Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Nov 19 09:18:18 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	333214	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1486775	20.00 ug/mL	0.00
5) Acenaphthene-d10	8.210	164	866729	20.00 ug/mL	0.00
10) Phenanthrene-d10	9.681	188	1320280	20.00 ug/mL	0.00
11) Chrysene-d12	13.963	240	690637	20.00 ug/mL	# 0.00
12) Perylene-d12	16.798	264	370644	20.00 ug/mL	0.00
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.575	172	7076m	0.13 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery =	~~1.04%#~~	
Target Compounds					Qvalue
2) MCHM	5.540	55	257627m	7.71 ug/mL	
4) PPH	6.881	94	26960m	1.02 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	642438m	18.80 ug/mL	

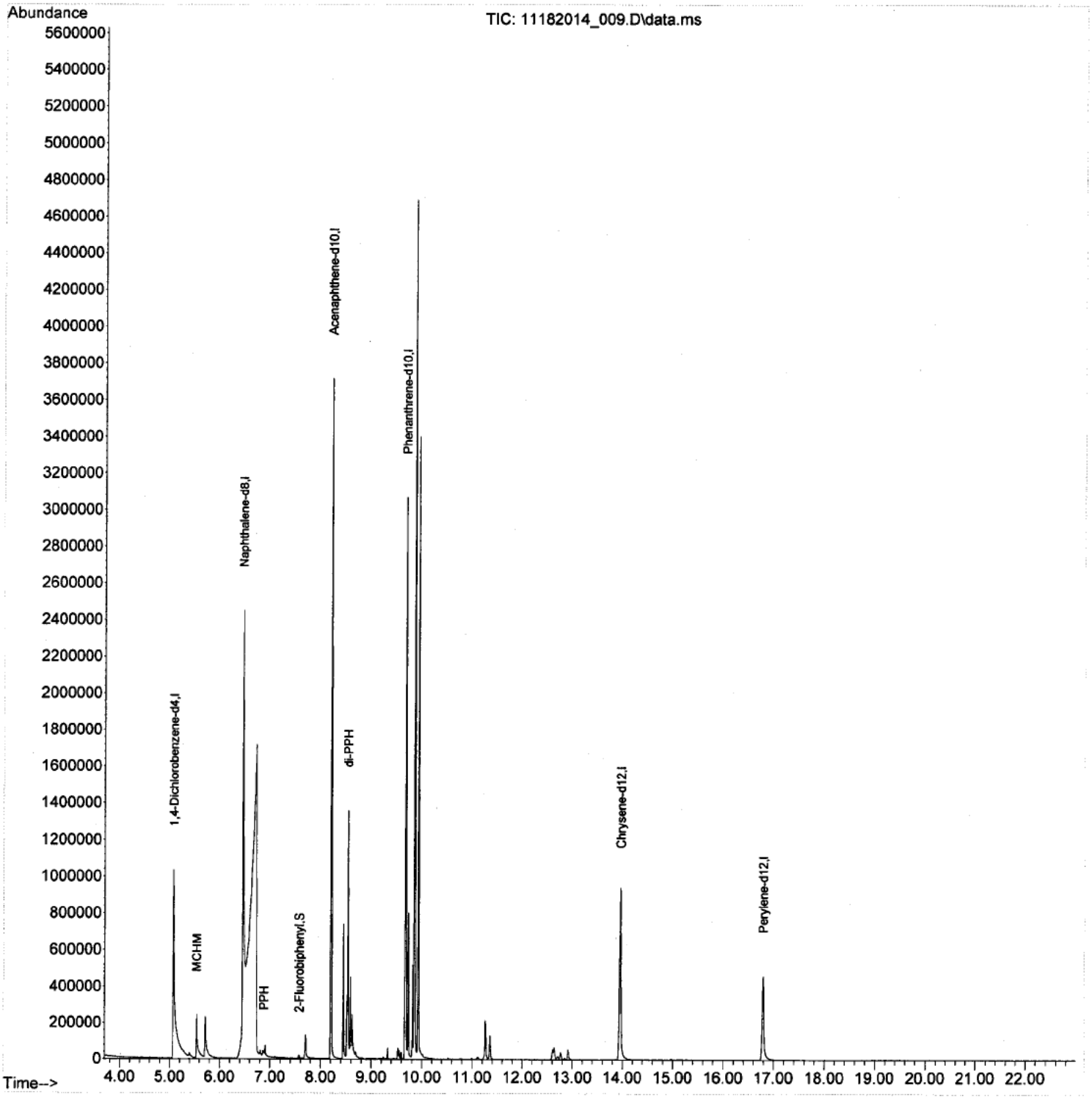
see Analyst Narrative, Surrogate Recovery [redacted] 11/21/14

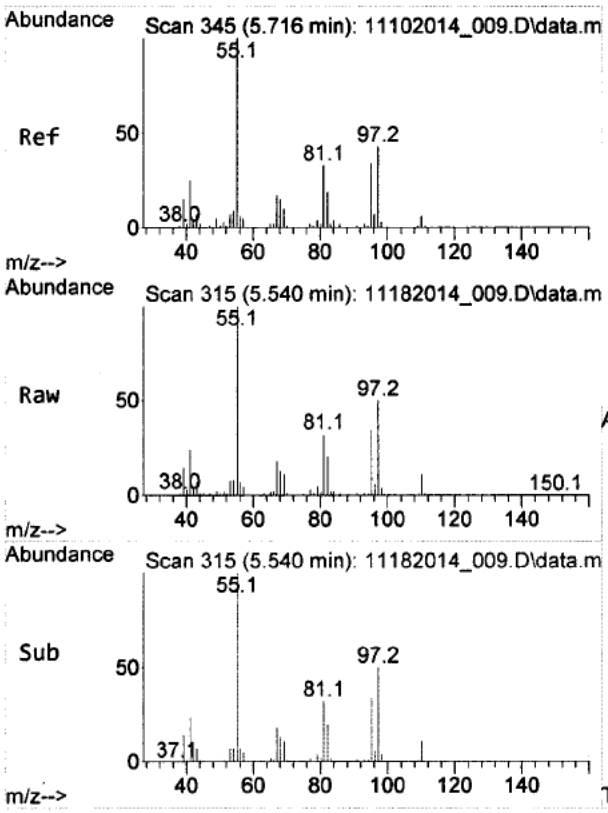
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Nov 19 09:18:18 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

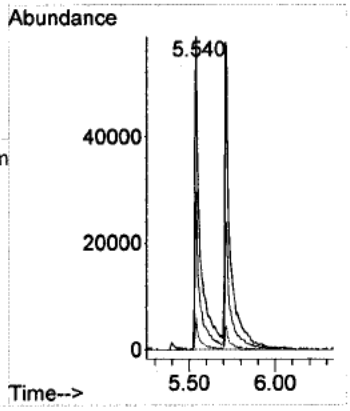


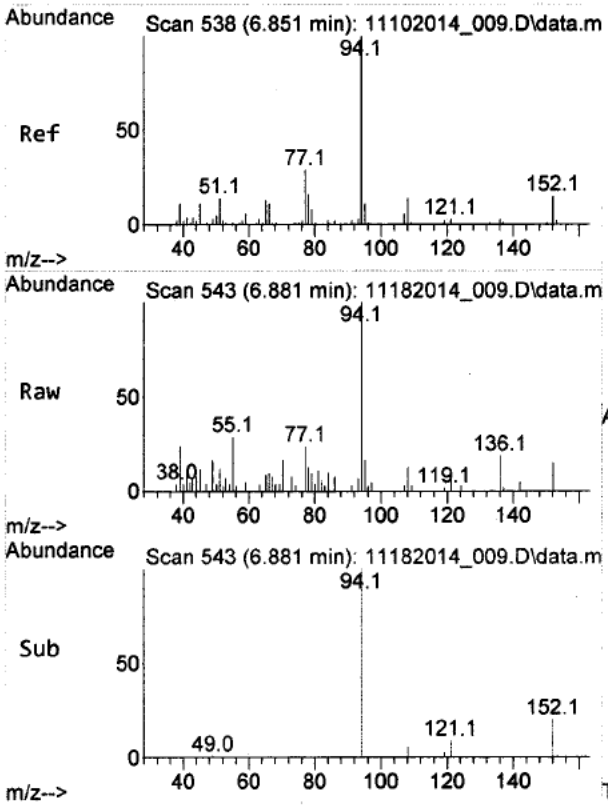


#2
MCHM
Concen: 7.71 ug/mL m
RT: 5.540 min Scan# 315
Delta R.T. -0.176 min
Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 55 Resp: 257627

Ion	Ratio	Lower	Upper
55	100		
97	18.8	34.6	51.8#
110	2.7	4.8	7.2#

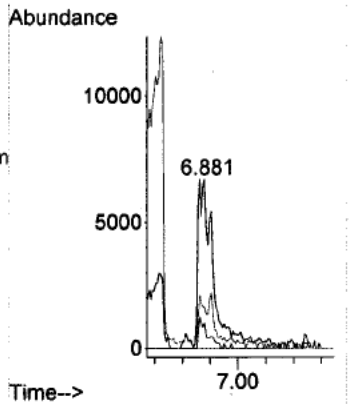


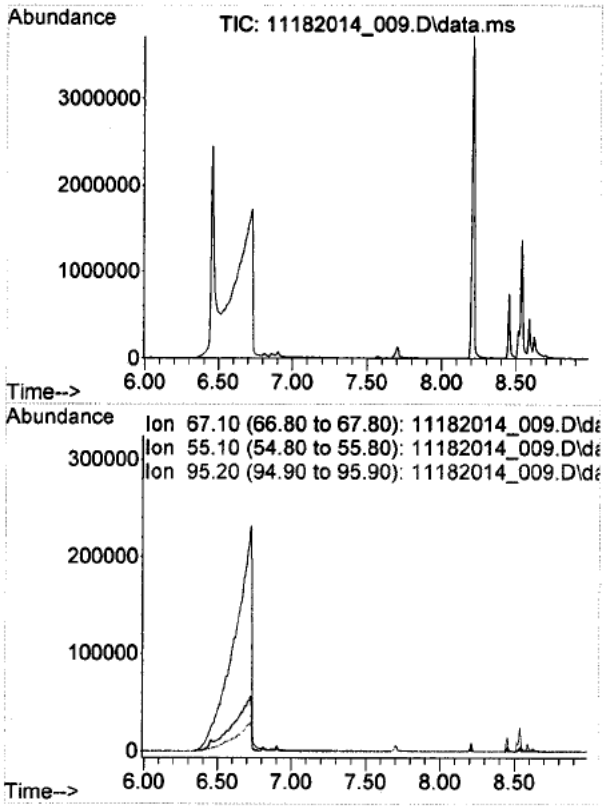


#4
PPH
Concen: 1.02 ug/mL m
RT: 6.881 min Scan# 543
Delta R.T. 0.024 min
Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 94 Resp: 26960

Ion	Ratio	Lower	Upper
94	100		
152	7.3	13.4	20.0#
77	15.4	21.2	31.8#



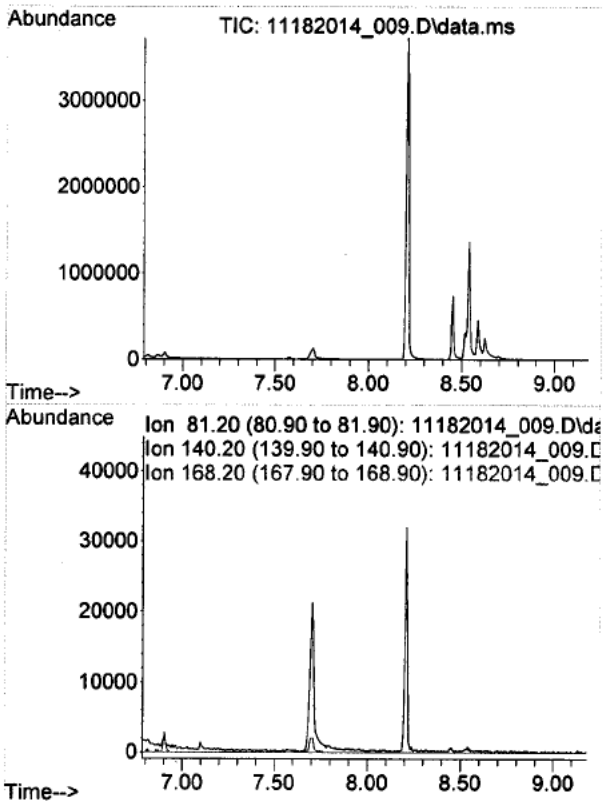


#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8

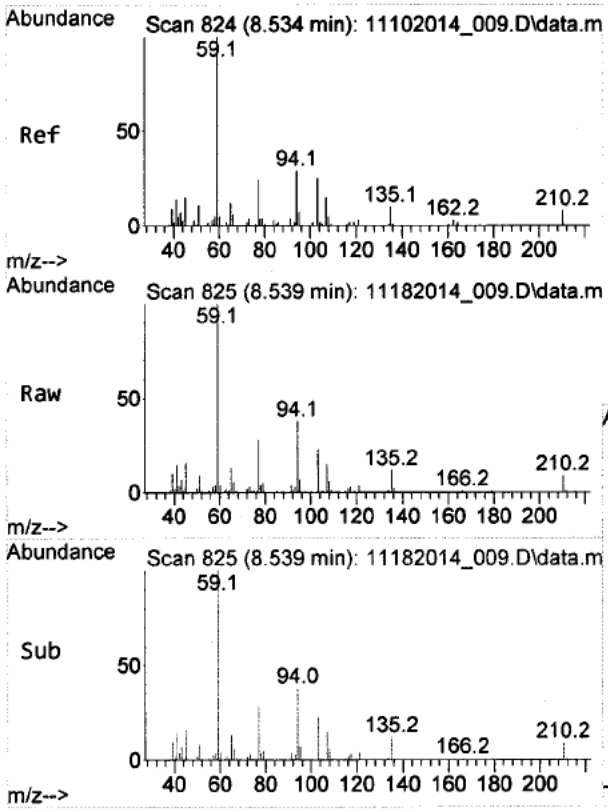


#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 81

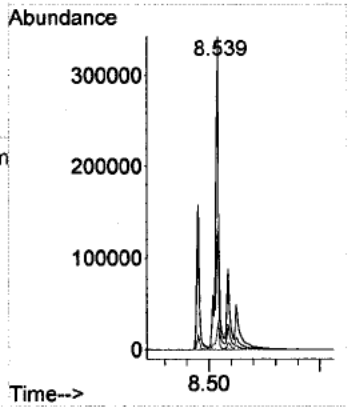
Sig	Exp Ratio
81	100
140	61.8
168	17.7



#9
di-PPH
Concen: 18.80 ug/mL m
RT: 8.539 min Scan# 825
Delta R.T. -0.001 min
Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 59 Resp: 642438

Ion	Ratio	Lower	Upper
59	100		
94	26.6	23.0	34.6
210	5.1	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Dec 01 14:10:08 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	571045	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1491725	20.00 ug/mL	0.00
24) Acenaphthene-d10	8.210	164	866729	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.681	188	1321205	20.00 ug/mL	0.00
49) Chrysene-d12	13.963	240	690637	20.00 ug/mL	#-0.01
58) Perylene-d12	16.798	264	376917	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. 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...	6.728	55	1864197	182.12 ug/mL	97
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	0.000		0	N.D. d	
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	0.000		0	N.D.	
23) n-Tetradecane	0.000		0	N.D. d	
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.	
30) 2,4-Dinitrotoluene	0.000		0	N.D. d	
31) n-Hexadecane	0.000		0	N.D. d	
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.	
35) N-Nitrosodiphenylamine	0.000		0	N.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	0.000		0	N.D. d	
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.	
45) n-Eicosane	0.000		0	N.D. d	

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Dec 01 14:10:08 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

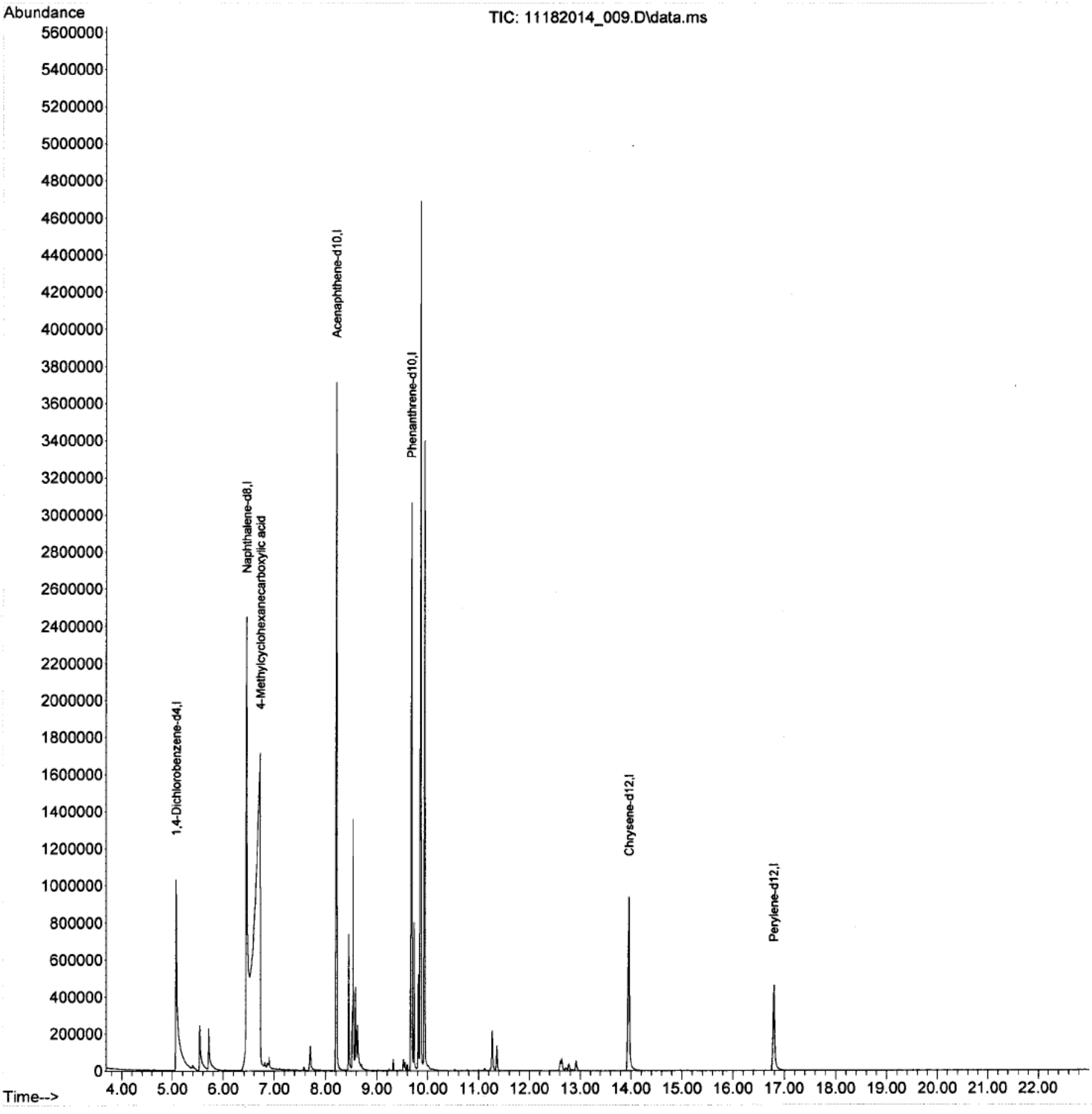
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	0.000		0	N.D.	
47) Pyrene	0.000		0	N.D.	
48) n-Docosane	0.000		0	N.D.	
50) Benzyl Butyl Phthalate	0.000		0	N.D.	
51) n-Tetracosane	0.000		0	N.D.	
52) n-Hexacosane	0.000		0	N.D. d	
53) n-Octacosane	0.000		0	N.D.	
54) Benz[a]anthracene	0.000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

