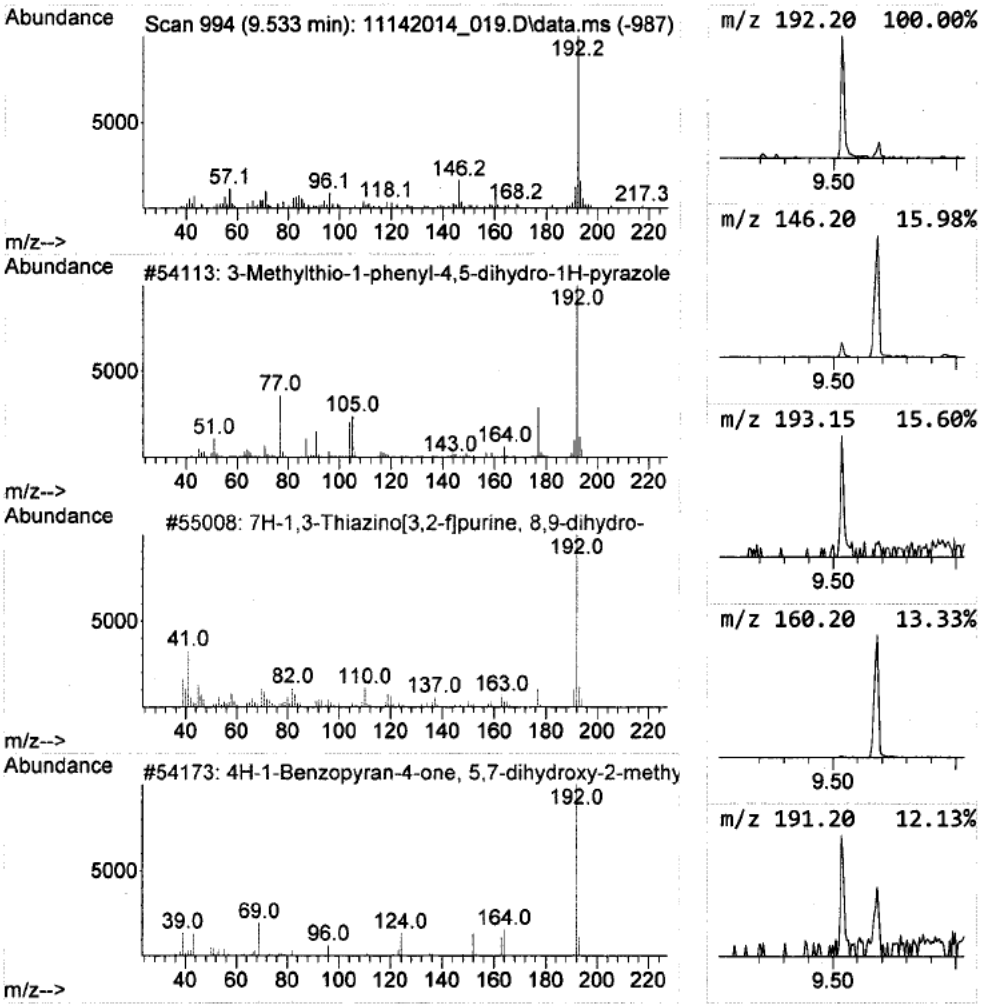
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 2 3-Methylthio-1-phenyl-4,5-d... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	1.30 ug/mL	289744	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylthio-1-phenyl-4,5-dihydr...	192	C10H12N2S	1000305-46-9	64
2	7H-1,3-Thiazino[3,2-f]purine, 8,...	192	C8H8N4S	339370-55-7	59
3	4H-1-Benzopyran-4-one, 5,7-dihyd...	192	C10H8O4	001013-69-0	53
4	D-Norleucine, N-(2-chloroethoxy)...	377	C19H36ClNO4	1000344-17-8	53
5	p-(2-Amino-4-thiazolyl)phenol	192	C9H8N2OS	057634-55-6	53



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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

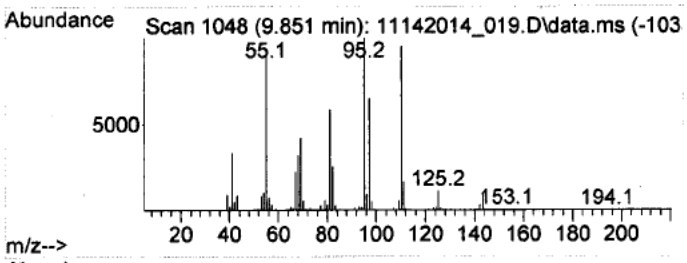
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

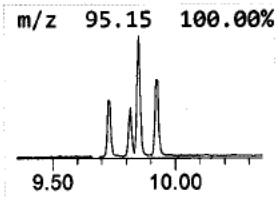
****

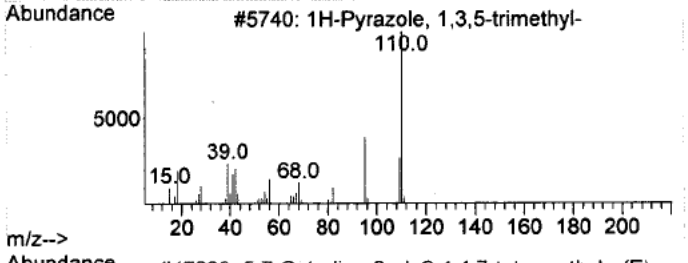
Peak Number 3 1H-Pyrazole, 1,3,5-trimethyl- Concentration Rank 2

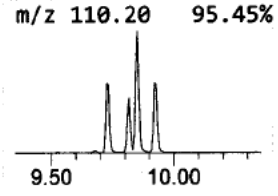
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	6.85 ug/mL	1523970	Phenanthrene-d10	9.680

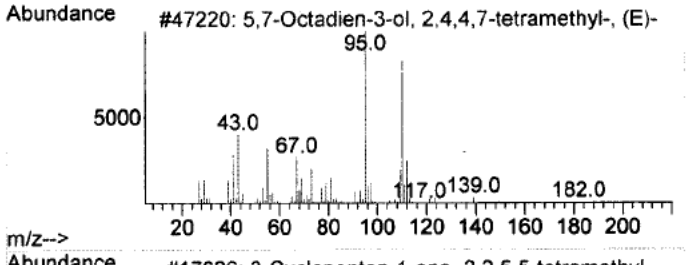
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	64
2	5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	53
3	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	50
4	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	43
5	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	42

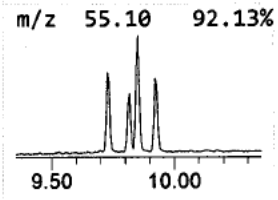


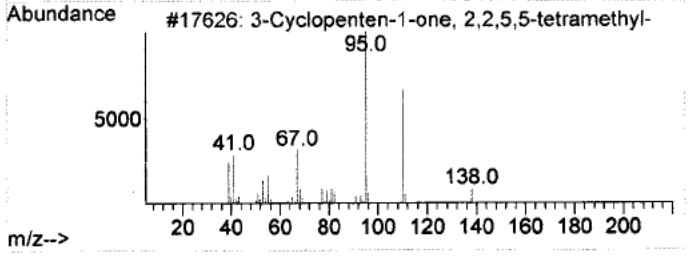


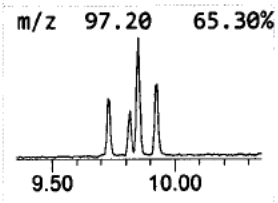


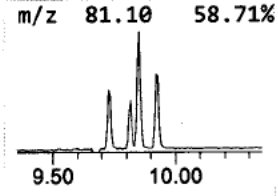












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

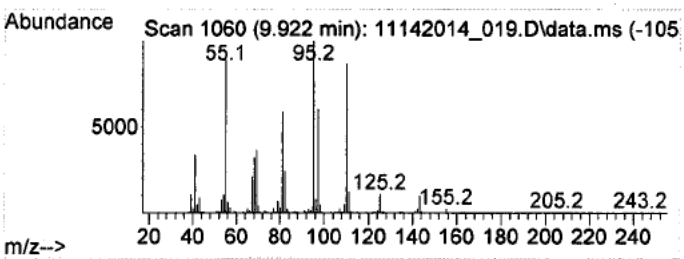
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

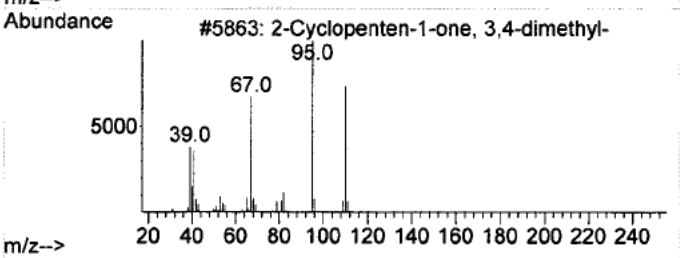
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

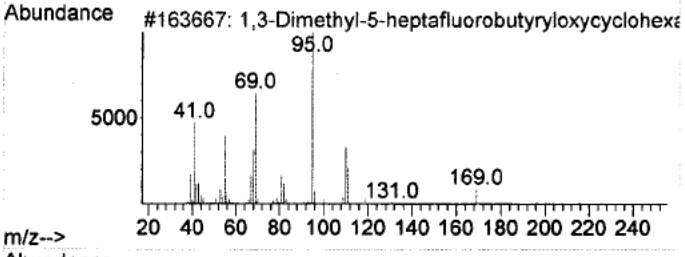
****
Peak Number 4 2-Cyclopenten-1-one, 3,4-di... Concentration Rank 3

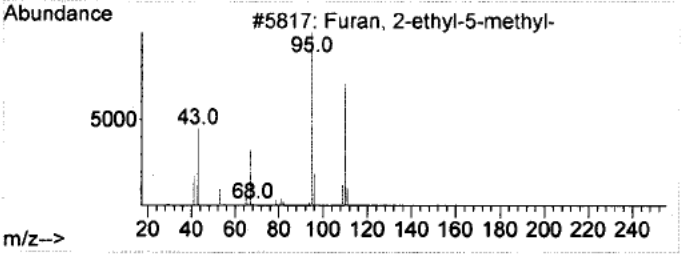
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	4.41 ug/mL	981174	Phenanthrene-d10	9.680