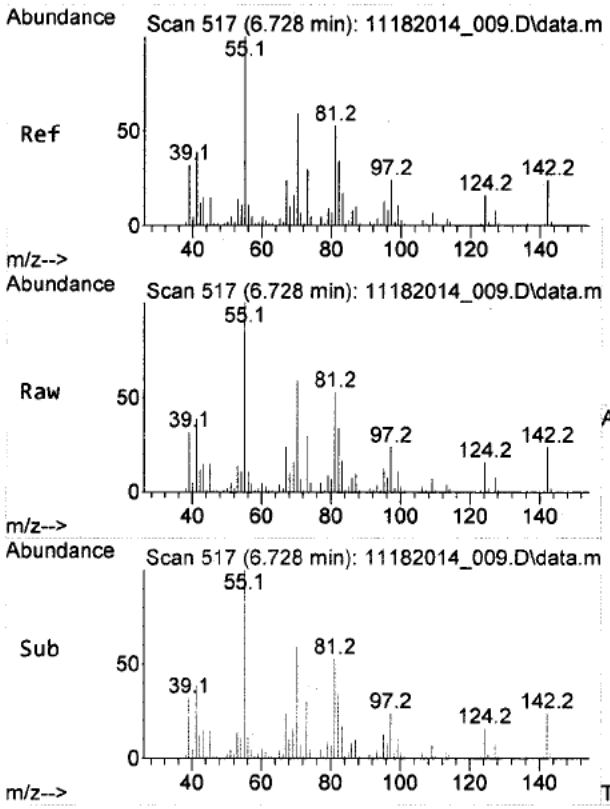
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Dec 01 14:10:08 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

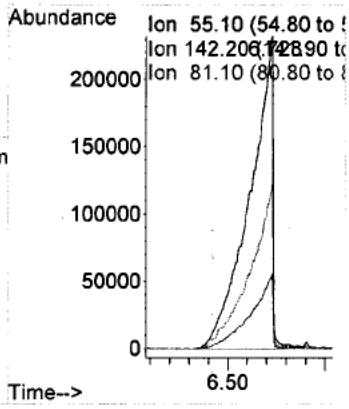




#12
4-Methylcyclohexanecarboxylic acid
Concen: 182.12 ug/mL
RT: 6.728 min Scan# 517
Delta R.T. 0.000 min
Lab File: 11182014_009.D
Acq: 18 Nov 2014 04:07 pm

Tgt Ion: 55 Resp: 1864197

Ion	Ratio	Lower	Upper
55	100		
142	22.5	19.1	28.7
81	51.0	42.3	63.5



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 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: 11182014_009.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.822	21	23	55	rVB7	5711	37491	0.29%	0.080%
2	5.075	229	236	285	rBV	1029061	2573972	20.03%	5.516%
3	5.398	285	291	307	rVB6	27800	84487	0.66%	0.181%
4	5.540	307	315	339	rBV	240250	493250	3.84%	1.057%
5	5.710	339	344	397	rVB	226038	509136	3.96%	1.091%
6	6.457	447	471	481	rBV	2448040	4658489	36.26%	9.983%
7	6.728	481	517	527	rVV2	1713056	12848563	100.00%	27.533%
8	6.810	527	531	537	rVV	44676	93055	0.72%	0.199%
9	6.904	537	547	577	rVV5	73312	245292	1.91%	0.526%
10	7.098	577	580	591	rVV8	10018	25609	0.20%	0.055%
11	7.181	591	594	601	rVV8	5452	13852	0.11%	0.030%
12	7.575	653	661	667	rBV	17794	19183	0.15%	0.041%
13	7.704	675	683	713	rBV	131186	239202	1.86%	0.513%
14	8.210	757	769	803	rBV	3715918	3830784	29.81%	8.209%
15	8.451	803	810	817	rVV	736561	604440	4.70%	1.295%
16	8.539	817	825	831	rVV	1356163	1539104	11.98%	3.298%
17	8.587	831	833	837	rVV	451765	442060	3.44%	0.947%
18	8.622	837	839	885	rVV	244185	476218	3.71%	1.020%
19	9.328	949	959	965	rVB	62705	54868	0.43%	0.118%
20	9.528	987	993	1001	rBV3	61108	117829	0.92%	0.252%
21	9.598	1001	1005	1011	rVB	37060	33417	0.26%	0.072%
22	9.681	1011	1019	1023	rBV	3067134	3513785	27.35%	7.530%
23	9.728	1023	1027	1037	rVV	800973	798484	6.21%	1.711%
24	9.863	1037	1050	1057	rVV	4689551	5734545	44.63%	12.289%
25	9.933	1057	1062	1117	rVB	3398576	3678006	28.63%	7.882%
26	11.122	1255	1264	1277	rVB5	11822	23279	0.18%	0.050%
27	11.269	1277	1289	1299	rBV2	215223	337361	2.63%	0.723%
28	11.357	1299	1304	1327	rVB	134548	184112	1.43%	0.395%
29	12.639	1499	1522	1529	rVV2	65974	199807	1.56%	0.428%
30	12.722	1529	1536	1539	rVV4	14367	36446	0.28%	0.078%
31	12.769	1539	1544	1553	rVV	39089	71864	0.56%	0.154%
32	12.916	1563	1569	1593	rVB	53066	95430	0.74%	0.204%
33	13.957	1735	1746	1797	rVV	941101	1983176	15.44%	4.250%
34	16.798	2215	2229	2285	rBV	461730	1068672	8.32%	2.290%

LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 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

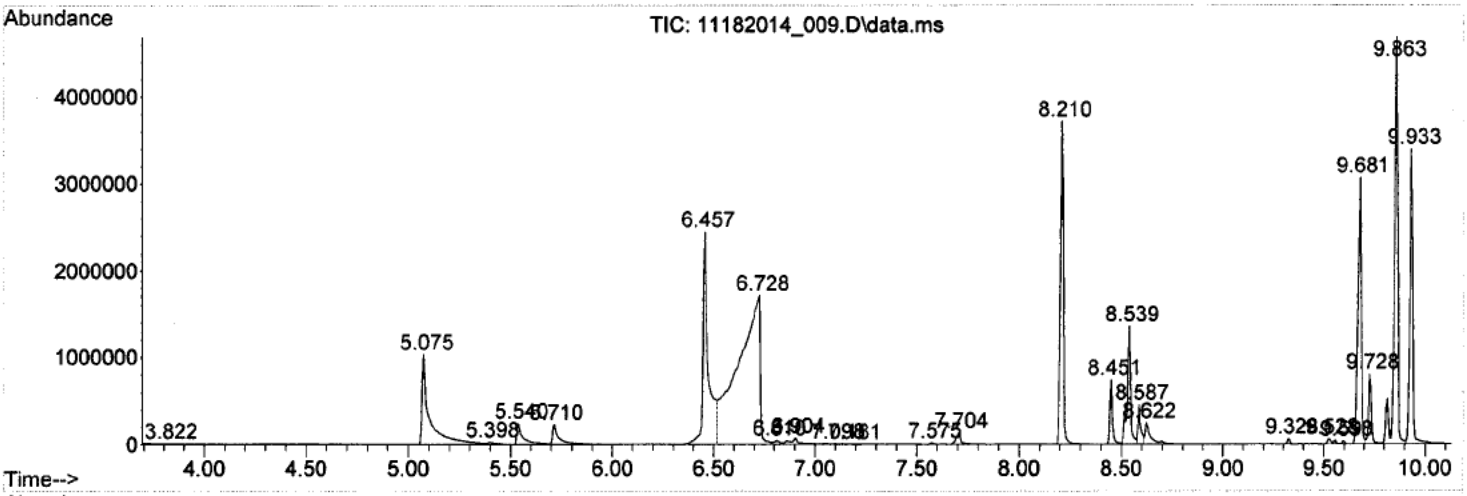
Sum of corrected areas: 46665268

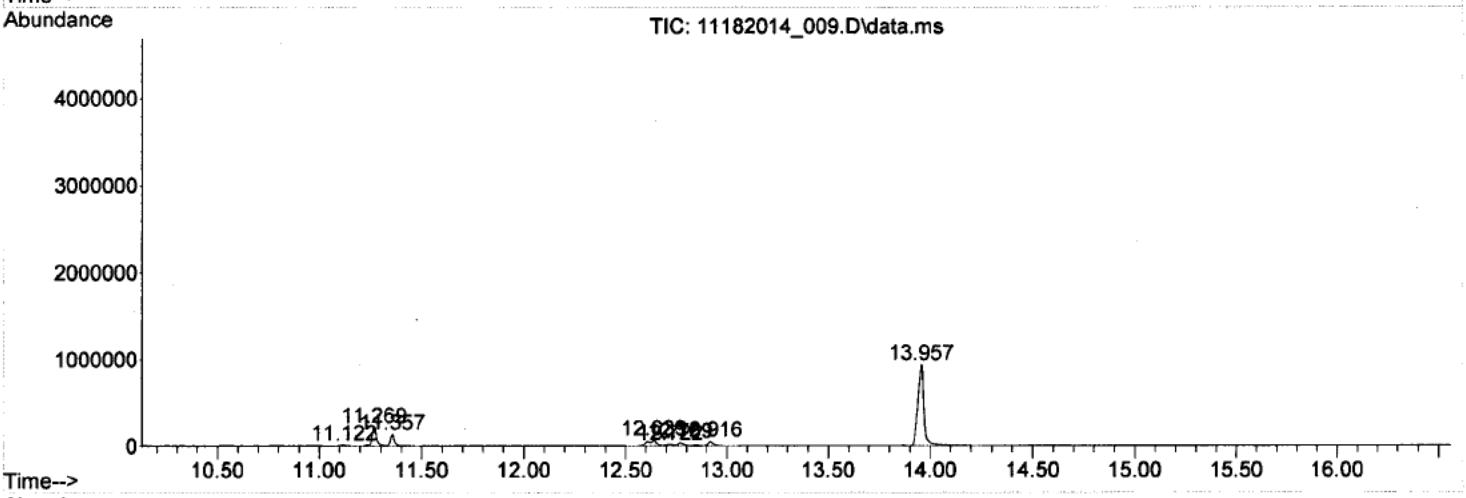
LSC Report - Integrated Chromatogram

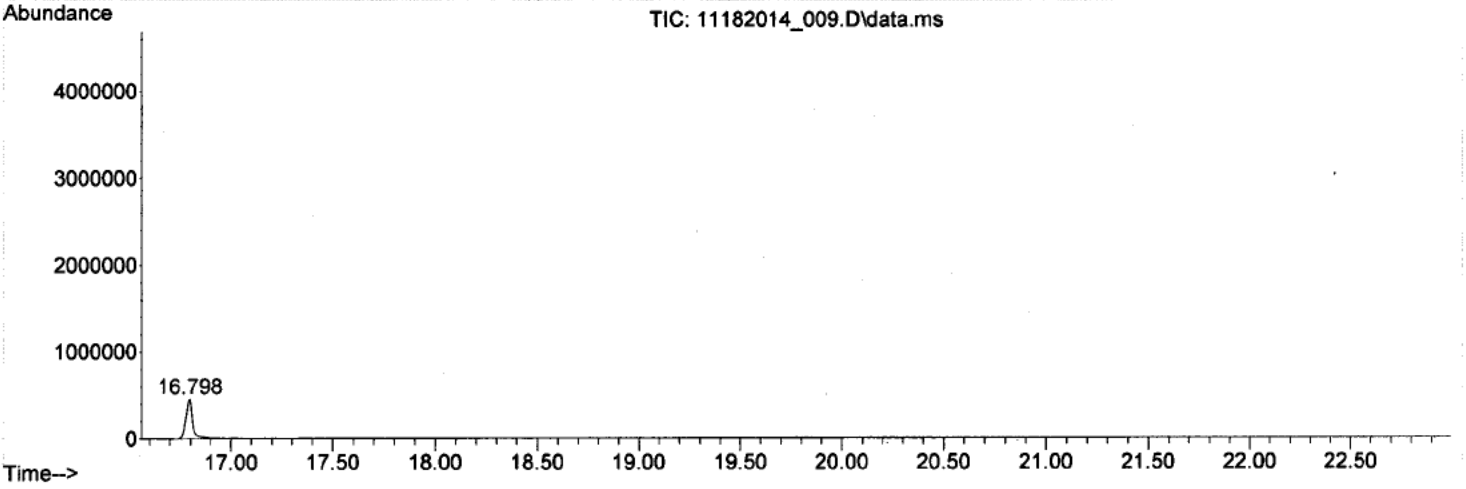
Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

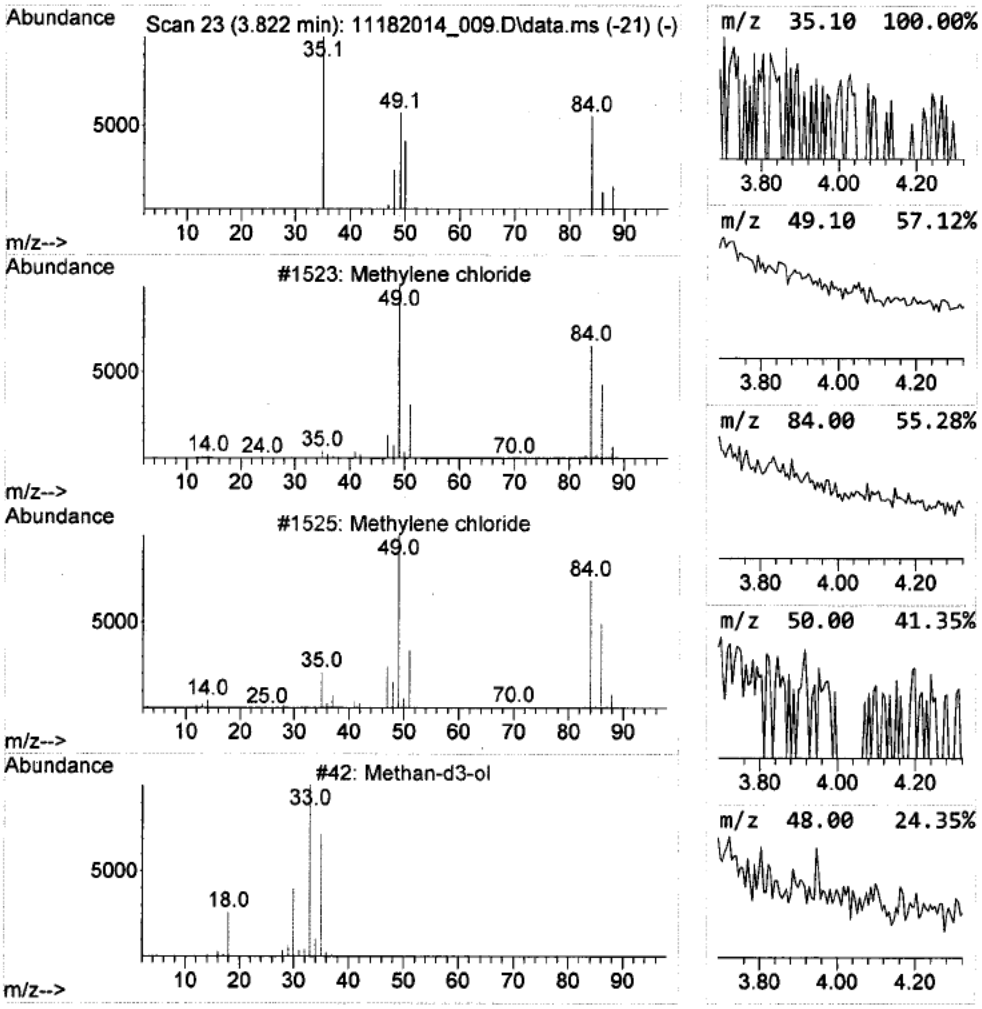
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 1 Methylene chloride Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.822	0.29 ug/mL	37491	1,4-Dichlorobenzene-d4	5.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylene chloride	84	CH2Cl2	000075-09-2	7
2	Methylene chloride	84	CH2Cl2	000075-09-2	7
3	Methan-d3-ol	35	CHD3O	001849-29-2	4
4	Methylene chloride	84	CH2Cl2	000075-09-2	4
5	Methan-d3-ol	35	CHD3O	001849-29-2	3



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

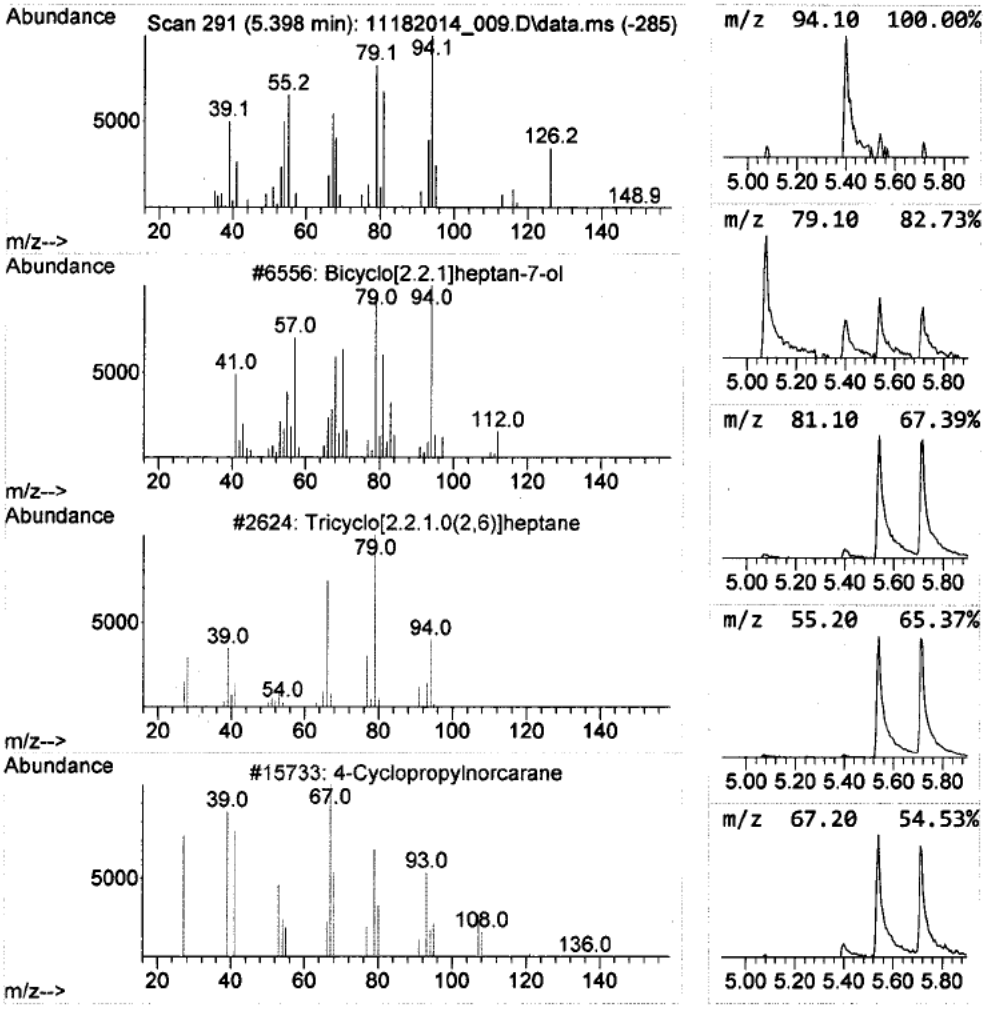
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 2 Bicyclo[2.2.1]heptan-7-ol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.398	0.66 ug/mL	84487	1,4-Dichlorobenzene-d4	5.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-7-ol	112	C7H12O	002566-48-5	47
2	Tricyclo[2.2.1.0(2,6)]heptane	94	C7H10	000279-19-6	43
3	4-Cyclopropylnorcarane	136	C10H16	1000222-73-9	35
4	Pentanal, 5-(methylenecyclopropyl)-	138	C9H14O	1000158-49-1	35
5	Oxirane, 5-hexenyl-	126	C8H14O	019600-63-6	27



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Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

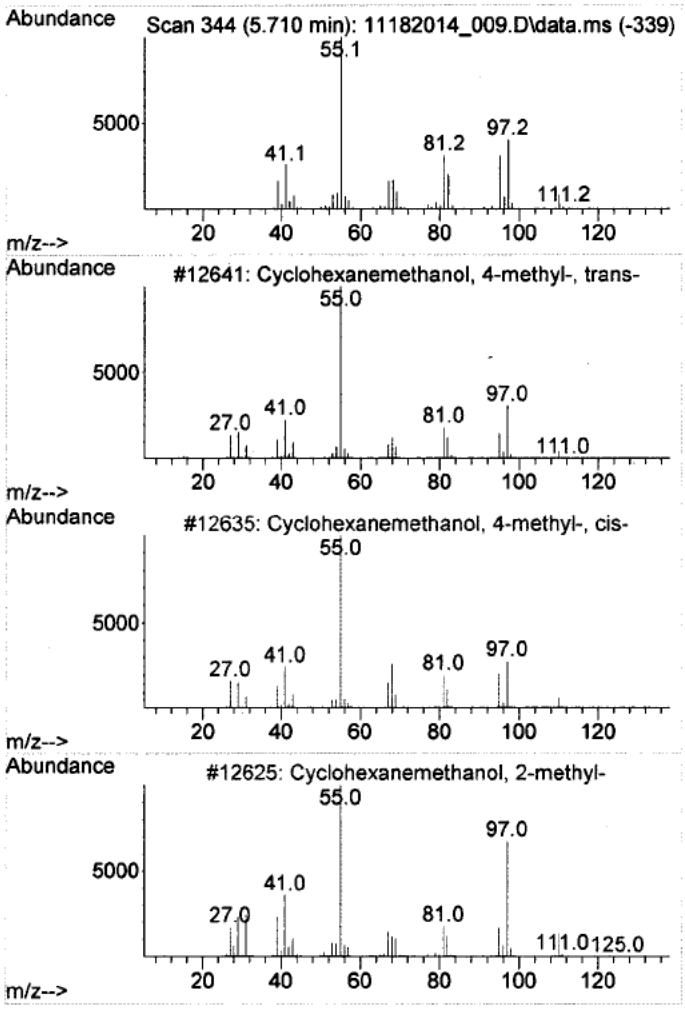
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

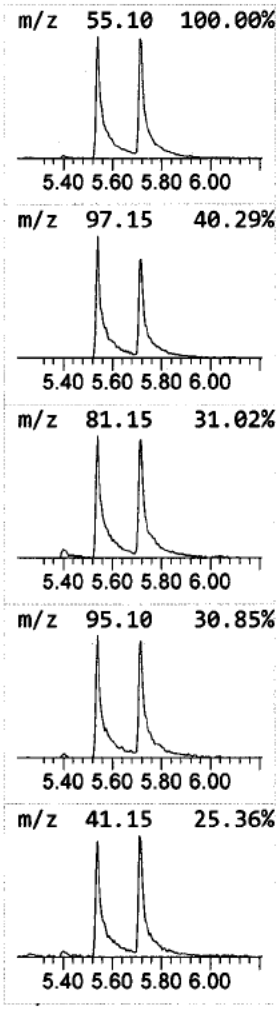
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.710	3.96 ug/mL	509136	1,4-Dichlorobenzene-d4	5.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	83
2	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	72
3	Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	59
4	Oxalic acid, di(cyclohexylmethyl...	282	C16H2604	1000309-68-5	50
5	Oxalic acid, cyclohexylmethyl et...	214	C11H1804	1000309-68-0	50





Library Search Compound Report

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Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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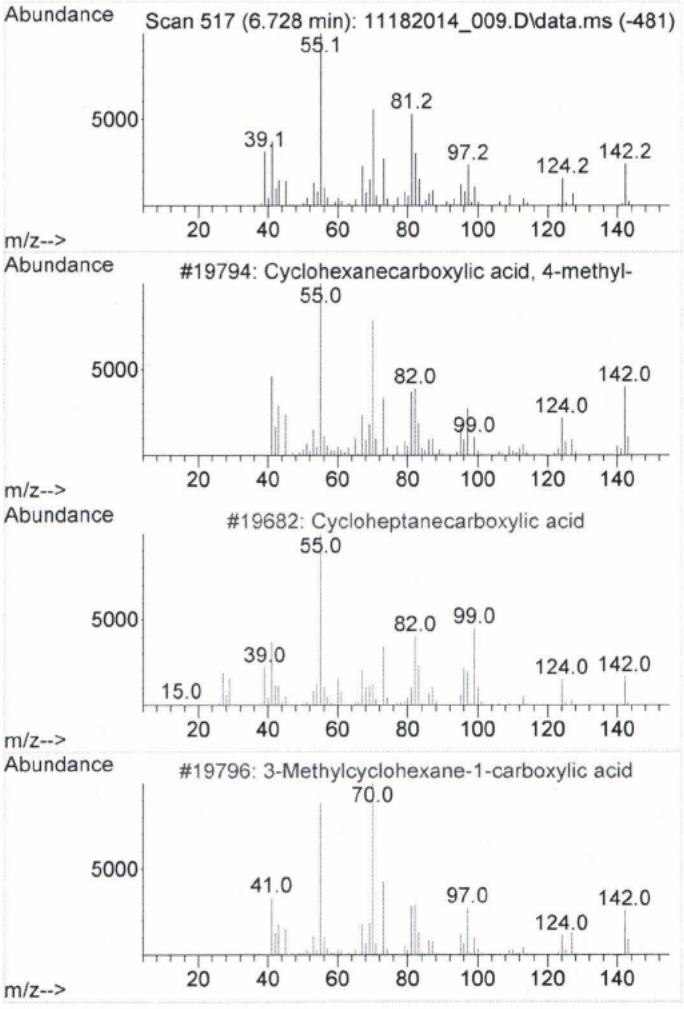
Quant Title : RP1616-MCHM Compounds

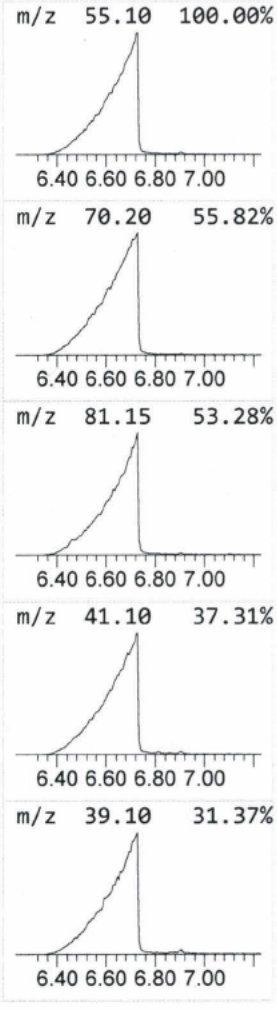
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	55.16 ug/mL	12848600	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	38
4	3-Pyrrolidin-2-yl-propionic acid	143	C7H13NO2	1000193-88-0	25
5	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	25





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Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

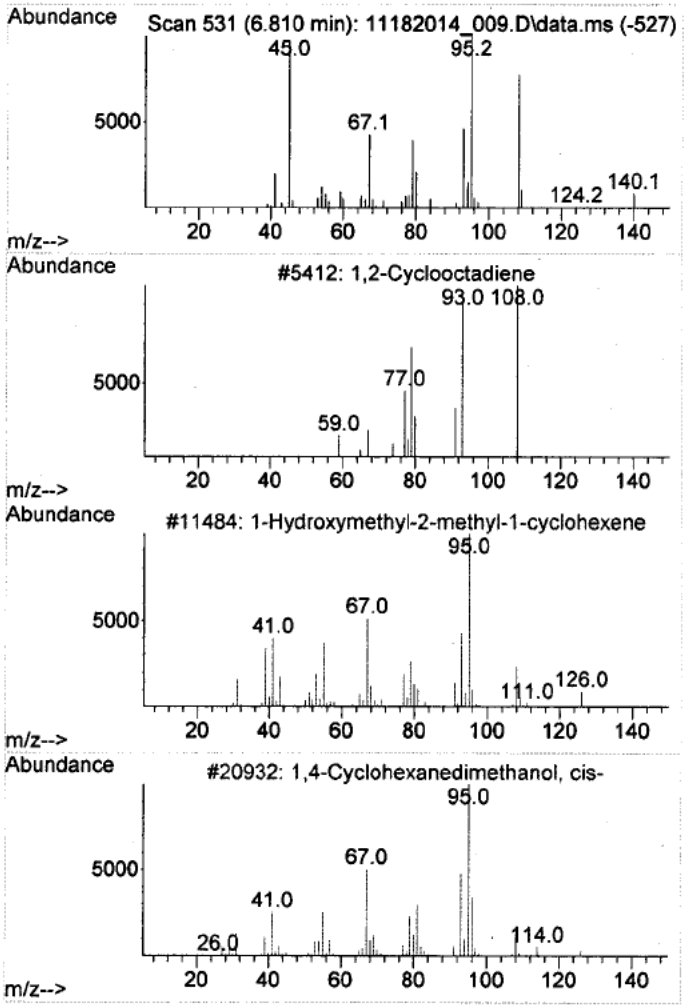
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

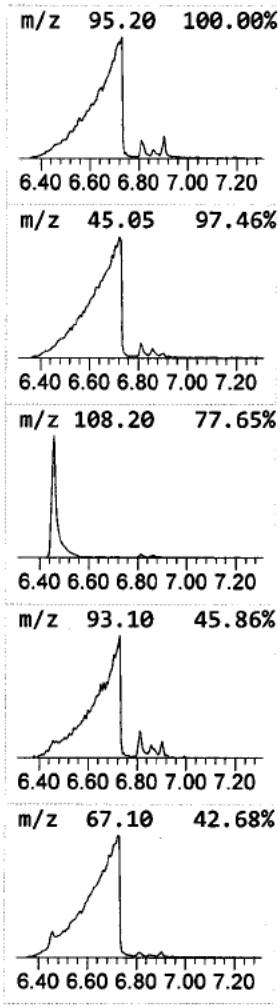
****

Peak Number 5 1,2-Cyclooctadiene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.810	0.40 ug/mL	93055	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclooctadiene	108	C8H12	007124-40-5	38
2	1-Hydroxymethyl-2-methyl-1-cyclo...	126	C8H14O	029474-11-1	25
3	1,4-Cyclohexanedimethanol, cis-	144	C8H16O2	003236-47-3	23
4	exo-2-Bromonorbornane	174	C7H11Br	002534-77-2	14
5	2,3,4-Hexatriene, 2,5-dimethyl-	108	C8H12	002431-31-4	12





Library Search Compound Report

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Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

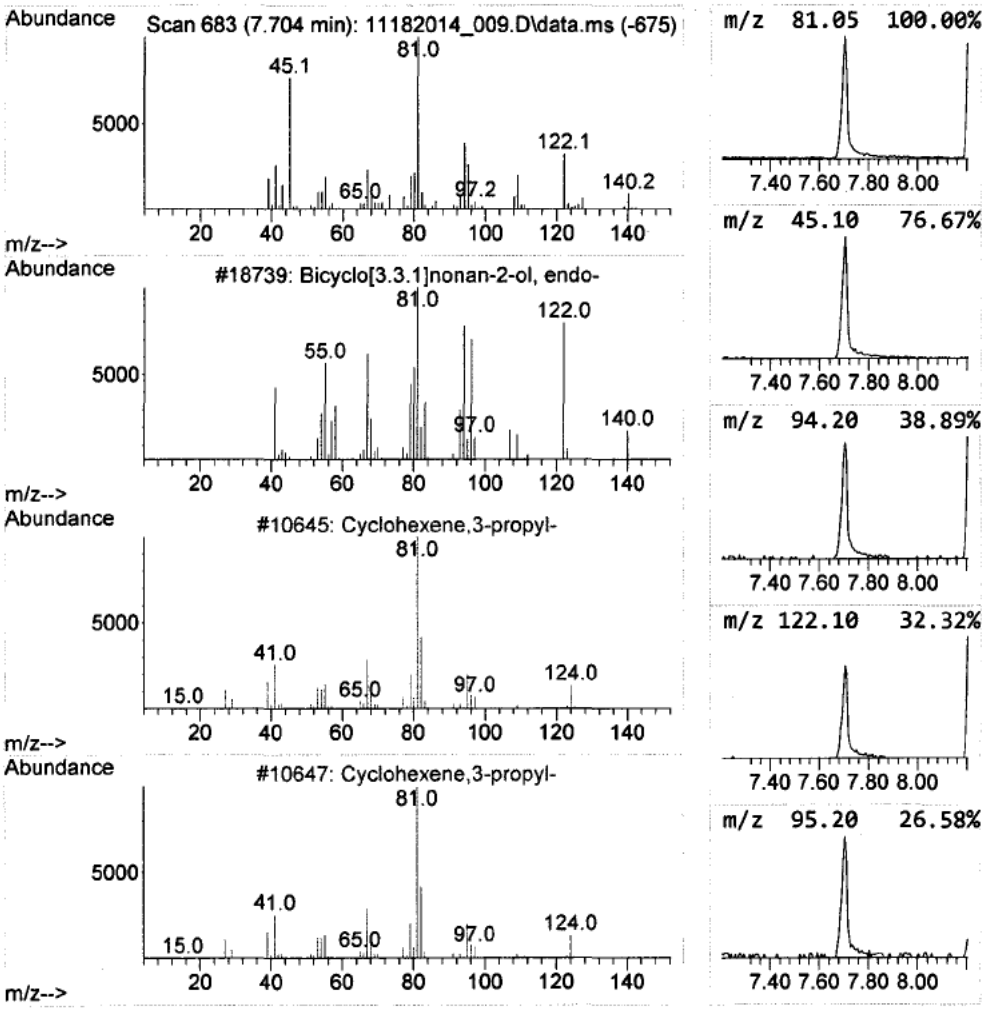
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 6 Bicyclo[3.3.1]nonan-2-ol, e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.704	1.25 ug/mL	239202	Acenaphthene-d10	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.3.1]nonan-2-ol, endo-	140	C9H16O	010036-25-6	38
2	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	27
3	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	27
4	Cyclohexene, 3-(1-methylethyl)-	124	C9H16	003983-08-2	27
5	Cyclohexene,3-(2-propenyl)-	122	C9H14	015232-95-8	22



Library Search Compound Report

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Operator : DBH
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Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

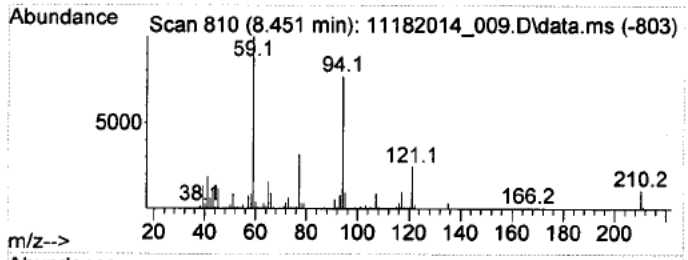
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

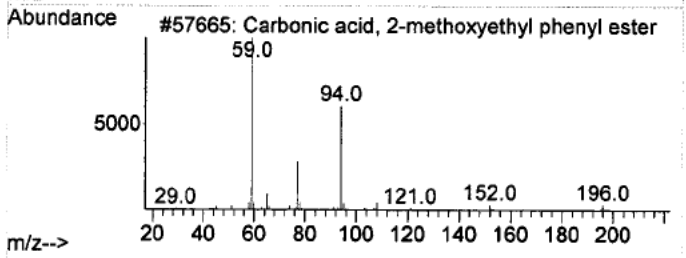
****

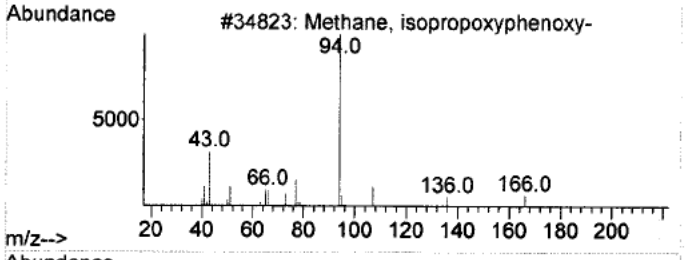
Peak Number 7 Carbonic acid, 2-methoxyeth... Concentration Rank 5

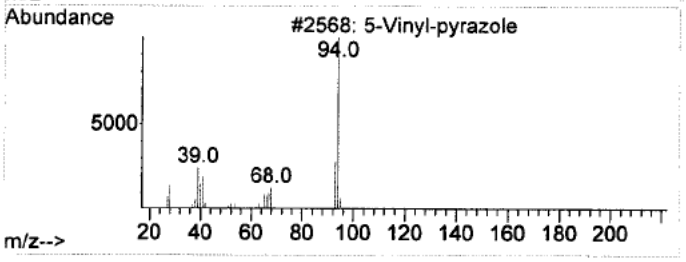
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	3.16 ug/mL	604440	Acenaphthene-d10	8.210