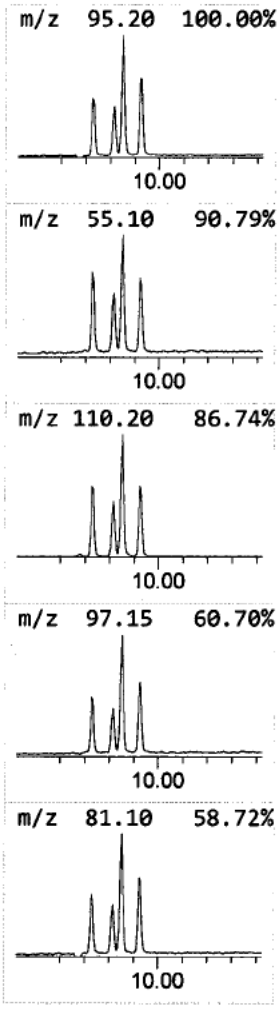
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
2	1,3-Dimethyl-5-heptafluorobutyry...	324	C12H15F7O2	1000216-63-8	38
3	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	38
4	Imidazole-5-carboxylic amide, N-...	125	C5H7N3O	053525-55-6	30
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	27











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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

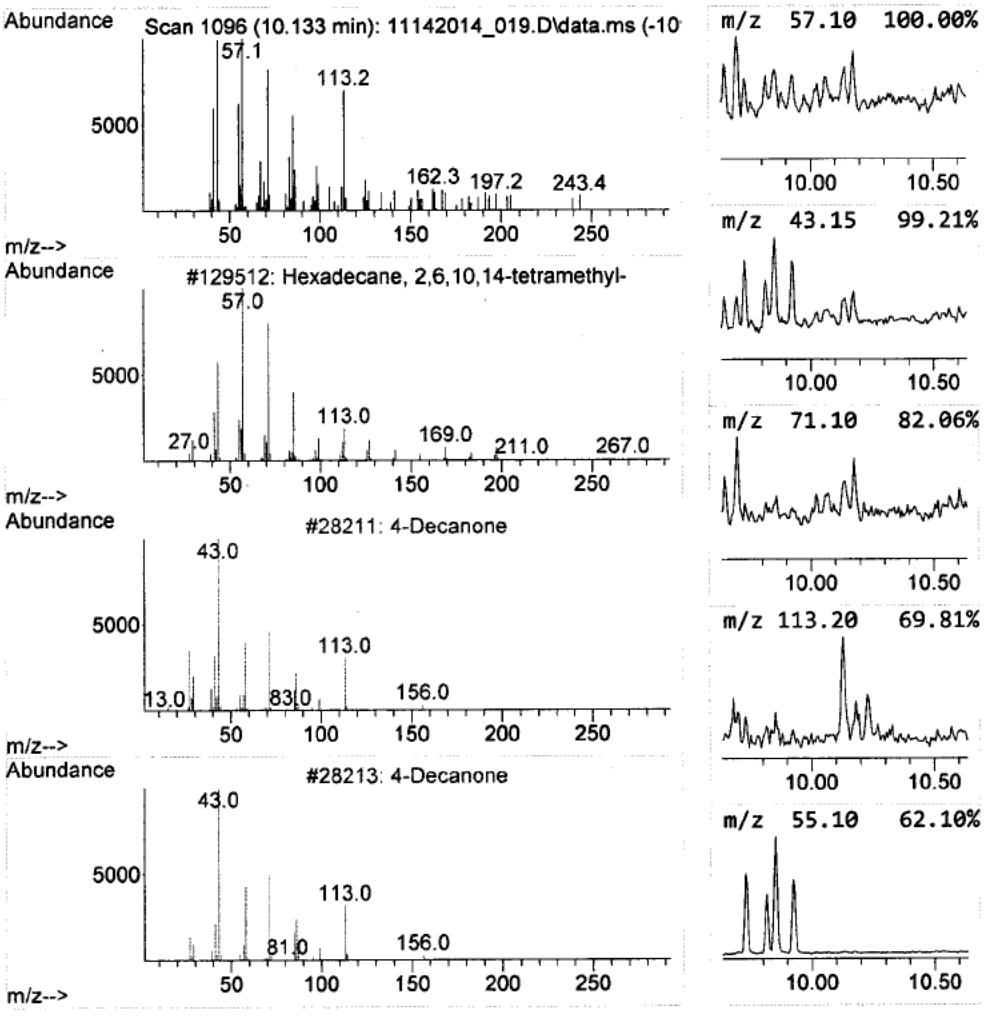
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 5 Hexadecane, 2,6,10,14-tetra... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	1.18 ug/mL	261516	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	49
2	4-Decanone	156	C10H20O	000624-16-8	46
3	4-Decanone	156	C10H20O	000624-16-8	46
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	43
5	Hentriacontane	437	C31H64	000630-04-6	43



Library Search Compound Report

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Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

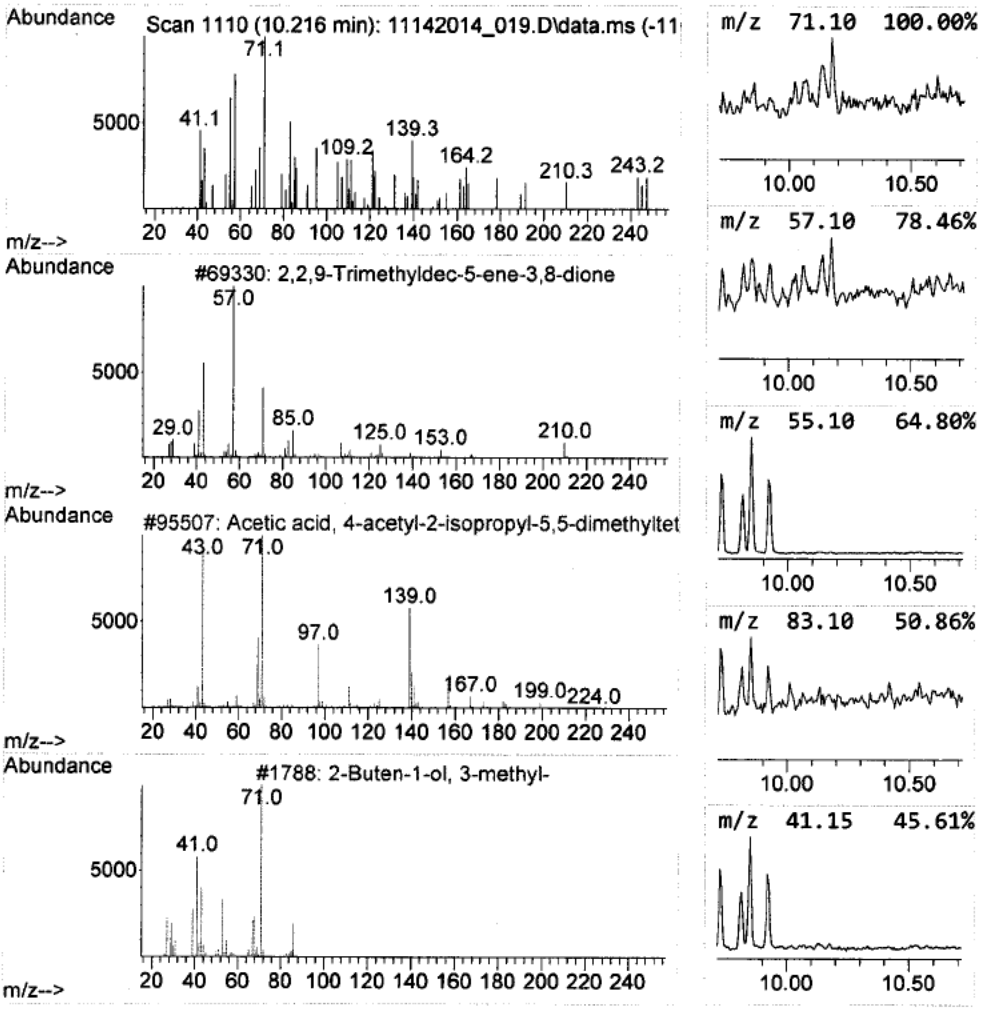
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 6 2,2,9-Trimethyldec-5-ene-3,... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.216	1.44 ug/mL	319709	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,9-Trimethyldec-5-ene-3,8-dione	210	C13H22O2	083040-81-7	27
2	Acetic acid, 4-acetyl-2-isopropy...	242	C13H22O4	1000192-07-0	23
3	2-Buten-1-ol, 3-methyl-	86	C5H10O	000556-82-1	14
4	9-Octadecene, 1,1-dimethoxy-, (Z)-	312	C20H40O2	015677-71-1	12
5	Oxalic acid, 6-ethyloct-3-yl eth...	258	C14H26O4	1000309-33-9	12