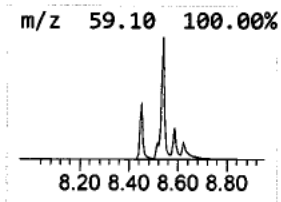
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	50
2	Methane, isopropoxyphenoxy-	166	C10H14O2	000828-12-6	38
3	5-Vinyl-pyrazole	94	C5H6N2	1000288-36-8	27
4	Benzene, [(3-methyl-2-butenyl)oxy]-	162	C11H14O	014309-15-0	27
5	Fampridine	94	C5H6N2	000504-24-5	27

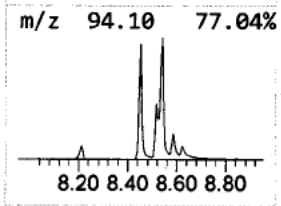


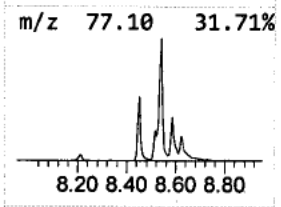


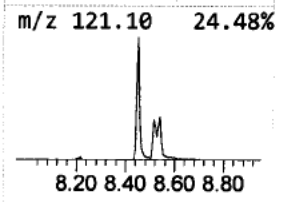


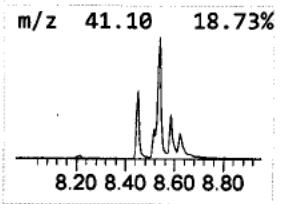












Library Search Compound Report

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Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

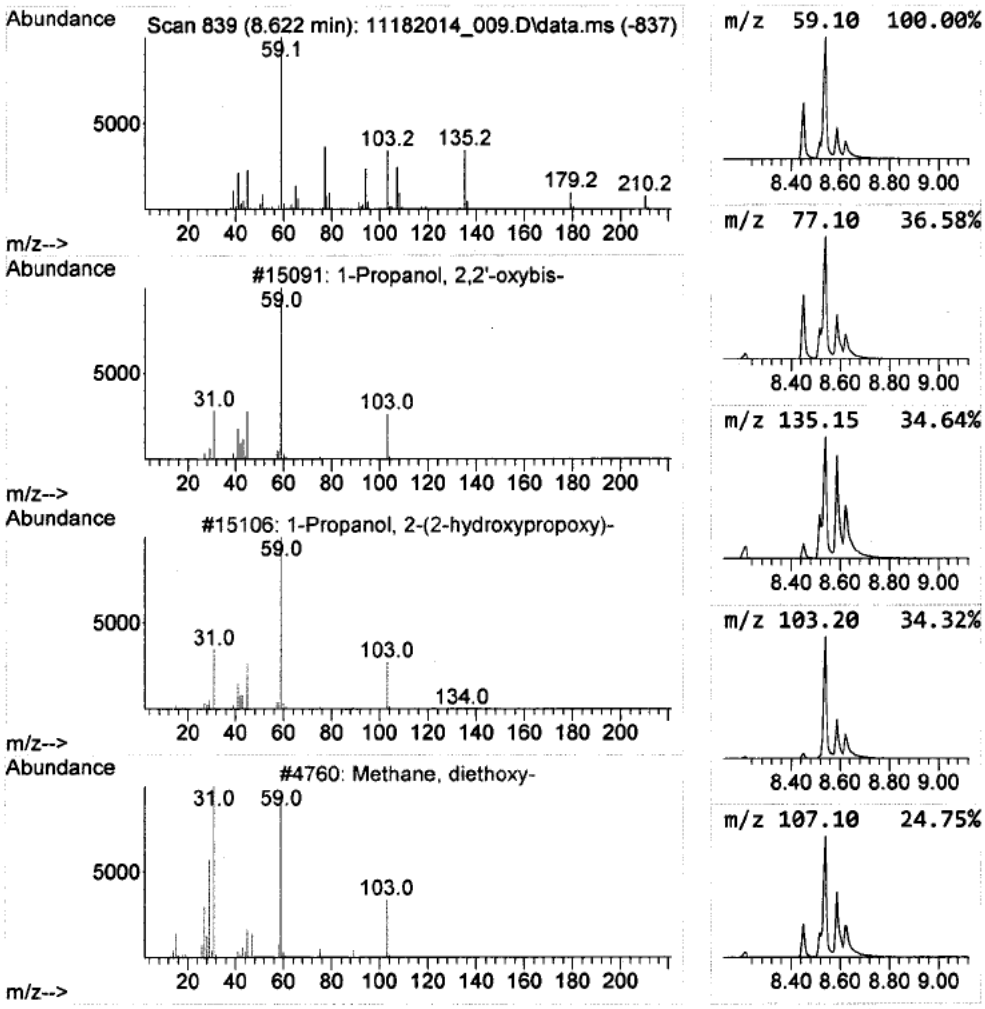
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 8 1-Propanol, 2,2'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	2.49 ug/mL	476218	Acenaphthene-d10	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	38
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	38
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	38
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	35
5	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	32



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Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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Quant Title : RP1616-MCHM Compounds

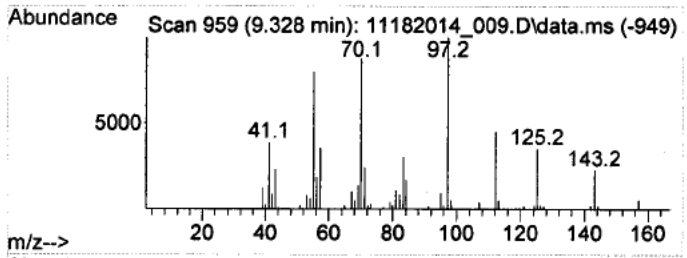
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

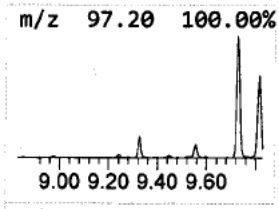
****

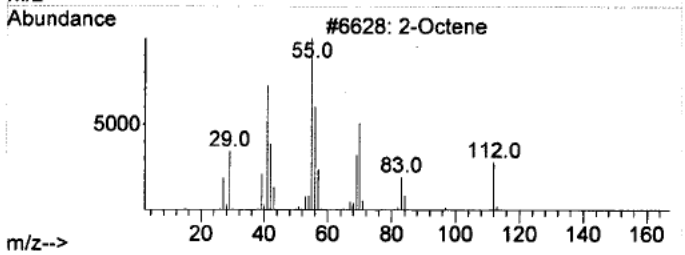
Peak Number 9 2-Octene Concentration Rank 17

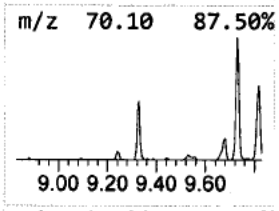
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	0.31 ug/mL	54868	Phenanthrene-d10	9.681

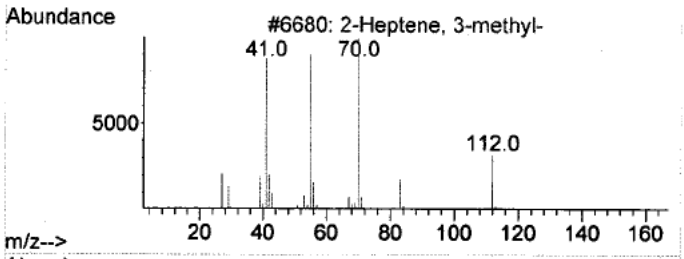
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene	112	C8H16	000111-67-1	38
2	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	38
3	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	38
4	4-Undecen-6-one	168	C11H20O	032064-74-7	38
5	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	35

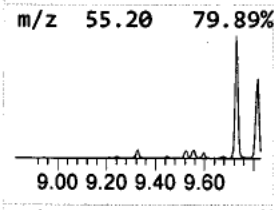


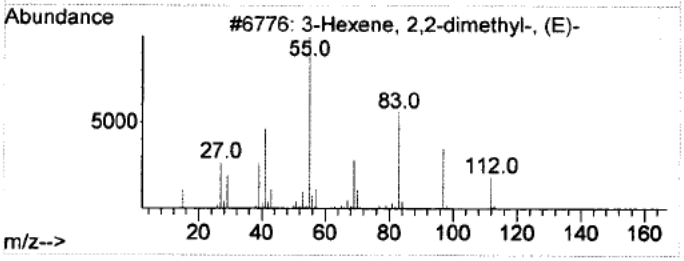


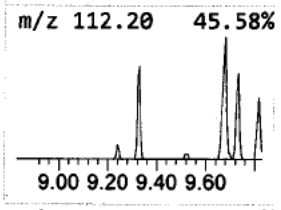


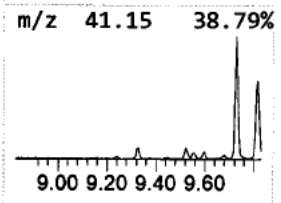












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Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

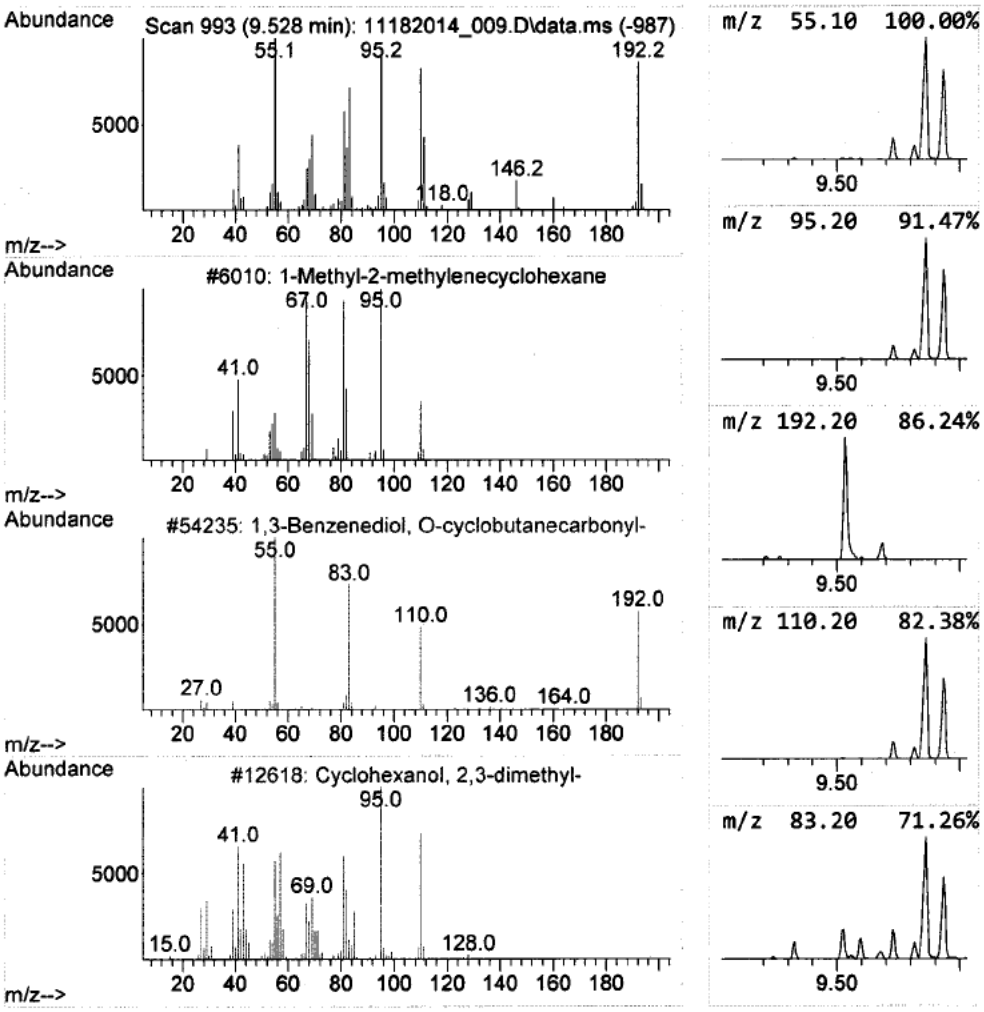
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 10 1-Methyl-2-methylenecyclohe... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	0.67 ug/mL	117829	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	45
2	1,3-Benzenediol, O-cyclobutaneca...	192	C11H12O3	1000345-51-7	43
3	Cyclohexanol, 2,3-dimethyl-	128	C8H16O	001502-24-5	38
4	Cyclohexanol, 2,3-dimethyl-	128	C8H16O	001502-24-5	35
5	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	35



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Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

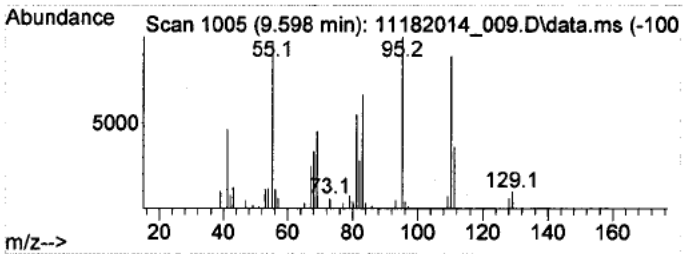
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

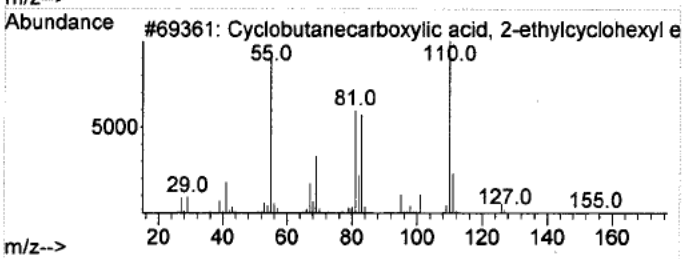
****

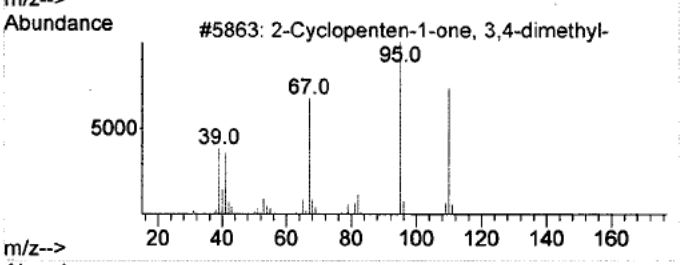
Peak Number 11 Cyclobutanecarboxylic acid,... Concentration Rank 19

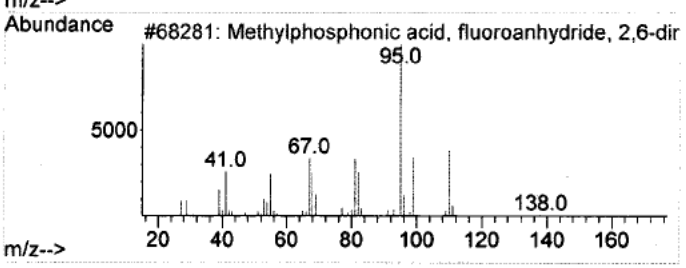
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	0.19 ug/mL	33417	Phenanthrene-d10	9.681

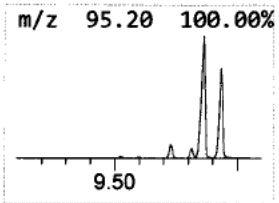
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanecarboxylic acid, 2-et...	210	C13H22O2	1000282-61-0	47
2	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
3	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	42
4	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	40
5	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	40

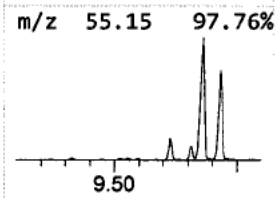


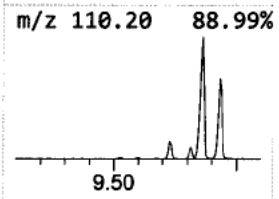


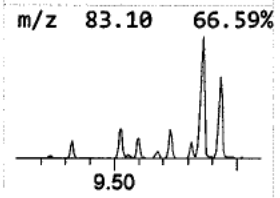


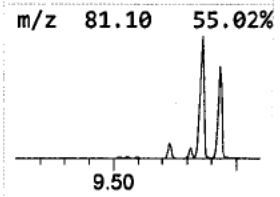












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

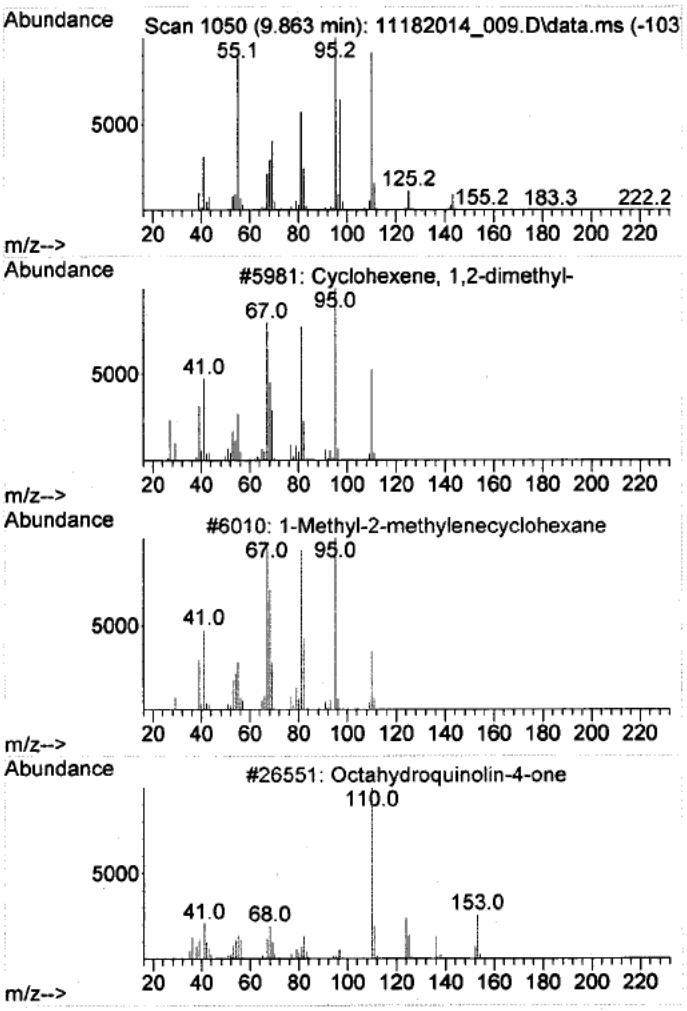
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

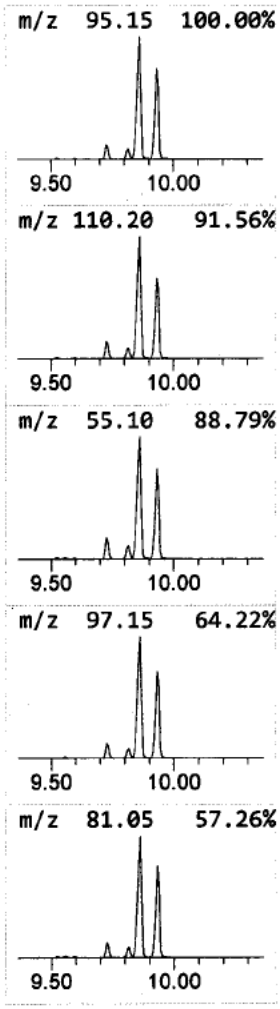
****

Peak Number 12 Cyclohexene, 1,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.863	32.64 ug/mL	5734550	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	53
2	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	53
3	Octahydroquinolin-4-one	153	C9H15NO	1000302-88-0	43
4	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	43
5	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	42





Library Search Compound Report

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Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

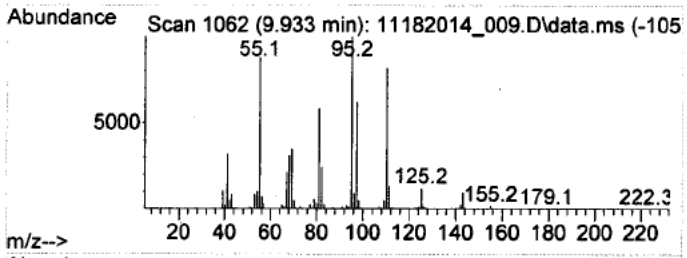
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

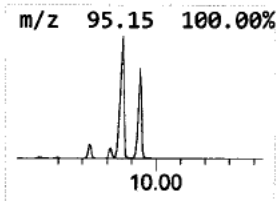
****

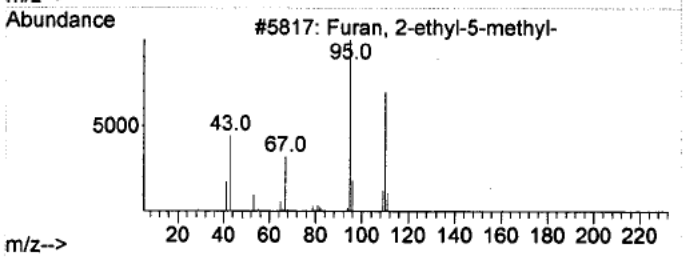
Peak Number 13 Furan, 2-ethyl-5-methyl- Concentration Rank 3

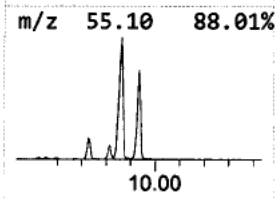
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.933	20.93 ug/mL	3678010	Phenanthrene-d10	9.681

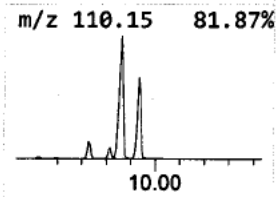
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	47
2	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	43
4	Cyclohexane, 1-methyl-4-(2-hydro...	142	C9H18O	004916-87-4	38
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	38

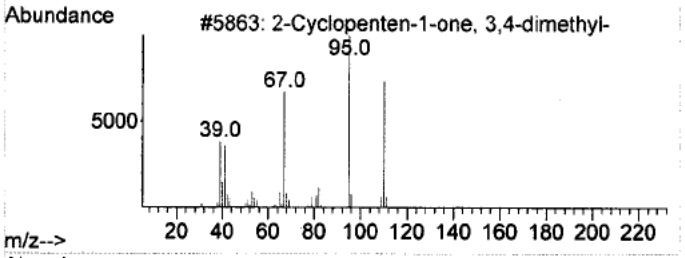


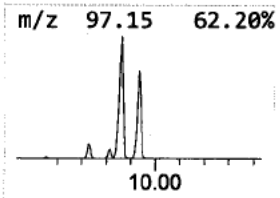


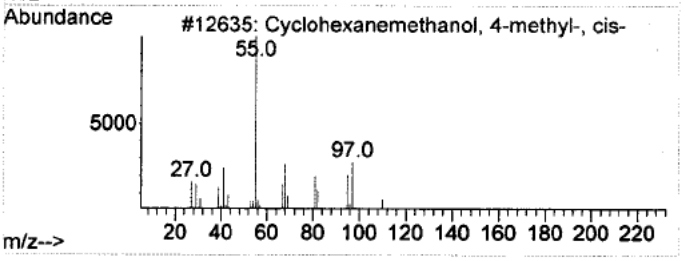


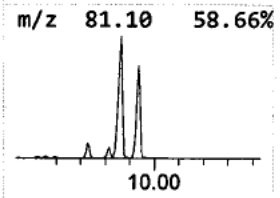












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

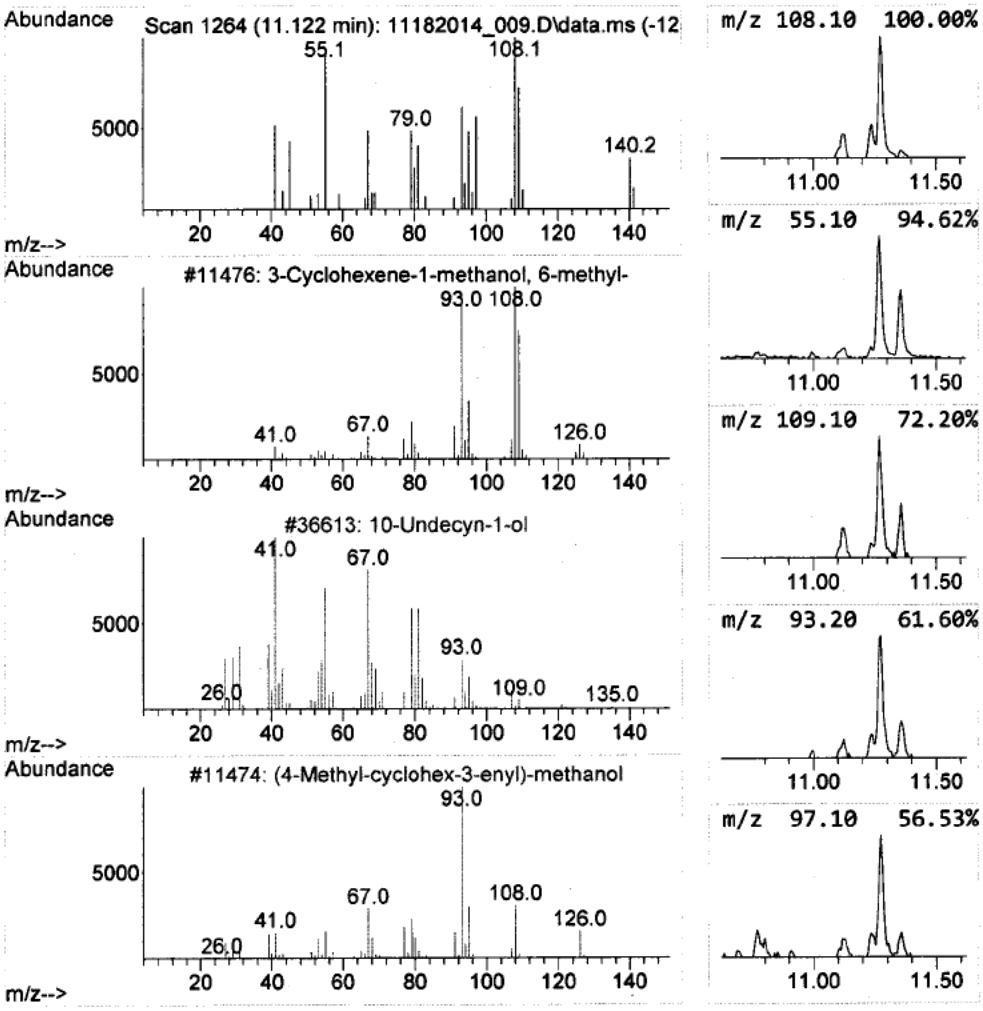
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 14 3-Cyclohexene-1-methanol, 6... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.122	0.13 ug/mL	23279	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-methanol, 6-methyl-	126	C8H14O	005259-31-4	40
2	10-Undecyn-1-ol	168	C11H20O	002774-84-7	32
3	(4-Methyl-cyclohex-3-enyl)-methanol	126	C8H14O	089690-46-0	32
4	1H-Pyrrole, 2,3,5-trimethyl-	109	C7H11N	002199-41-9	27
5	1,2,5-Trimethylpyrrole	109	C7H11N	000930-87-0	27



Library Search Compound Report

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Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

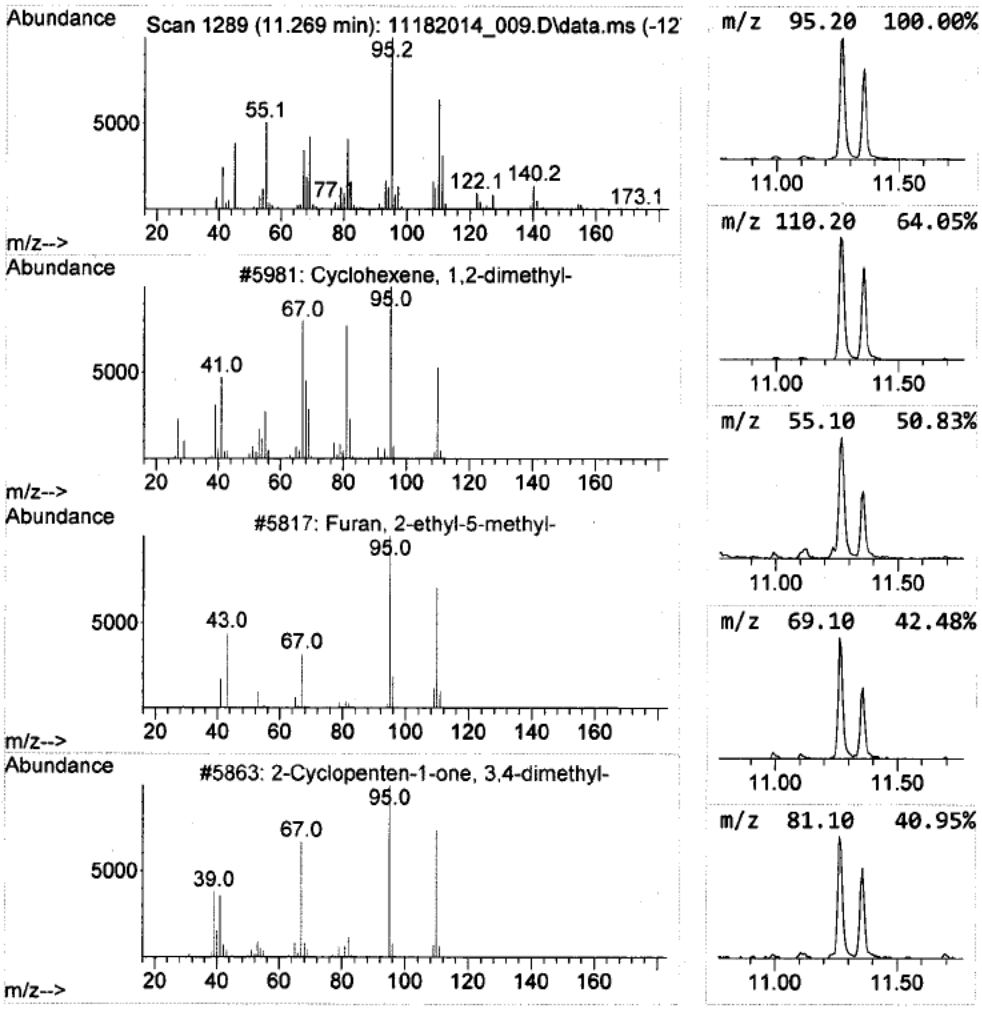
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 15 Cyclohexene, 1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	1.92 ug/mL	337361	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	46
2	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	46
3	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
4	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	43
5	Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	43



Library Search Compound Report

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Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

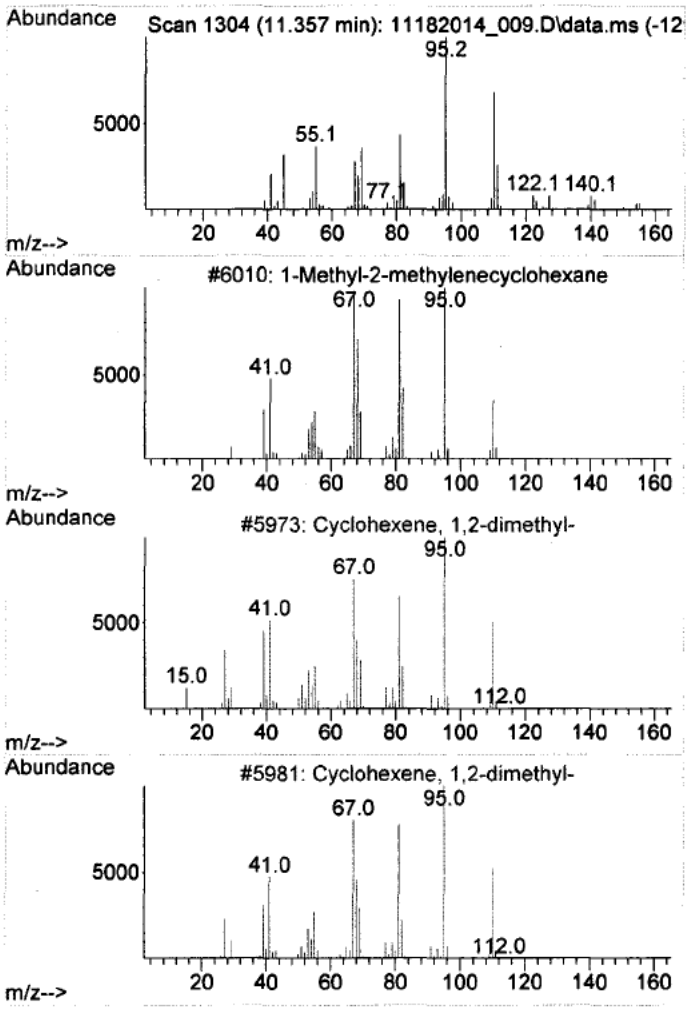
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

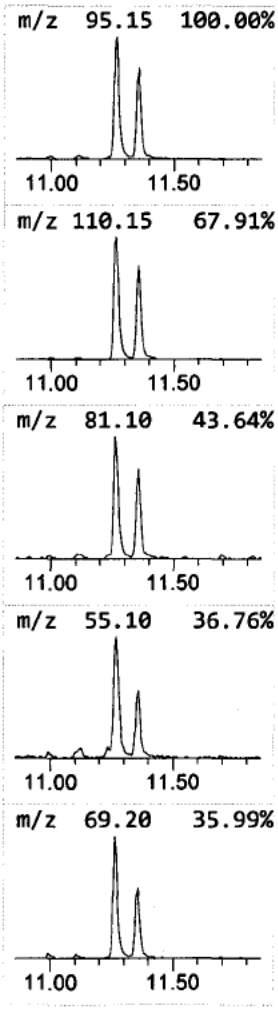
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 16 1-Methyl-2-methylenecyclohe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.357	1.05 ug/mL	184112	Phenanthrene-d10	9.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	76
2	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	62
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	62
4	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	50
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	50





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Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

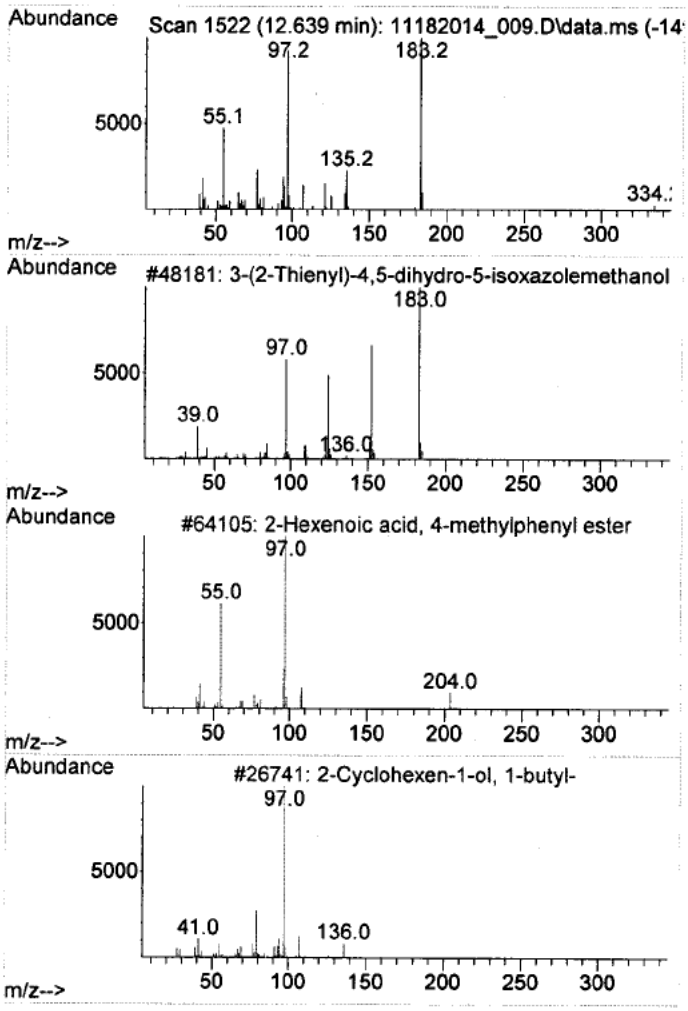
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

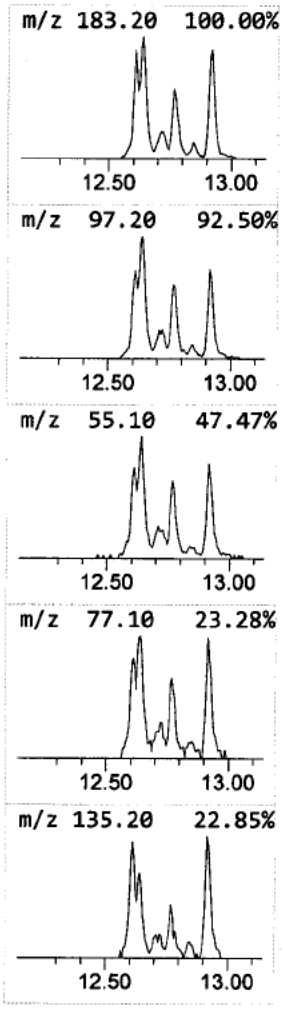
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 17 3-(2-Thienyl)-4,5-dihydro-5... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.02 ug/mL	199807	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Thienyl)-4,5-dihydro-5-isox...	183	C8H9NO2S	022353-85-1	47
2	2-Hexenoic acid, 4-methylphenyl ...	204	C13H16O2	069687-91-8	22
3	2-Cyclohexen-1-ol, 1-butyl-	154	C10H18O	088116-46-5	22
4	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	22
5	Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	14





Library Search Compound Report

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Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