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

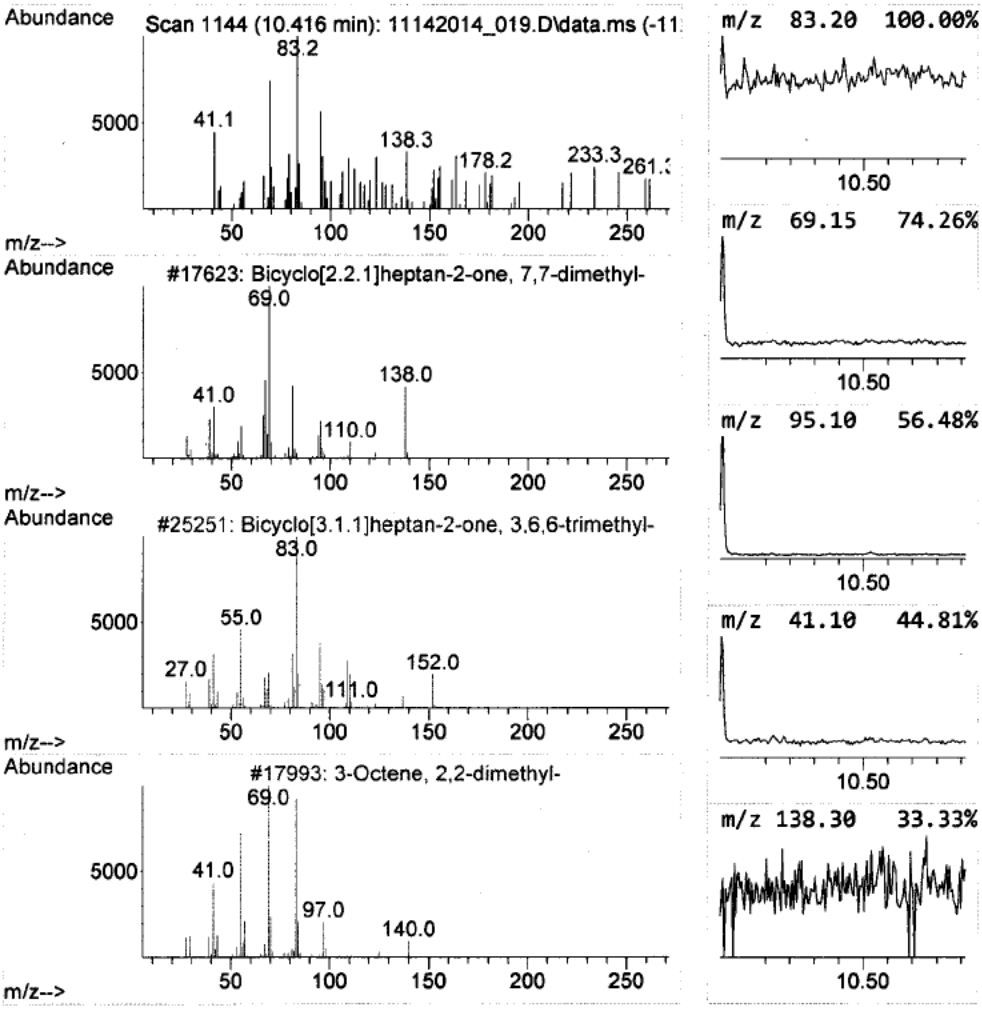
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.416	2.39 ug/mL	532249	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 7,7-...	138	C9H14O	000514-15-8	27
2	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	18
3	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	16
4	3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	16
5	2-sec-Butyl-3-methyl-1-pentene	140	C10H20	075144-24-0	16



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

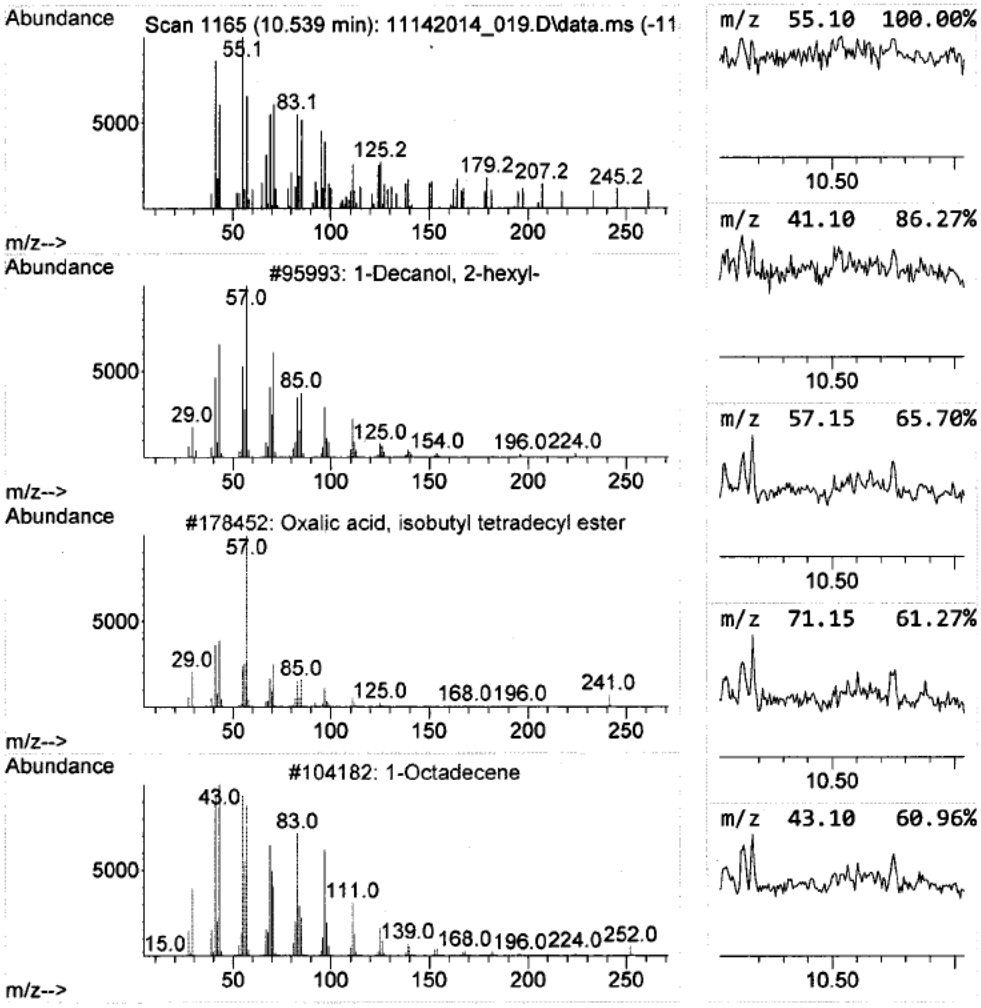
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.539	3.47 ug/mL	770906	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	43
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	38
3	1-Octadecene	252	C18H36	000112-88-9	30
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	30
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	30



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

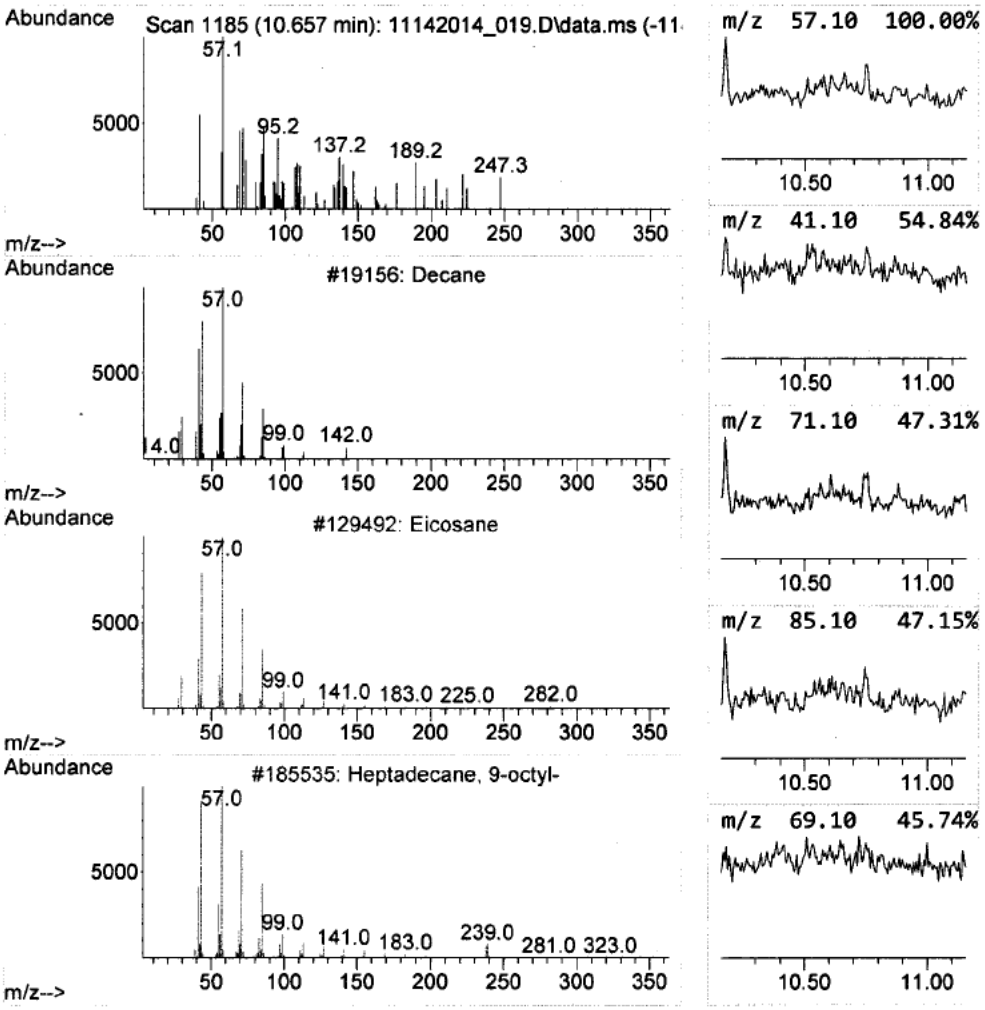
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 9 Decane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	1.83 ug/mL	407490	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	10
2	Eicosane	282	C20H42	000112-95-8	10
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	10
4	Sulfurous acid, butyl decyl ester	278	C14H3003S	1000309-17-7	10
5	9-methylheptadecane	254	C18H38	026741-18-4	10