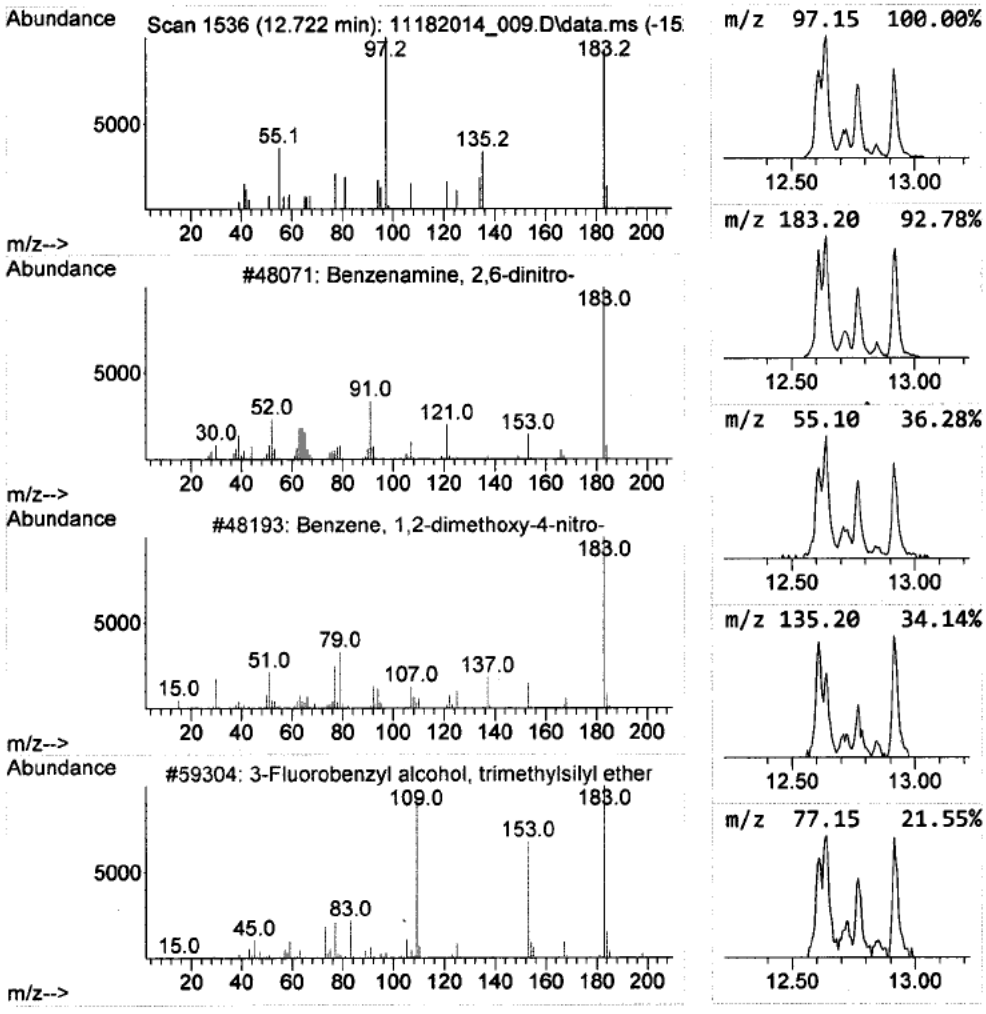
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 18 Benzenamine, 2,6-dinitro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	0.37 ug/mL	36446	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,6-dinitro-	183	C6H5N3O4	000606-22-4	27
2	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	25
3	3-Fluorobenzyl alcohol, trimethy...	198	C10H15FOSi	1000365-10-1	16
4	5-Hydroxy-2-nitrobenzoic acid	183	C7H5NO5	000610-37-7	16
5	Benzene, 1,3-dimethoxy-2-nitro-	183	C8H9NO4	006665-97-0	16



Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

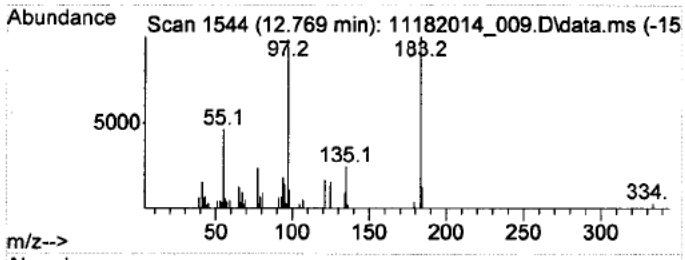
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

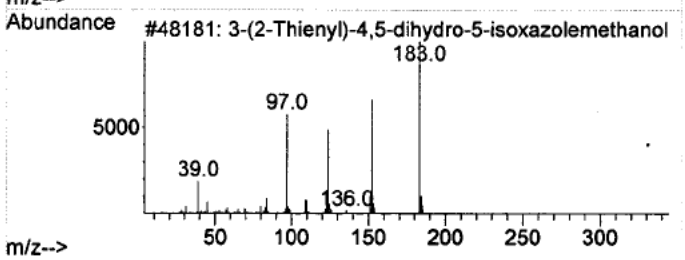
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

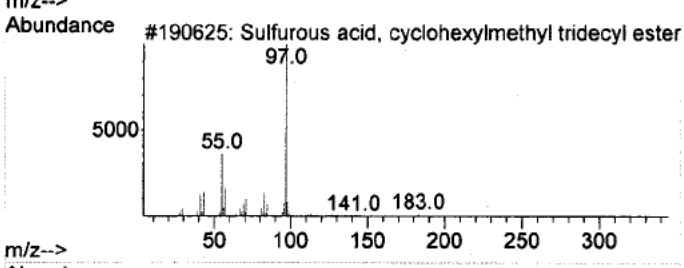
****
Peak Number 19 3-(2-Thienyl)-4,5-dihydro-5... Concentration Rank 12

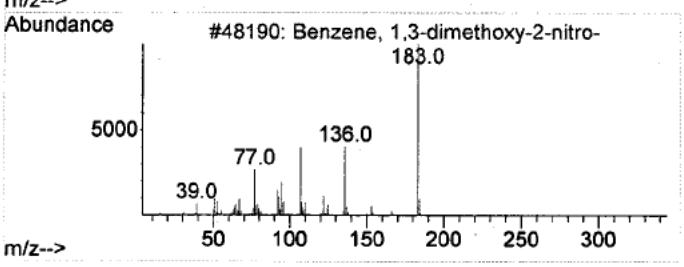
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	0.72 ug/mL	71864	Chrysene-d12	13.963

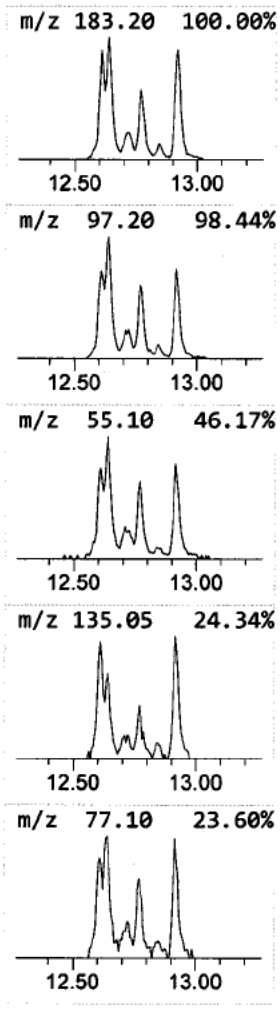
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Thienyl)-4,5-dihydro-5-isox...	183	C8H9NO2S	022353-85-1	58
2	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	40
3	Benzene, 1,3-dimethoxy-2-nitro-	183	C8H9NO4	006665-97-0	38
4	5,8-Methano-4H-3,1-benzoxazine-2...	183	C9H13NOS	1000142-76-8	27
5	2-Thiopheneacetic acid, isopropy...	184	C9H12O2S	068100-13-0	27











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

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

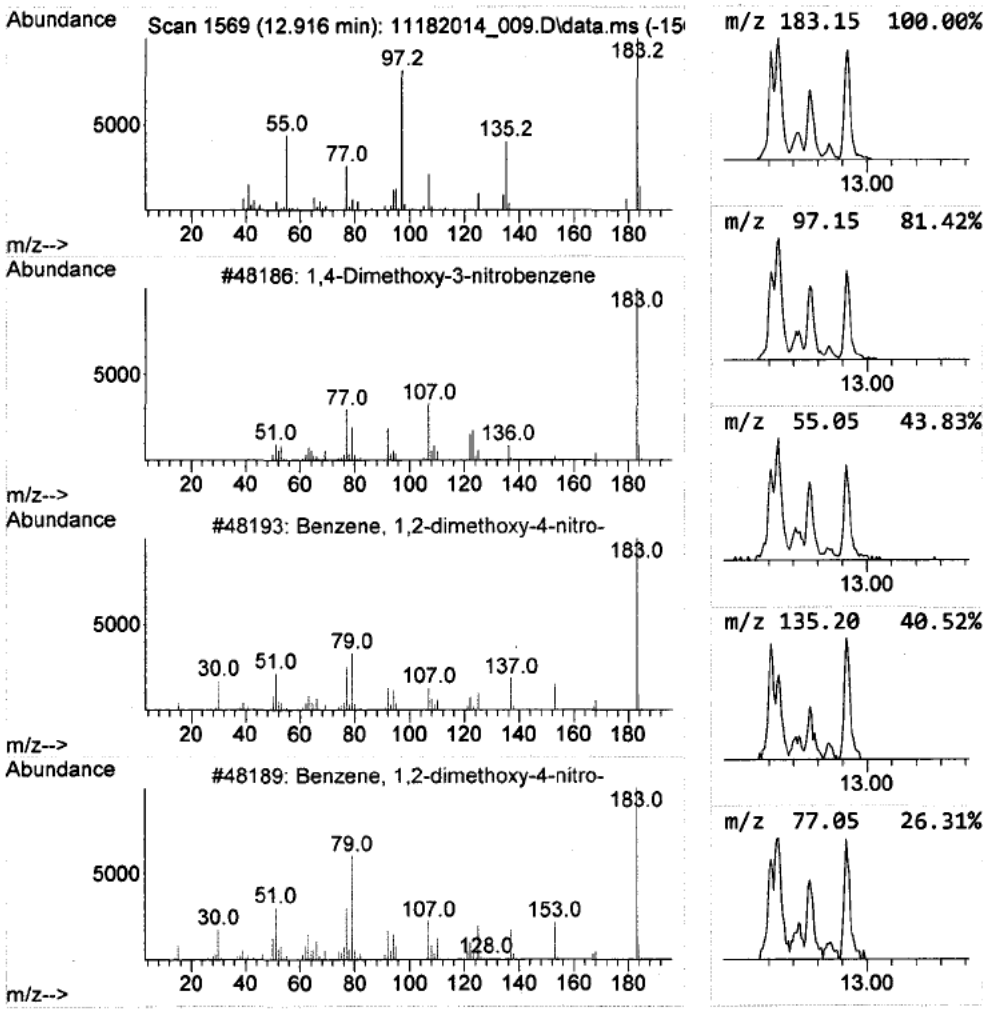
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 20 1,4-Dimethoxy-3-nitrobenzene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	0.96 ug/mL	95430	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethoxy-3-nitrobenzene	183	C8H9NO4	000089-39-4	17
2	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	16
3	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	16
4	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	12
5	Methyl benzilate	242	C15H14O3	000076-89-1	12



Tentatively Identified Compound (LSC) summary

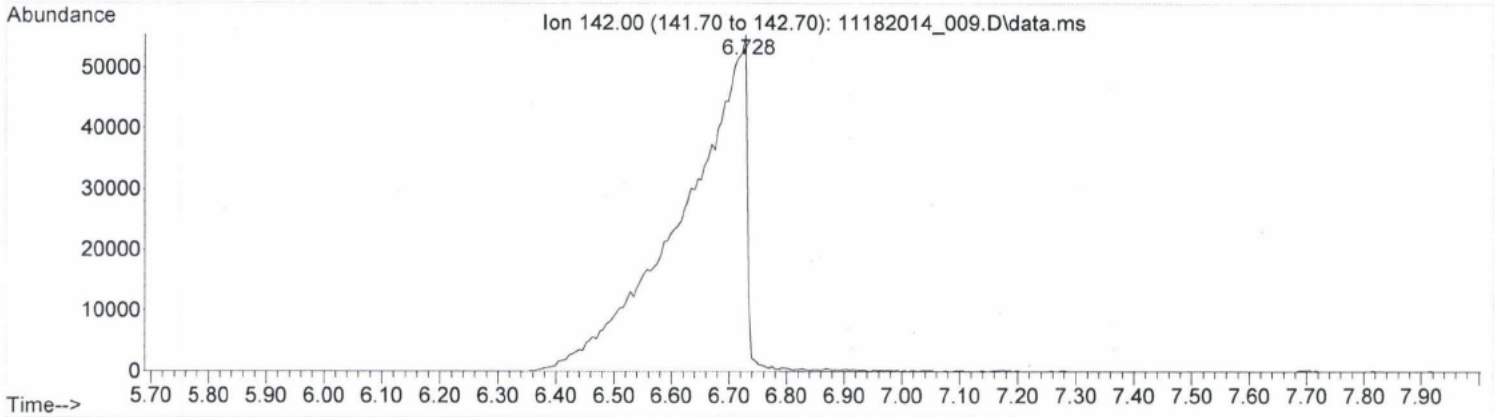
Data Path : D:\[redacted]\RP1616\11182014_Run\
Data File : 11182014_009.D
Acq On : 18 Nov 2014 04:07 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 100X
ALS Vial : 7 Sample Multiplier: 1

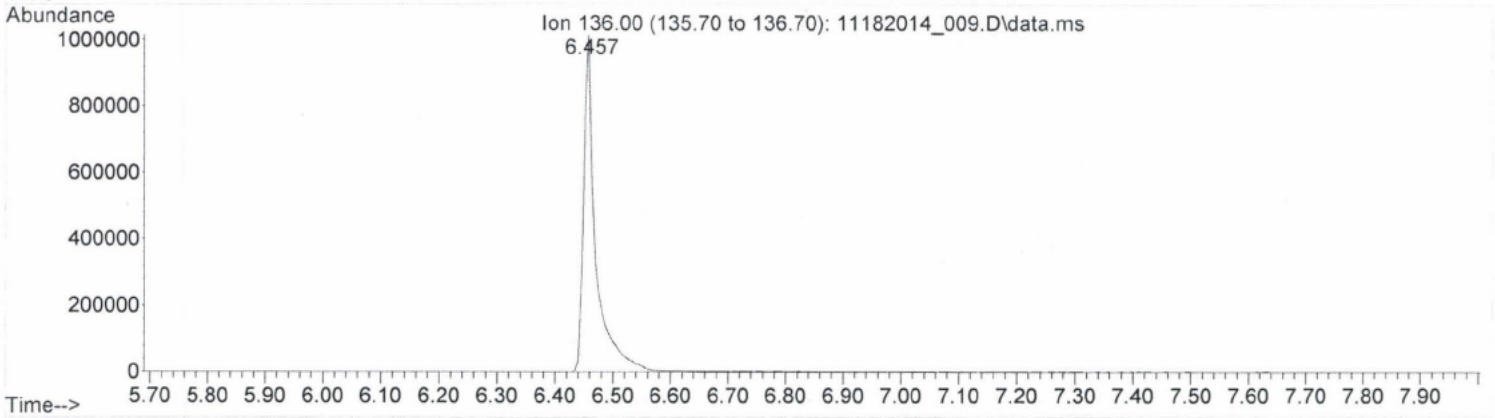
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

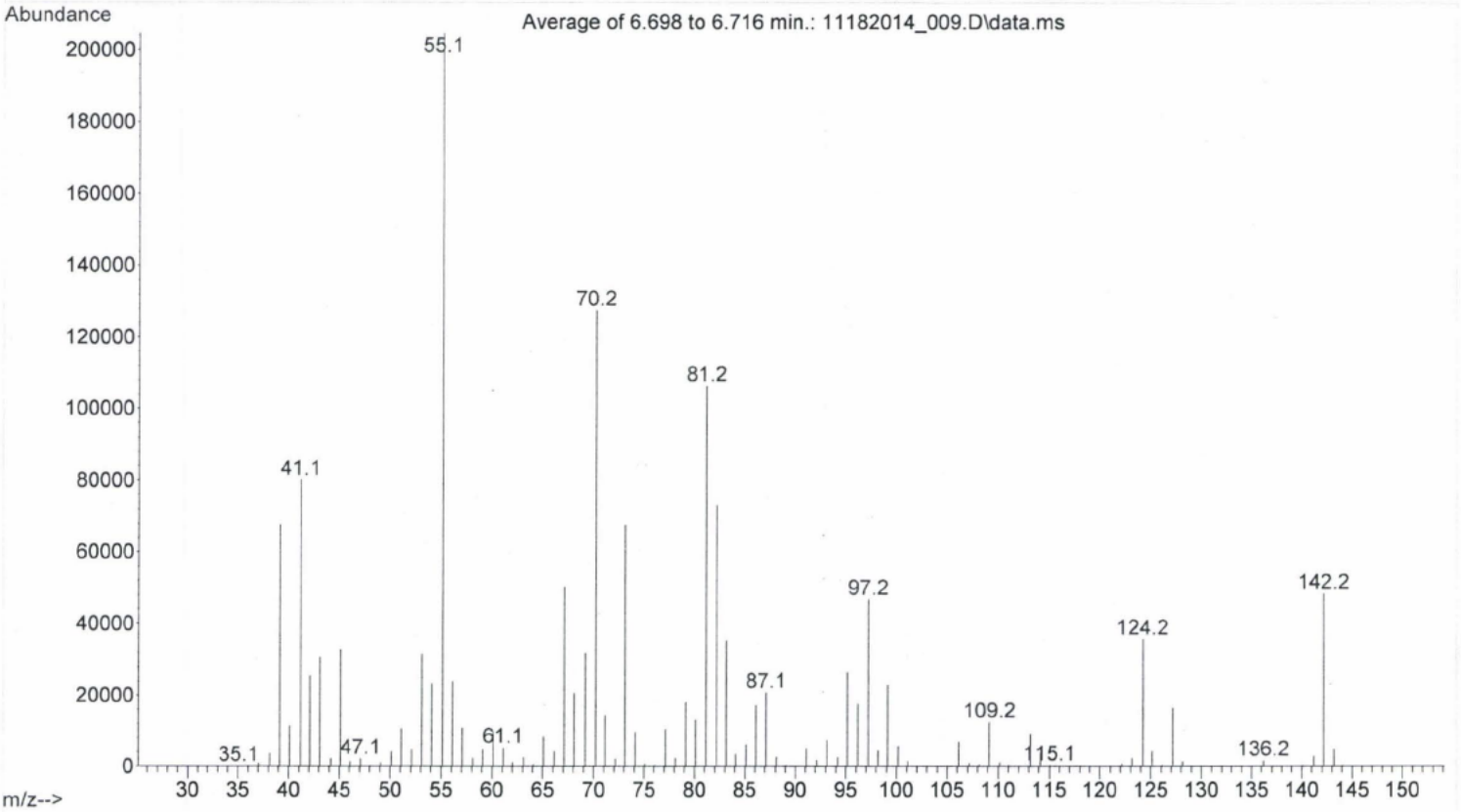
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Methylene chloride	3.822	0.3	ug/mL	37491	1	5.075	2573970	20.0
Bicyclo[2.2.1]h...	5.398	0.7	ug/mL	84487	1	5.075	2573970	20.0
Cyclohexanemeth...	5.710	4.0	ug/mL	509136	1	5.075	2573970	20.0
Cyclohexanecarb...	6.728	55.2	ug/mL	12848600	2	6.457	4658490	20.0
1,2-Cyclooctadiene	6.810	0.4	ug/mL	93055	2	6.457	4658490	20.0
Bicyclo[3.3.1]n...	7.704	1.2	ug/mL	239202	3	8.210	3830780	20.0
Carbonic acid, ...	8.451	3.2	ug/mL	604440	3	8.210	3830780	20.0
1-Propanol, 2,2...	8.622	2.5	ug/mL	476218	3	8.210	3830780	20.0
2-Octene	9.328	0.3	ug/mL	54868	4	9.681	3513790	20.0
1-Methyl-2-meth...	9.528	0.7	ug/mL	117829	4	9.681	3513790	20.0
Cyclobutanecarb...	9.598	0.2	ug/mL	33417	4	9.681	3513790	20.0
Cyclohexene, 1,...	9.863	32.6	ug/mL	5734550	4	9.681	3513790	20.0
Furan, 2-ethyl-...	9.933	20.9	ug/mL	3678010	4	9.681	3513790	20.0
3-Cyclohexene-1...	11.122	0.1	ug/mL	23279	4	9.681	3513790	20.0
Cyclohexene, 1,...	11.269	1.9	ug/mL	337361	4	9.681	3513790	20.0
1-Methyl-2-meth...	11.357	1.0	ug/mL	184112	4	9.681	3513790	20.0
3-(2-Thienyl)-4...	12.639	2.0	ug/mL	199807	5	13.963	1983180	20.0
Benzenamine, 2,...	12.722	0.4	ug/mL	36446	5	13.963	1983180	20.0
3-(2-Thienyl)-4...	12.769	0.7	ug/mL	71864	5	13.963	1983180	20.0
1,4-Dimethoxy-3...	12.916	1.0	ug/mL	95430	5	13.963	1983180	20.0