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

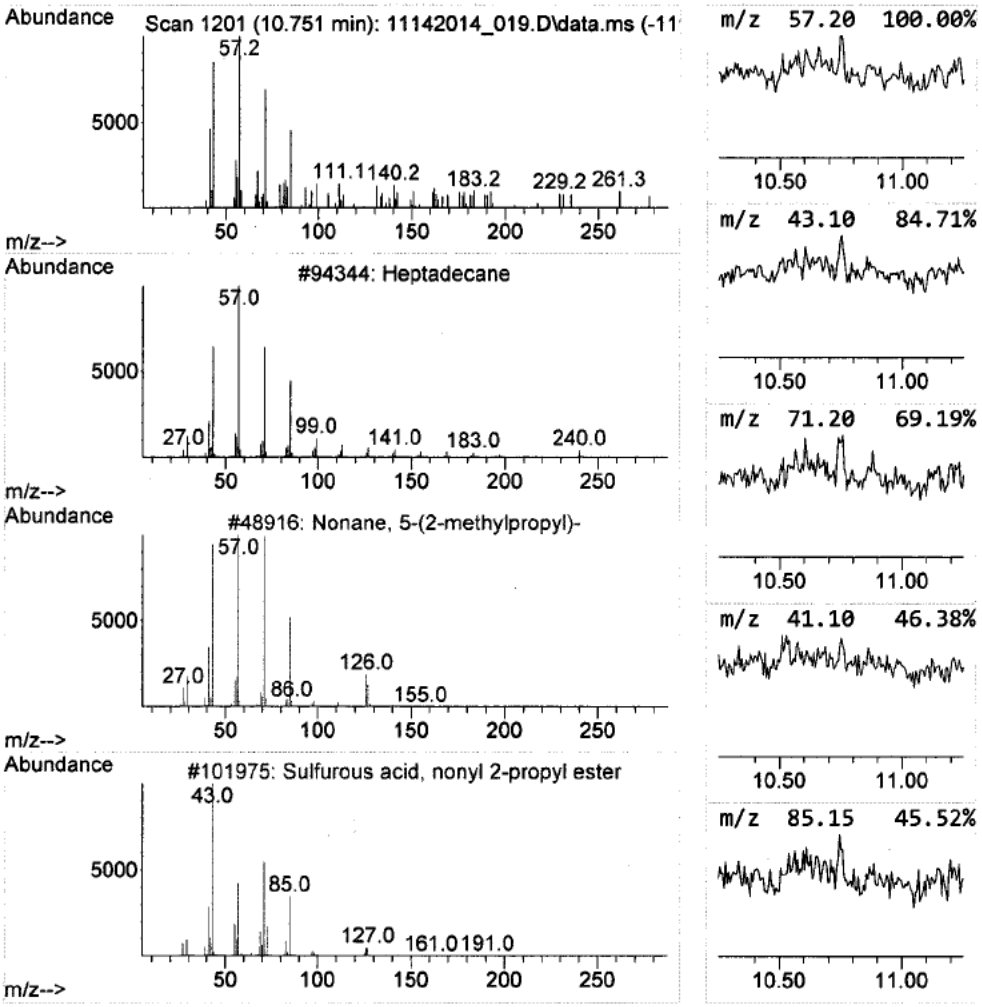
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 10 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.751	2.23 ug/mL	496549	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	43
2	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	38
3	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	38
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	38
5	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	38



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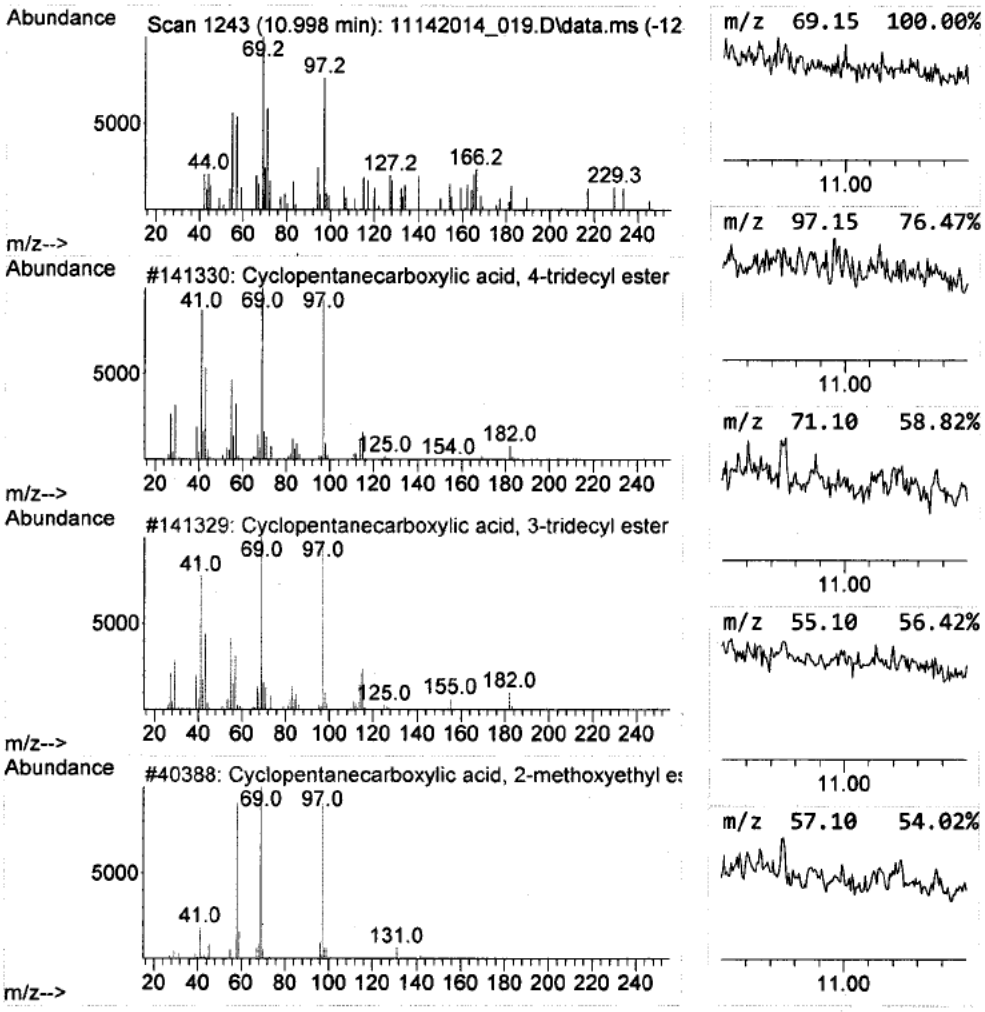
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 11 Cyclopentanecarboxylic acid... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	2.70 ug/mL	600163	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 4-t...	296	C19H36O2	1000280-58-6	27
2	Cyclopentanecarboxylic acid, 3-t...	296	C19H36O2	1000280-58-5	27
3	Cyclopentanecarboxylic acid, 2-m...	172	C9H16O3	1000331-06-9	27
4	Cyclopentene, 3,5-dimethoxy-	128	C7H12O2	089897-05-2	27
5	Cyclopentanecarboxylic acid, 3-p...	324	C21H40O2	1000280-59-1	27



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Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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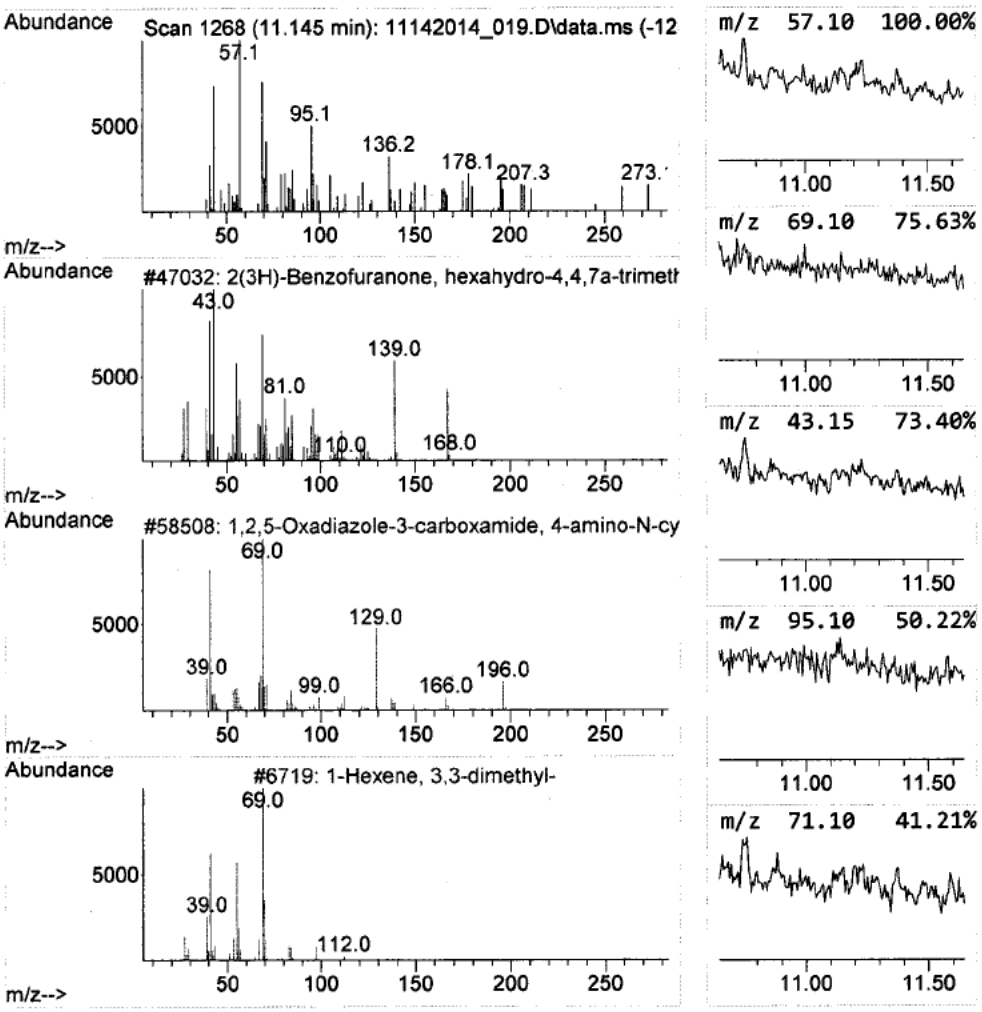
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 12 2(3H)-Benzofuranone, hexahy... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	1.48 ug/mL	330060	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzofuranone, hexahydro-4...	182	C11H18O2	016778-27-1	32
2	1,2,5-Oxadiazole-3-carboxamide, ...	196	C8H12N4O2	1000351-71-7	22
3	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	14
4	8-Bromo-1octanol, trifluoroacetate	304	C10H16BrF3O2	1000365-19-4	10
5	2,6a-Methano-6aH-indeno[4,5-b]ox...	150	C10H14O	016489-32-0	10



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

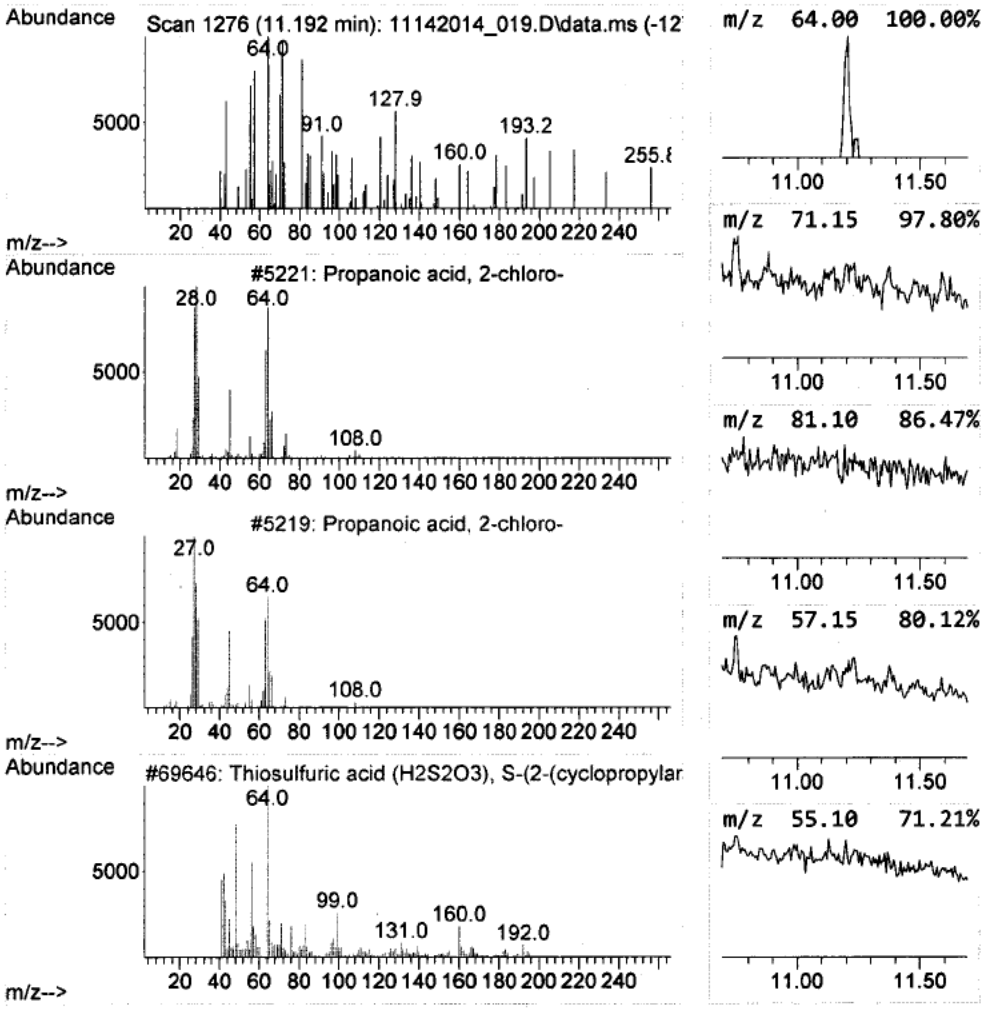
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 13 Propanoic acid, 2-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.192	2.85 ug/mL	634044	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	43
2	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	43
3	Thiosulfuric acid (H2S2O3), S-(2...	210	C5H10N2O3S2	040283-52-1	25
4	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	17
5	S-2-[3-Succinimidopropylamino]et...	296	C9H16N2O5S2	031701-75-4	12



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Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

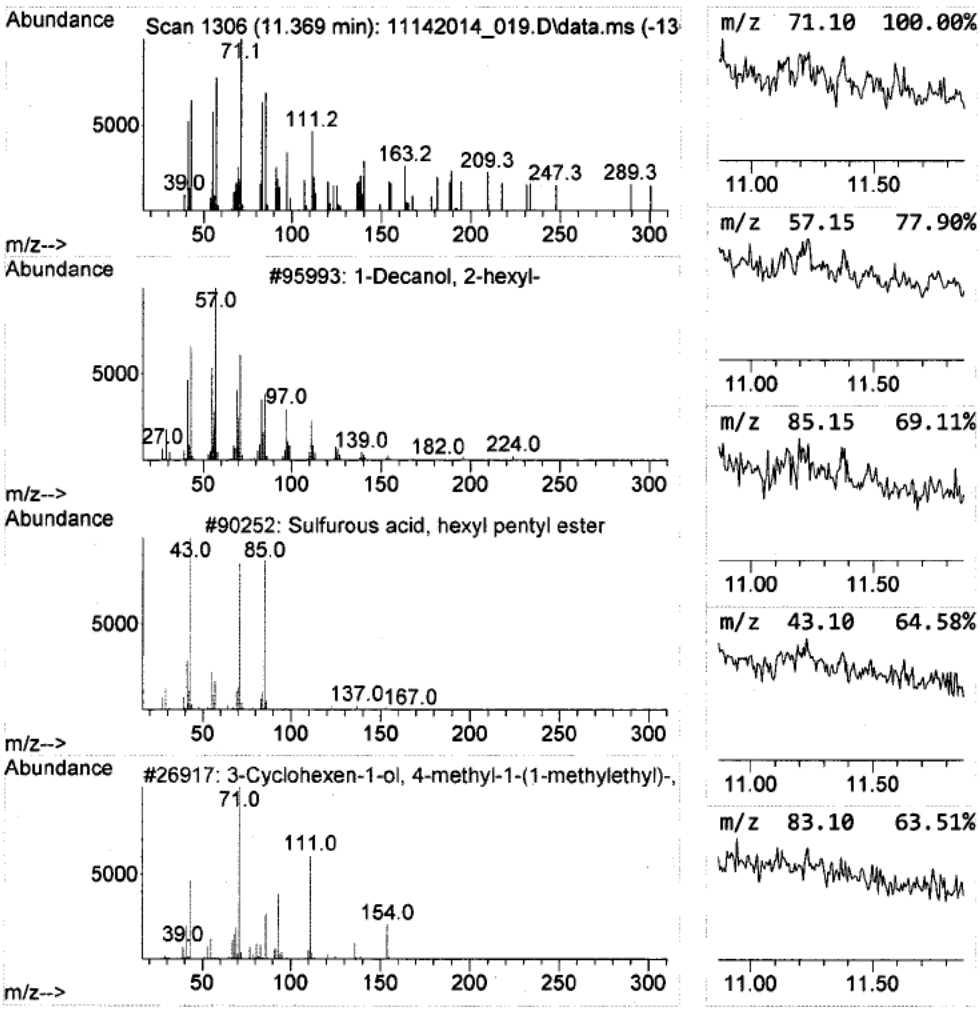
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 14 1-Decanol, 2-hexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.369	1.69 ug/mL	375035	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47
2	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	35
3	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	35
4	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	14
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	14



Library Search Compound Report

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Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

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

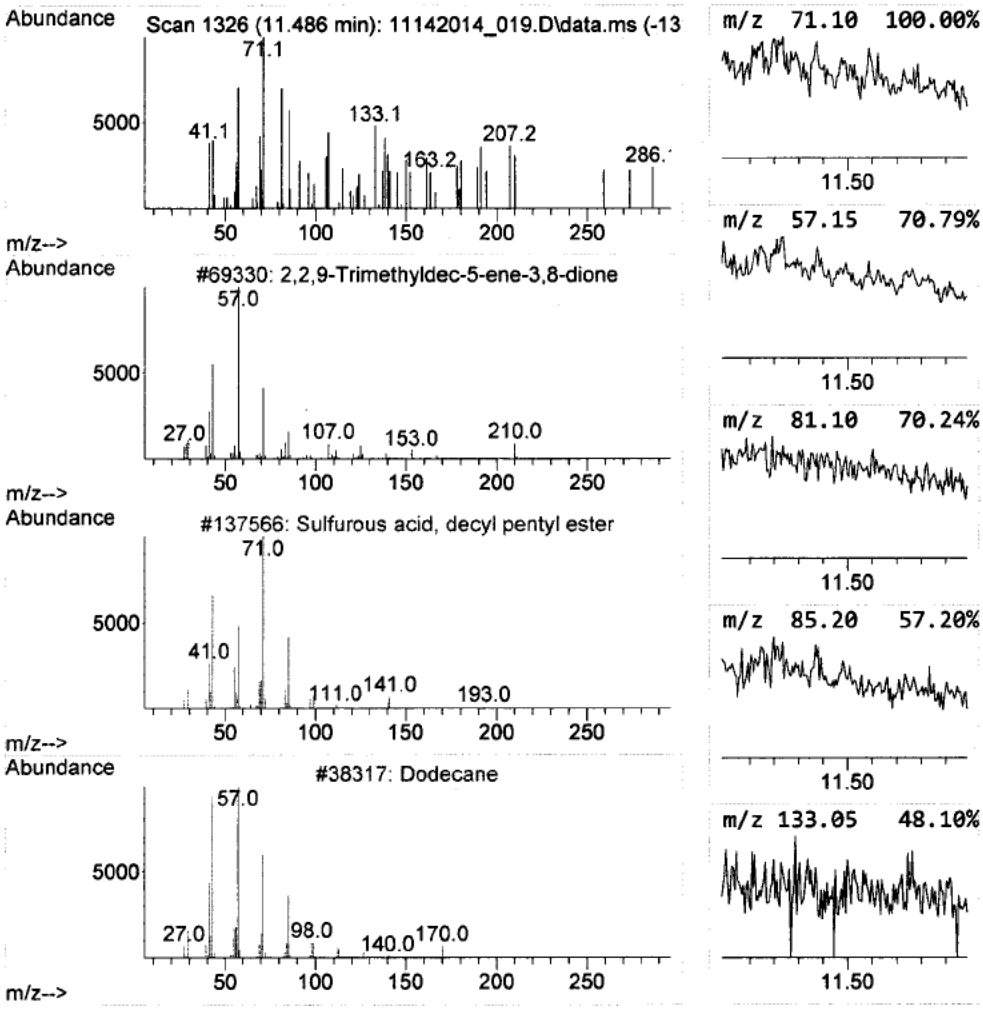
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 15 2,2,9-Trimethyldec-5-ene-3,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.486	1.76 ug/mL	392064	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,9-Trimethyldec-5-ene-3,8-dione	210	C13H22O2	083040-81-7	32
2	Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	22
3	Dodecane	170	C12H26	000112-40-3	12
4	Dotriacontane	451	C32H66	000544-85-4	12
5	Pentadecane	212	C15H32	000629-62-9	12