File :D:[redacted]\RP1616\11182014_Run\11182014_009.D
Operator : [redacted]
Acquired : 18 Nov 2014 04:07 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36691
Misc Info : Tag # NE36691, 100X
Vial Number: 7







[redacted] RP1616 12/17/14

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

Quant Time: Nov 17 10:40:30 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	424125	20.00 ug/mL	0.00
3) Naphthalene-d8	6.457	136	1875168	20.00 ug/mL	# 0.00
5) Acenaphthene-d10	8.222	164	1057509	20.00 ug/mL	0.01
10) Phenanthrene-d10	9.698	188	1657784	20.00 ug/mL	0.02
11) Chrysene-d12	13.969	240	932264	20.00 ug/mL	0.01
12) Perylene-d12	16.804	264	551399	20.00 ug/mL	0.01
System Monitoring Compounds					
7) 2-Fluorobiphenyl	7.581	172	94644	1.46 ug/mL	0.00
Spiked Amount 12.500	Range 25 - 150		Recovery =	~~11.68%#~~ see	
Target Compounds					Qvalue
2) MCHM	5.557	55	3392356m	77.87 ug/mL	
4) PPH	6.869	94	308766	6.41 ug/mL	95
6) 1,4-CHDM	0.000		0	N.D. d	
8) DM-1,4-CHDC	0.000		0	N.D. d	
9) di-PPH	8.593	59	7113490m	166.23 ug/mL	

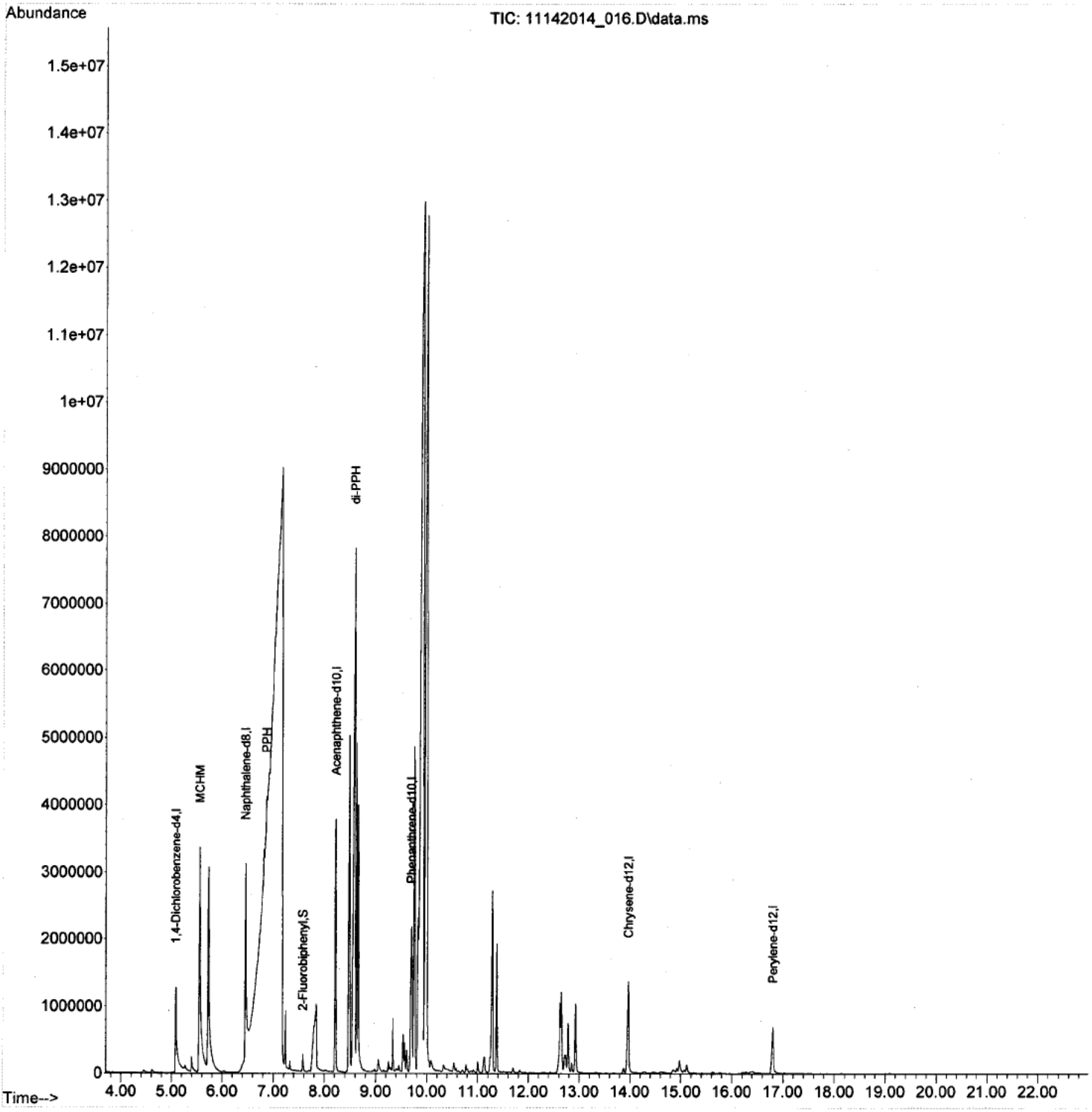
Narrative pld
Analyst ~~Recovery~~, 1/7/15
Surrogat Recovery
[redacted] 1/7/15

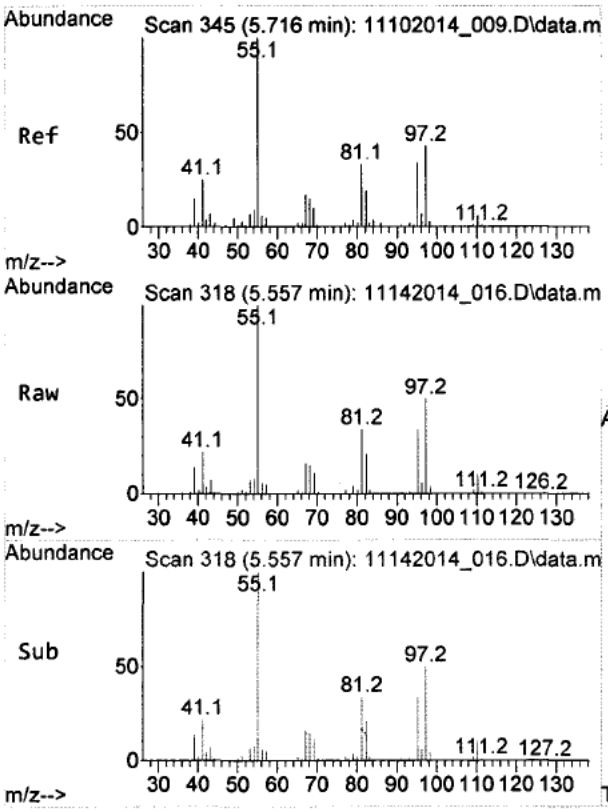
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

Quant Time: Nov 17 10:40:30 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

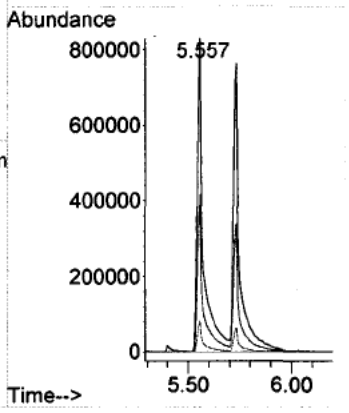


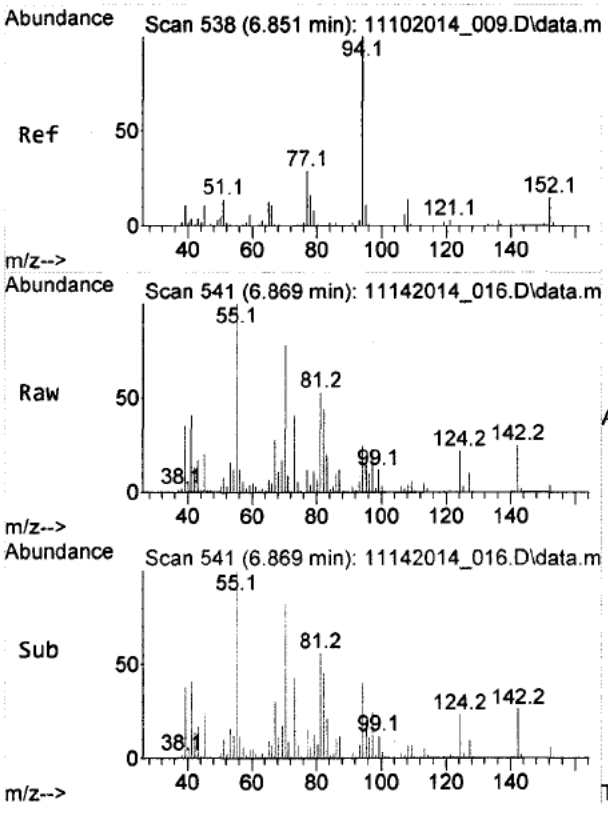


#2
MCHM
Concen: 77.87 ug/mL m
RT: 5.557 min Scan# 318
Delta R.T. -0.159 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 55 Resp: 3392356

Ion	Ratio	Lower	Upper
55	100		
97	20.3	34.6	51.8#
110	3.5	4.8	7.2#

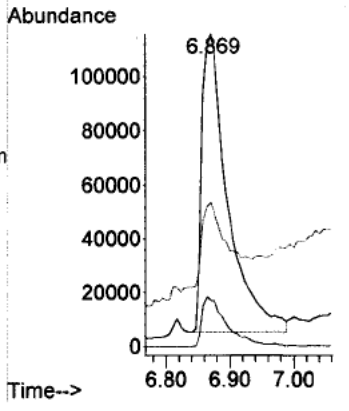


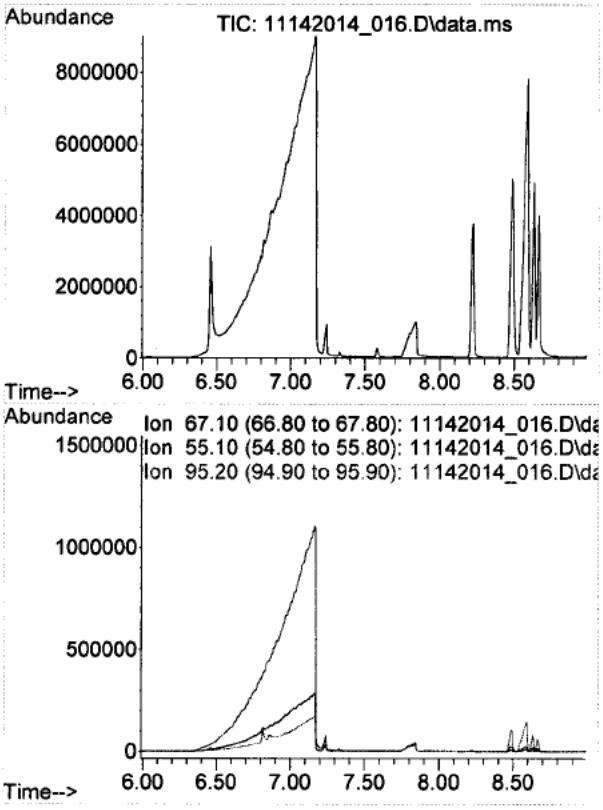


#4
PPH
Concen: 6.41 ug/mL
RT: 6.869 min Scan# 541
Delta R.T. 0.012 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 94 Resp: 308766

Ion	Ratio	Lower	Upper
94	100		
152	15.8	13.4	20.0
77	30.3	21.2	31.8



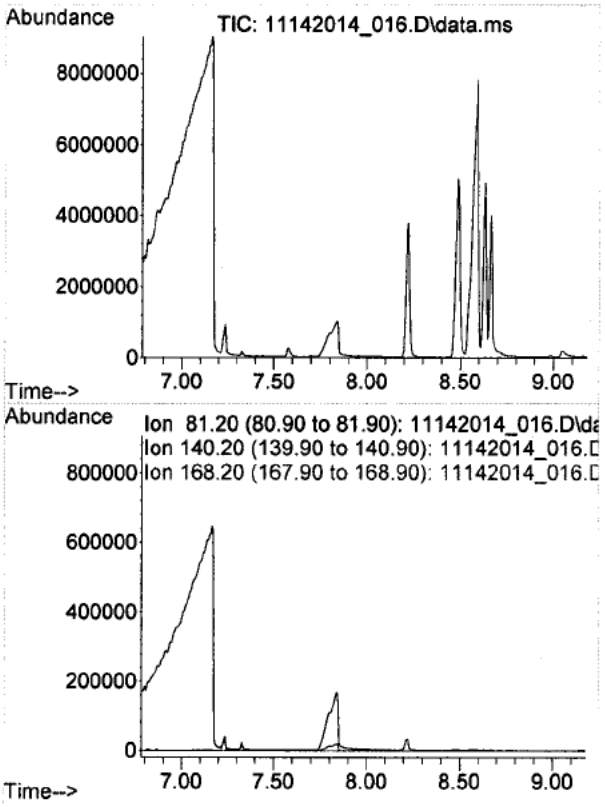


#6
1,4-CHDM
Concen: N.D.
Expected RT: 7.49 min

Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 67

Sig	Exp Ratio
67	100
55	59.7
95	255.8

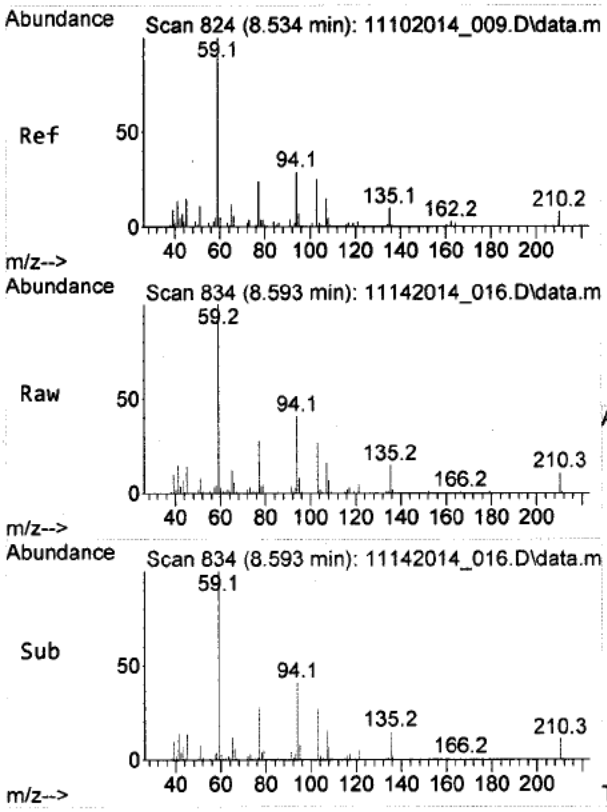


#8
DM-1,4-CHDC
Concen: N.D.
Expected RT: 7.98 min

Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 81

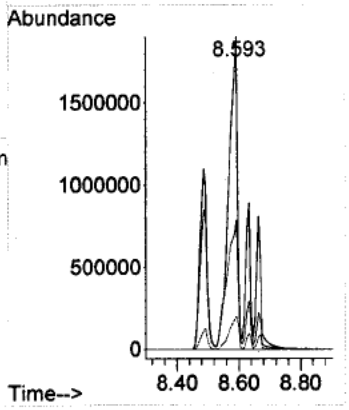
Sig	Exp Ratio
81	100
140	61.8
168	17.7



#9
di-PPH
Concen: 166.23 ug/mL m
RT: 8.593 min Scan# 834
Delta R.T. 0.053 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 59 Resp: 7113490

Ion	Ratio	Lower	Upper
59	100		
94	18.4	23.0	34.6#
210	2.6	6.1	9.1#



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

Quant Time: Dec 01 11:27:12 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	732217	20.00 ug/mL	0.00
13) Naphthalene-d8	6.457	136	1875168	20.00 ug/mL	# 0.00
24) Acenaphthene-d10	8.222	164	1057509	20.00 ug/mL	0.00
37) Phenanthrene-d10	9.698	188	1657784	20.00 ug/mL	0.01
49) Chrysene-d12	13.969	240	932264	20.00 ug/mL	0.00
58) Perylene-d12	16.804	264	553744	20.00 ug/mL	0.00
Target Compounds					Qvalue
2) Bis(2-chloroethyl) ether	0.000		0	N.D. 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...	7.163	55	19229188	1465.05 ug/mL#	96
14) n-Dodecane	6.528	57	6496	0.13 ug/mL#	96
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	7.281	142	2334	0.03 ug/mL	89
21) Hexachlorocyclopentadiene	0.000		0	N.D.	
22) 2-Chloronapthalene	0.000		0	N.D. d	
23) n-Tetradecane	0.000		0	N.D. d	
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	8.710	57	3598	0.06 ug/mL#	97
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.	
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	0.000		0	N.D. d	
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	0.000		0	N.D. d	