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Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

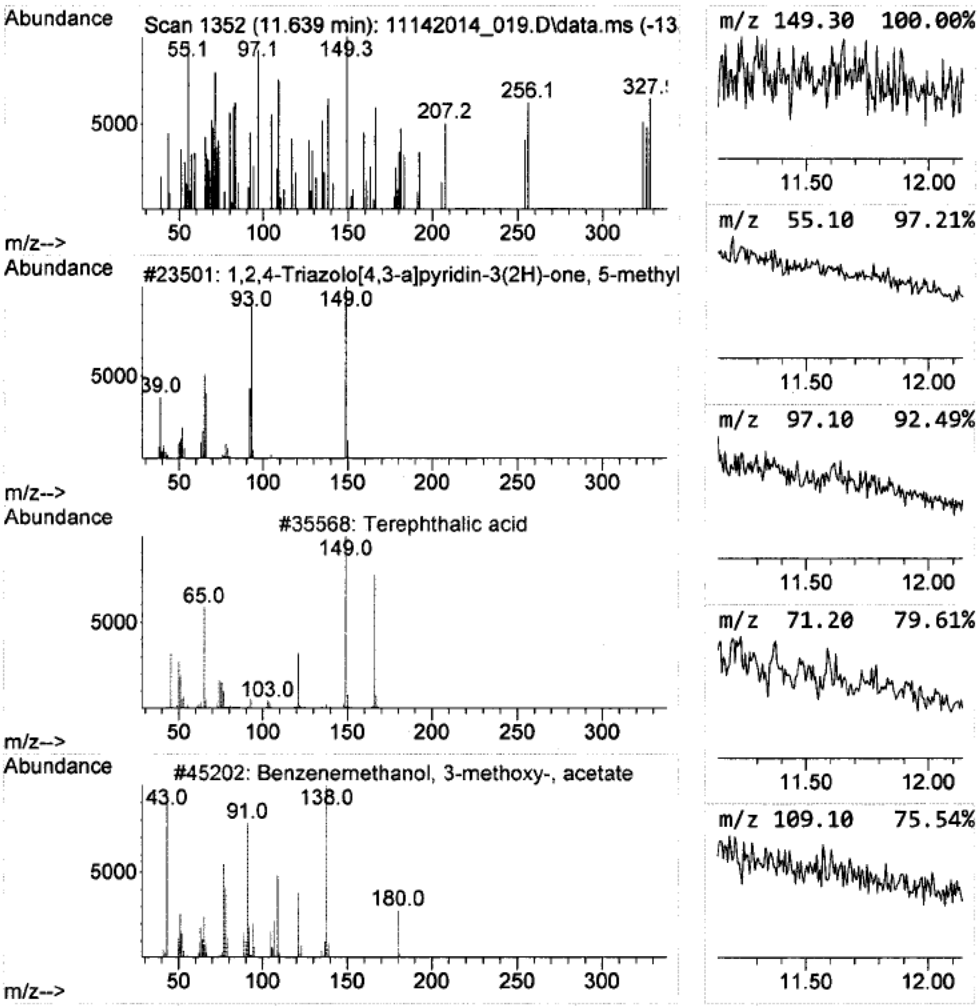
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 16 1,2,4-Triazolo[4,3-a]pyridi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.639	2.04 ug/mL	454476	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazolo[4,3-a]pyridin-3(2...	149	C7H7N3O	004926-18-5	35
2	Terephthalic acid	166	C8H6O4	000100-21-0	22
3	Benzenemethanol, 3-methoxy-, ace...	180	C10H12O3	035480-26-3	12
4	Cyclopenteno[4.3-b]tetrahydrofur...	358	C19H18O5S	1000211-22-7	12
5	Terephthalic acid	166	C8H6O4	000100-21-0	12



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ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

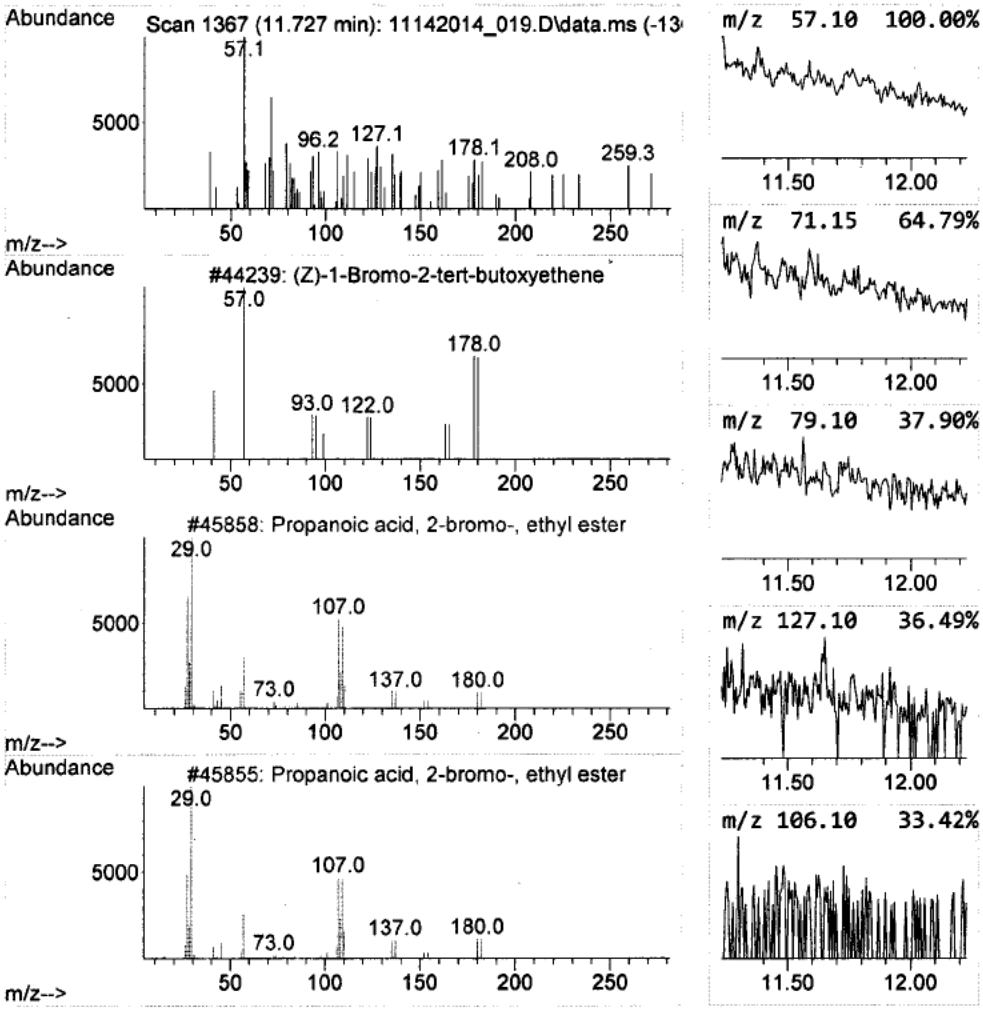
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 17 (Z)-1-Bromo-2-tert-butoxyet... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.727	1.58 ug/mL	352141	Phenanthrene-d10	9.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Bromo-2-tert-butoxyethene	178	C6H11BrO	113279-39-3	10
2	Propanoic acid, 2-bromo-, ethyl ...	180	C5H9BrO2	000535-11-5	5
3	Propanoic acid, 2-bromo-, ethyl ...	180	C5H9BrO2	000535-11-5	5
4	Cyclopentane, 1-bromo-2-methoxy-...	178	C6H11BrO	051475-11-7	4
5	Propanedioic acid, bromomethyl-,...	252	C8H13BrO4	029263-94-3	2



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Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

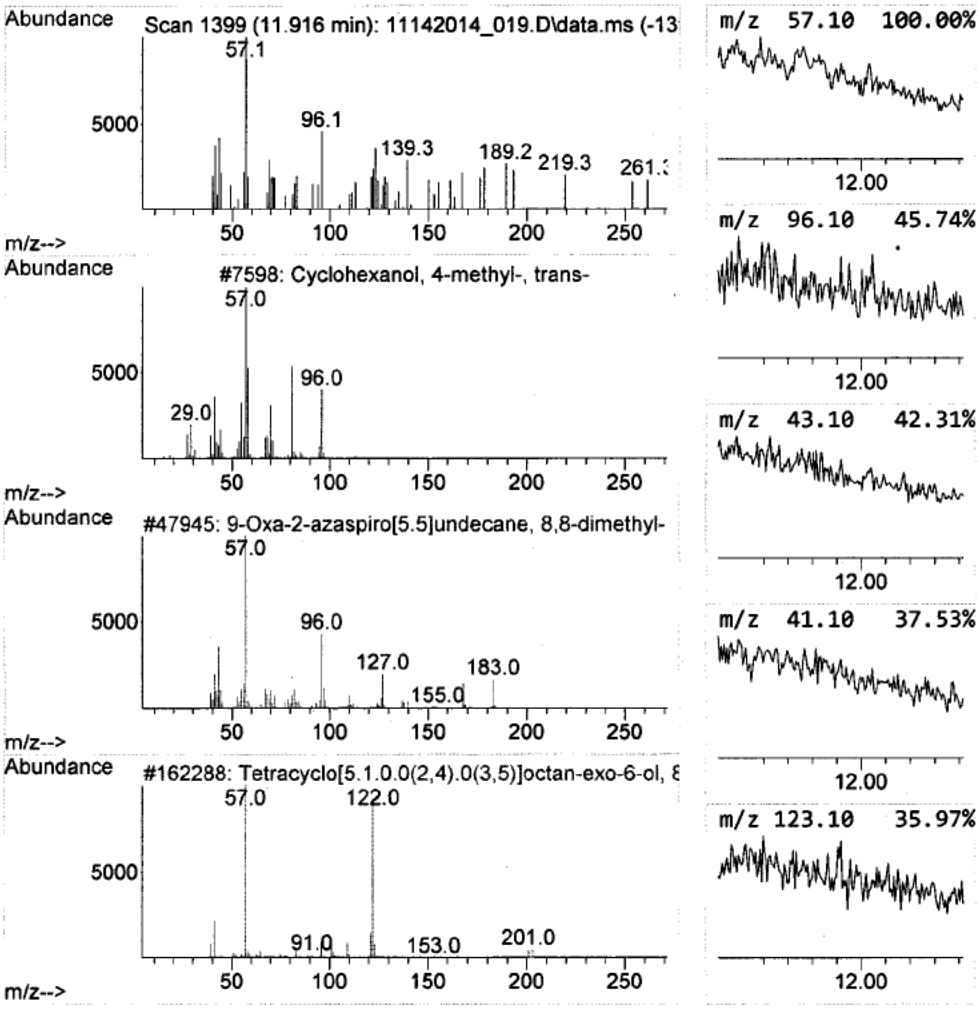
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 18 Cyclohexanol, 4-methyl-, tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.66 ug/mL	354444	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 4-methyl-, trans-	114	C7H14O	007731-29-5	9
2	9-Oxa-2-azaspiro[5.5]undecane, 8...	183	C11H21NO	057117-92-7	9
3	Tetracyclo[5.1.0.0(2,4).0(3,5)]o...	322	C12H16BrFO2S	1000143-00-7	9
4	Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	9
5	Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	9



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ALS Vial : 18 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

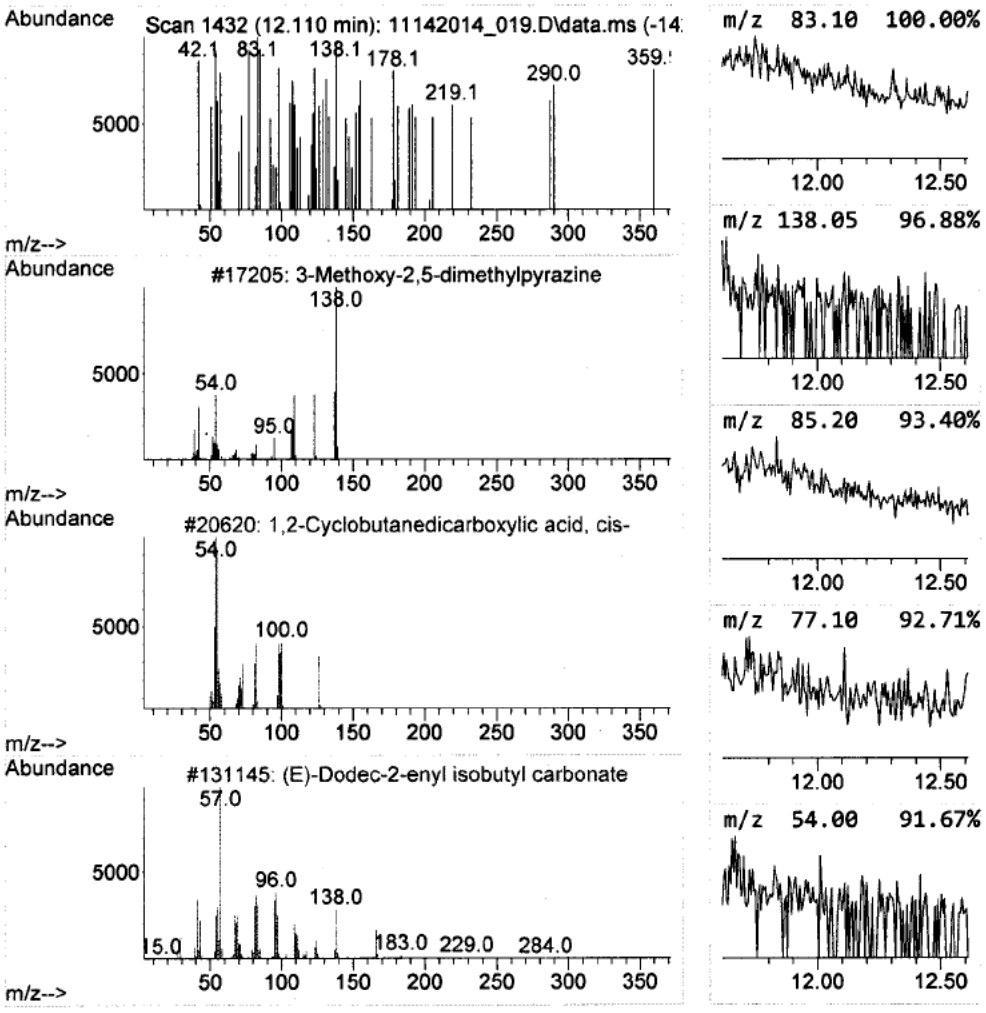
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 19 3-Methoxy-2,5-dimethylpyrazine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	3.15 ug/mL	420098	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methoxy-2,5-dimethylpyrazine	138	C7H10N2O	019846-22-1	23
2	1,2-Cyclobutanedicarboxylic acid...	144	C6H8O4	001461-94-5	22
3	(E)-Dodec-2-enyl isobutyl carbonate	284	C17H32O3	1000372-78-7	17
4	p-Benzoquinone	108	C6H4O2	000106-51-4	12
5	Xanthine	152	C5H4N4O2	000069-89-6	12



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Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

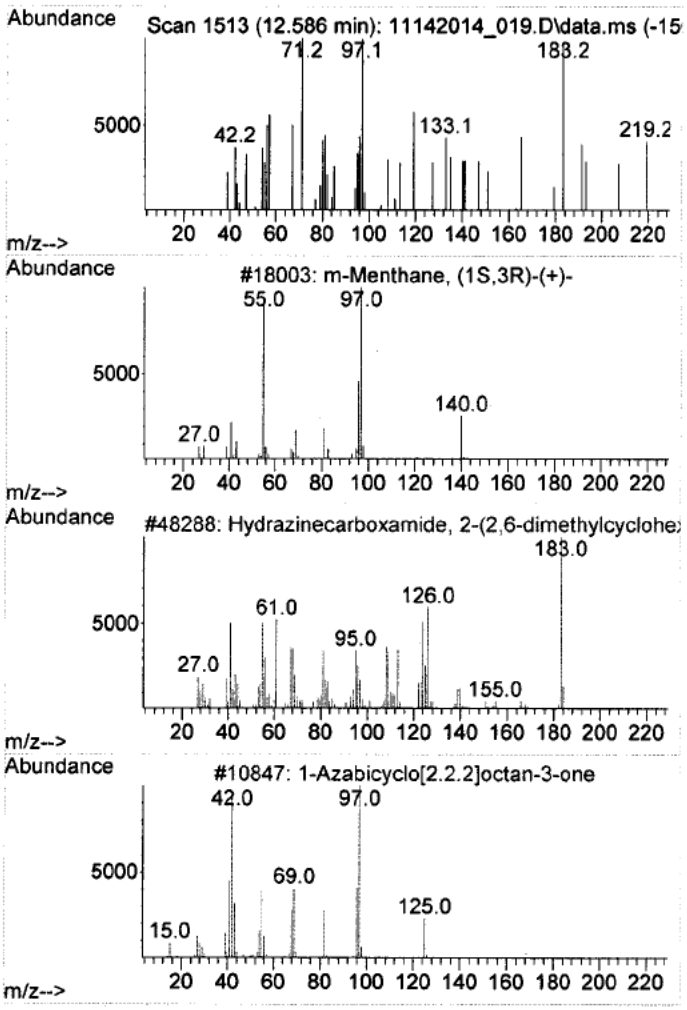
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

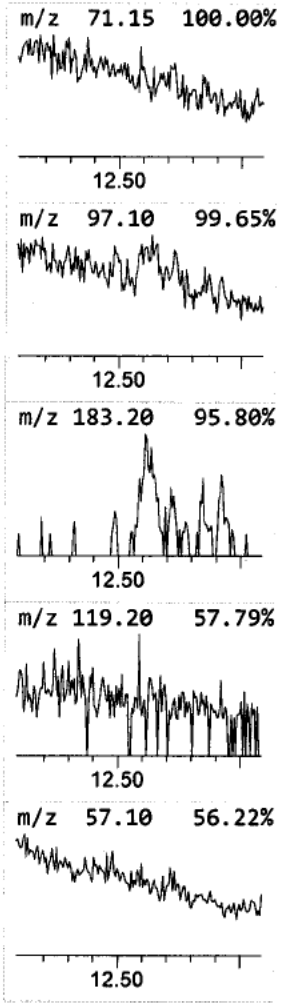
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 20 m-Menthane, (1S,3R)-(+)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	1.59 ug/mL	212082	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	10
2	Hydrazinecarboxamide, 2-(2,6-dim...	183	C9H17N3O	057174-11-5	10
3	1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	003731-38-2	10
4	4-Hydroxy-1-methyloctahydro-2(1H...	183	C10H17NO2	1005254-62-5	9
5	Aminoperimidine	183	C11H9N3	028832-64-6	9





Tentatively Identified Compound (LSC) summary

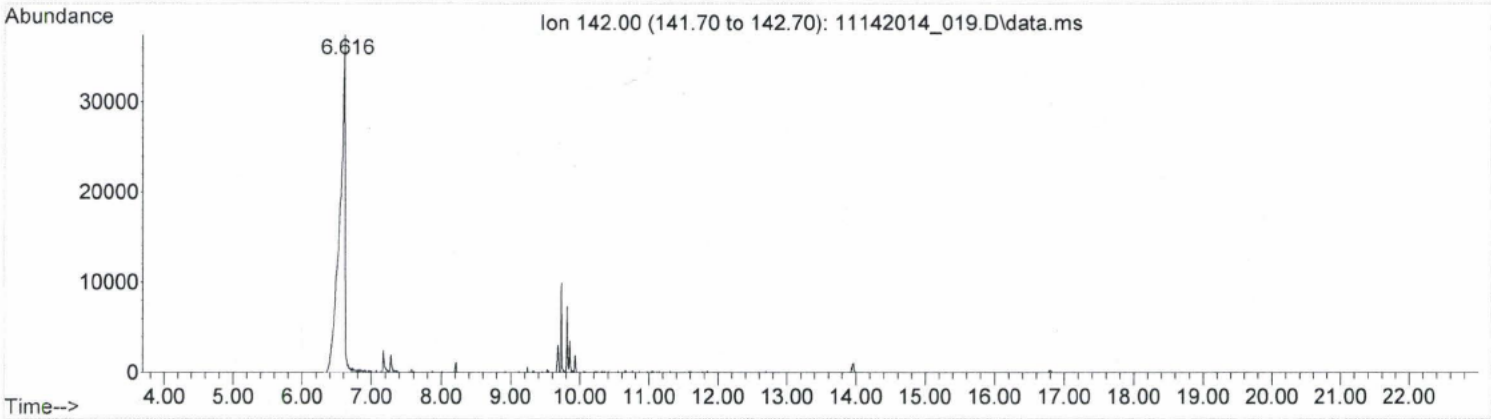
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_019.D
Acq On : 14 Nov 2014 06:41 pm
Operator : [redacted]
Sample : NE36692-A
Misc : Tag # NE36692-A, Lab Rep #1, 1X
ALS Vial : 18 Sample Multiplier: 1

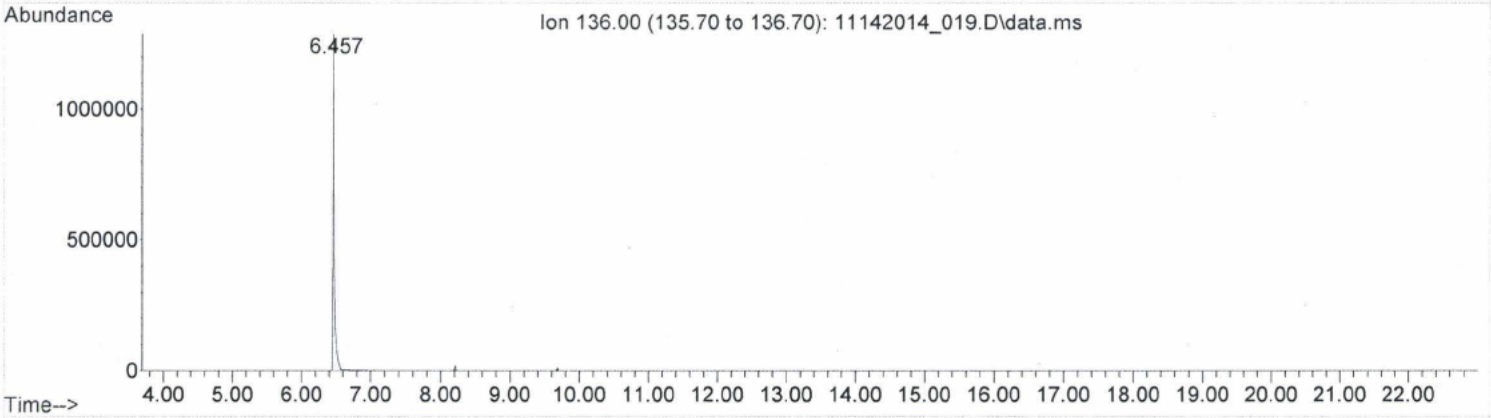
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

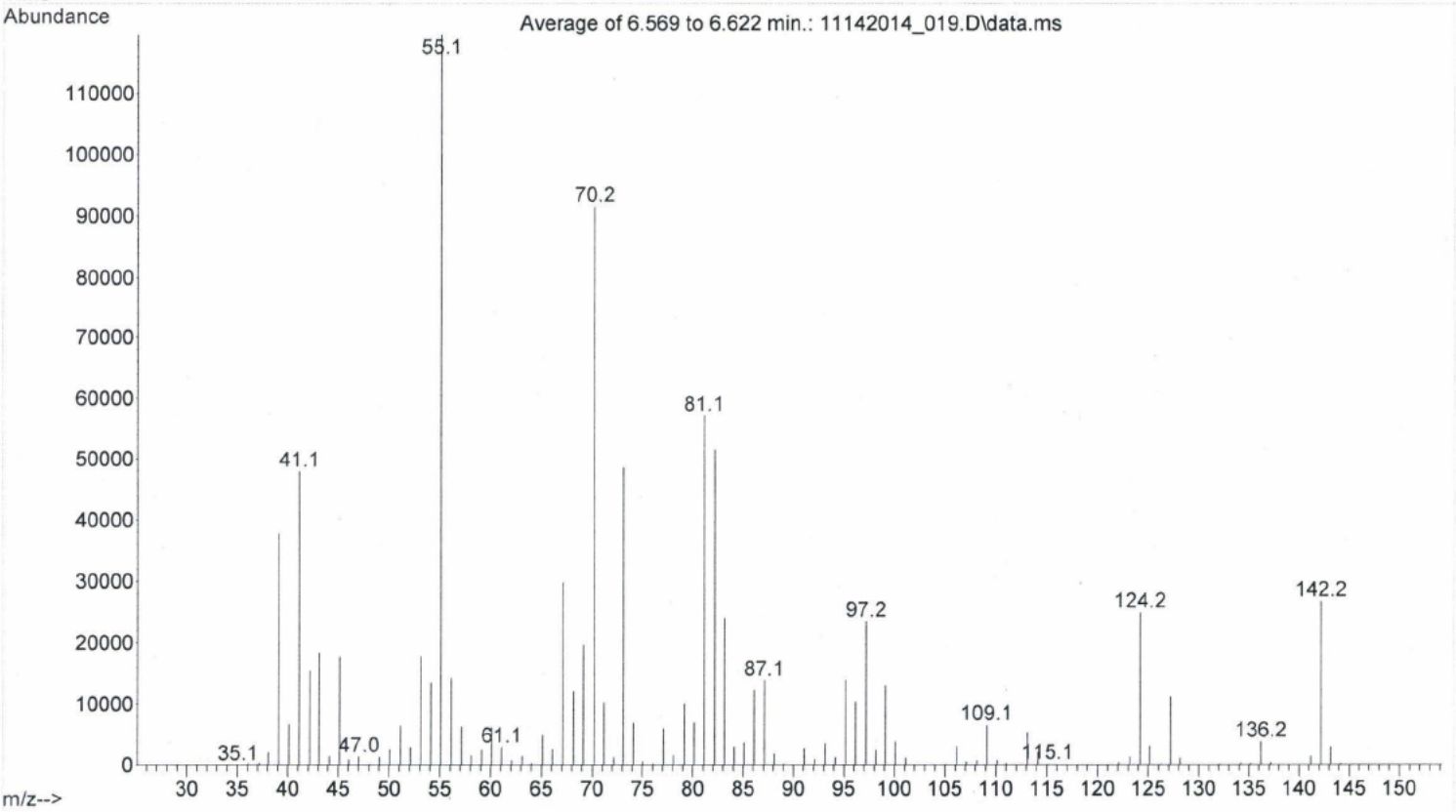
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Cyclohexanecarb...	6.616	16.1	ug/mL	5011520	2	6.457	6211780	20.0
3-Methylthio-1-...	9.533	1.3	ug/mL	289744	4	9.680	4449100	20.0
1H-Pyrazole, 1,...	9.851	6.9	ug/mL	1523970	4	9.680	4449100	20.0
2-Cyclopenten-1...	9.922	4.4	ug/mL	981174	4	9.680	4449100	20.0
Hexadecane, 2,6...	10.133	1.2	ug/mL	261516	4	9.680	4449100	20.0
2,2,9-Trimethyl...	10.216	1.4	ug/mL	319709	4	9.680	4449100	20.0
Bicyclo[2.2.1]h...	10.416	2.4	ug/mL	532249	4	9.680	4449100	20.0
1-Decanol, 2-he...	10.539	3.5	ug/mL	770906	4	9.680	4449100	20.0
Decane	10.657	1.8	ug/mL	407490	4	9.680	4449100	20.0
Heptadecane	10.751	2.2	ug/mL	496549	4	9.680	4449100	20.0
Cyclopentanecar...	10.998	2.7	ug/mL	600163	4	9.680	4449100	20.0
2(3H)-Benzofura...	11.145	1.5	ug/mL	330060	4	9.680	4449100	20.0
Propanoic acid,...	11.192	2.9	ug/mL	634044	4	9.680	4449100	20.0
1-Decanol, 2-he...	11.369	1.7	ug/mL	375035	4	9.680	4449100	20.0
2,2,9-Trimethyl...	11.486	1.8	ug/mL	392064	4	9.680	4449100	20.0
1,2,4-Triazolo[...	11.639	2.0	ug/mL	454476	4	9.680	4449100	20.0
(Z)-1-Bromo-2-t...	11.727	1.6	ug/mL	352141	4	9.680	4449100	20.0
Cyclohexanol, 4...	11.916	2.7	ug/mL	354444	5	13.963	2663420	20.0
3-Methoxy-2,5-d...	12.110	3.2	ug/mL	420098	5	13.963	2663420	20.0
m-Menthane, (1S...	12.586	1.6	ug/mL	212082	5	13.963	2663420	20.0

File :D:[redacted]\RP1616\11142014_Run\11142014_019.D
Operator : [redacted]
Acquired : 14 Nov 2014 06:41 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36692-A
Misc Info : Tag # NE36692-A, Lab Rep #1, 1X
Vial Number: 18







[redacted] RP1616 12/17/14