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

Quant Time: Dec 01 11:27:12 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

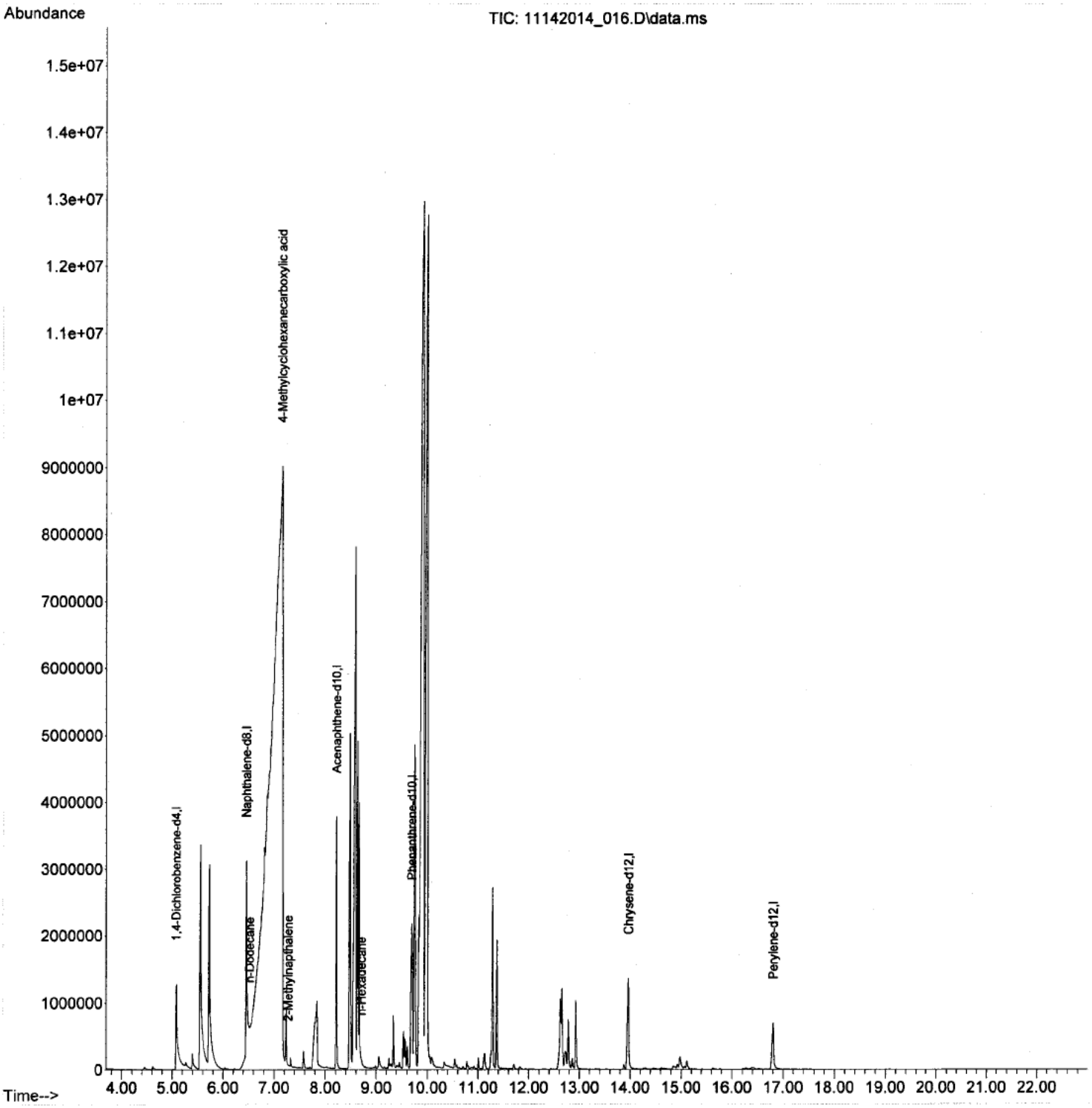
Compound	R.T.	QIon	Response	Conc Units	Dev(Min)
46) Fluoranthene	0.000		0	N.D.	d
47) Pyrene	0.000		0	N.D.	d
48) n-Docosane	0.000		0	N.D.	d
50) Benzyl Butyl Phthalate	0.000		0	N.D.	
51) n-Tetracosane	0.000		0	N.D.	d
52) n-Hexacosane	0.000		0	N.D.	d
53) n-Octacosane	0.000		0	N.D.	d
54) Benz[a]anthracene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

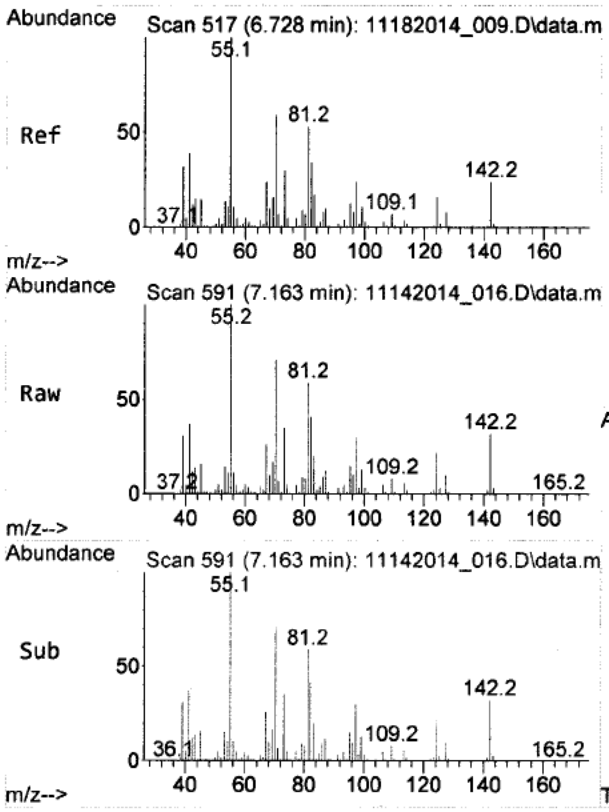
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

Quant Time: Dec 01 11:27:12 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

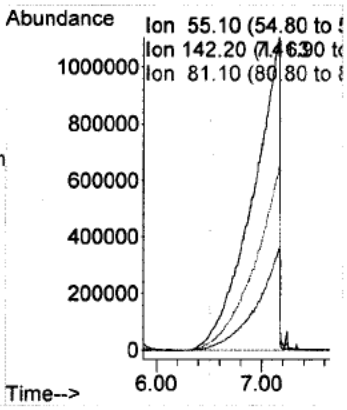


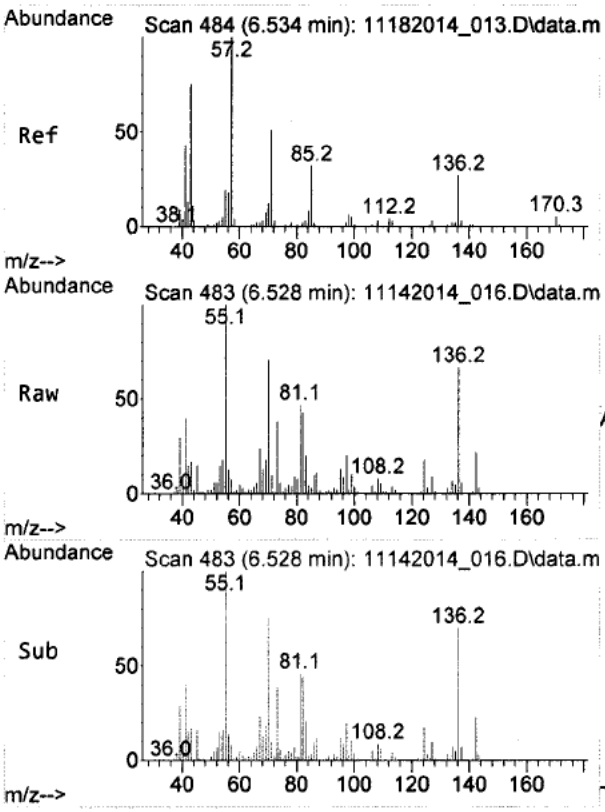


#12
4-Methylcyclohexanecarboxylic acid
Concen: 1465.05 ug/mL
RT: 7.163 min Scan# 591
Delta R.T. 0.435 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 55 Resp:19229188

Ion	Ratio	Lower	Upper
55	100		
142	18.4	19.1	28.7#
81	53.9	42.3	63.5

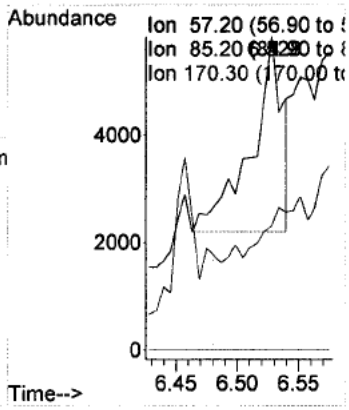


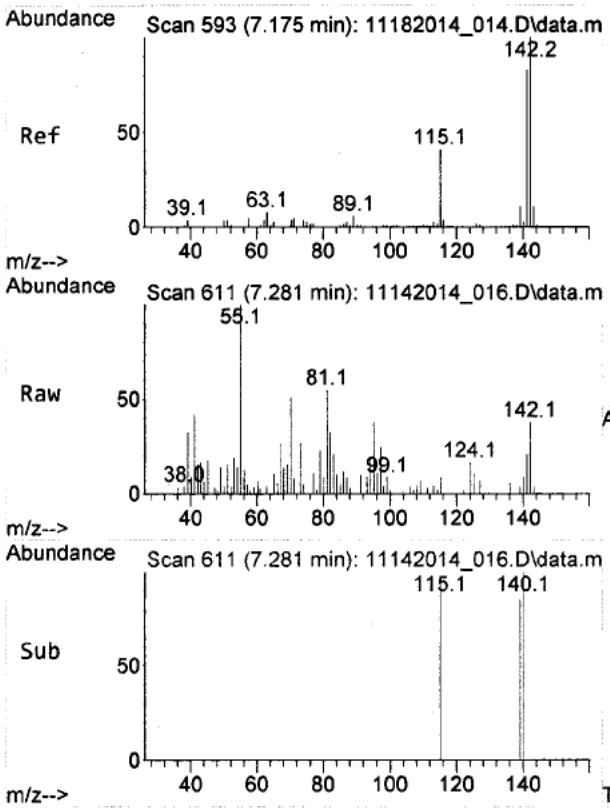


#14
n-Dodecane
Concen: 0.13 ug/mL
RT: 6.528 min Scan# 483
Delta R.T. -0.007 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 57 Resp: 6496

Ion	Ratio	Lower	Upper
57	100		
85	32.7	25.3	37.9
170	0.0	4.2	6.2#

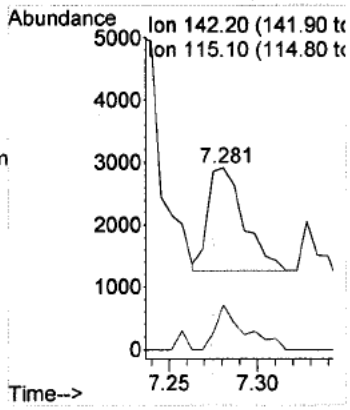


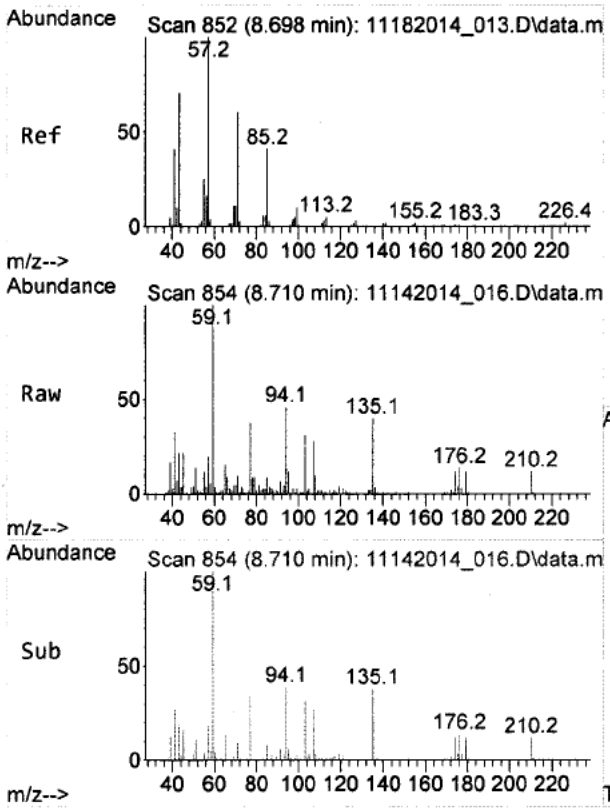


#20
2-Methylnapthalene
Concen: 0.03 ug/mL
RT: 7.281 min Scan# 611
Delta R.T. 0.106 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion:142 Resp: 2334

Ion	Ratio	Lower	Upper
142	100		
115	34.4	33.0	49.4

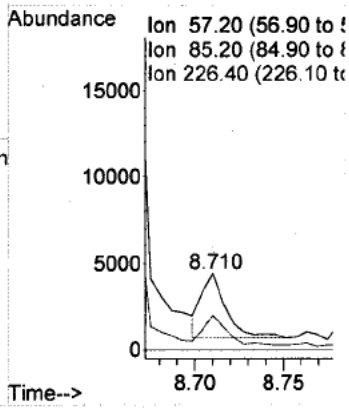




#31
n-Hexadecane
Concen: 0.06 ug/mL
RT: 8.710 min Scan# 854
Delta R.T. 0.012 min
Lab File: 11142014_016.D
Acq: 14 Nov 2014 05:13 pm

Tgt Ion: 57 Resp: 3598

Ion	Ratio	Lower	Upper
57	100		
85	42.5	35.1	52.7
226	0.0	3.1	4.7#



LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 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_016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	225	237	263	rBV	1266610	2866894	1.85%	0.845%
2	5.557	309	318	341	rVV	3359572	6952965	4.49%	2.050%
3	5.734	341	348	393	rVV	3062605	6444917	4.16%	1.900%
4	6.457	441	471	481	rVV	3112704	6000021	3.88%	1.769%
5	7.163	481	591	599	rVV	9011315	154807279	100.00%	45.637%
6	7.240	599	604	615	rVV	923539	1259857	0.81%	0.371%
7	7.328	615	619	655	rVV	171647	550585	0.36%	0.162%
8	7.840	685	706	731	rVV	1020051	4140608	2.67%	1.221%
9	8.222	763	771	791	rVV	3781396	4787264	3.09%	1.411%
10	8.487	803	816	823	rVV	5029763	7839802	5.06%	2.311%
11	8.593	823	834	837	rVV	7815669	16340046	10.56%	4.817%
12	8.634	837	841	887	rVV2	4914712	10011265	6.47%	2.951%
13	9.334	955	960	969	rVV	807811	943846	0.61%	0.278%
14	9.534	989	994	1003	rVV3	575398	1342372	0.87%	0.396%
15	9.610	1003	1007	1013	rVV	343451	503614	0.33%	0.148%
16	9.698	1013	1022	1025	rVV	2175592	4437727	2.87%	1.308%
17	9.751	1025	1031	1039	rVV	4860096	8130682	5.25%	2.397%
18	9.928	1039	1061	1065	rVV	12973781	51113283	33.02%	15.068%
19	10.004	1065	1074	1085	rVV	12766158	30303668	19.58%	8.934%
20	10.087	1085	1088	1107	rVV2	189236	643988	0.42%	0.190%
21	10.334	1121	1130	1159	rVV5	114616	658022	0.43%	0.194%
22	11.128	1257	1265	1275	rVV3	238335	531060	0.34%	0.157%
23	11.292	1275	1293	1301	rVV2	2716304	4680653	3.02%	1.380%
24	11.375	1301	1307	1323	rVV	1924748	2440798	1.58%	0.720%
25	12.651	1501	1524	1531	rVV2	1204013	3715970	2.40%	1.095%
26	12.722	1531	1536	1541	rVV4	271298	681715	0.44%	0.201%
27	12.781	1541	1546	1553	rVV	745771	1148980	0.74%	0.339%
28	12.928	1565	1571	1603	rVV	1028621	1639572	1.06%	0.483%
29	13.969	1737	1748	1769	rVV	1359763	2687179	1.74%	0.792%
30	16.804	2217	2230	2261	rVV	692255	1607120	1.04%	0.474%

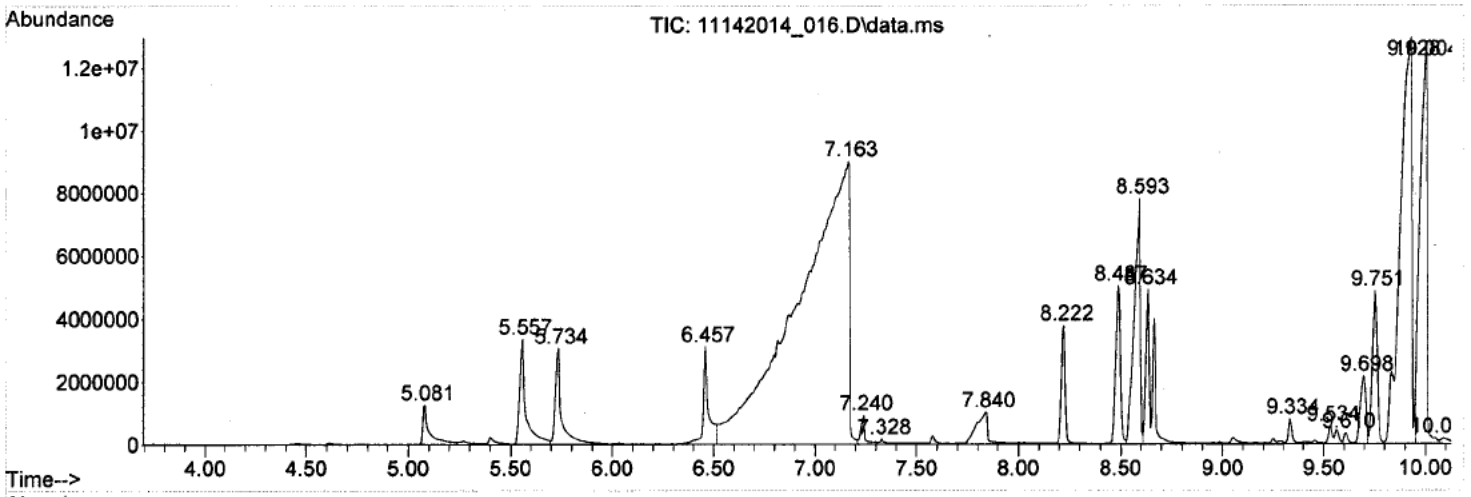
Sum of corrected areas: 339211752

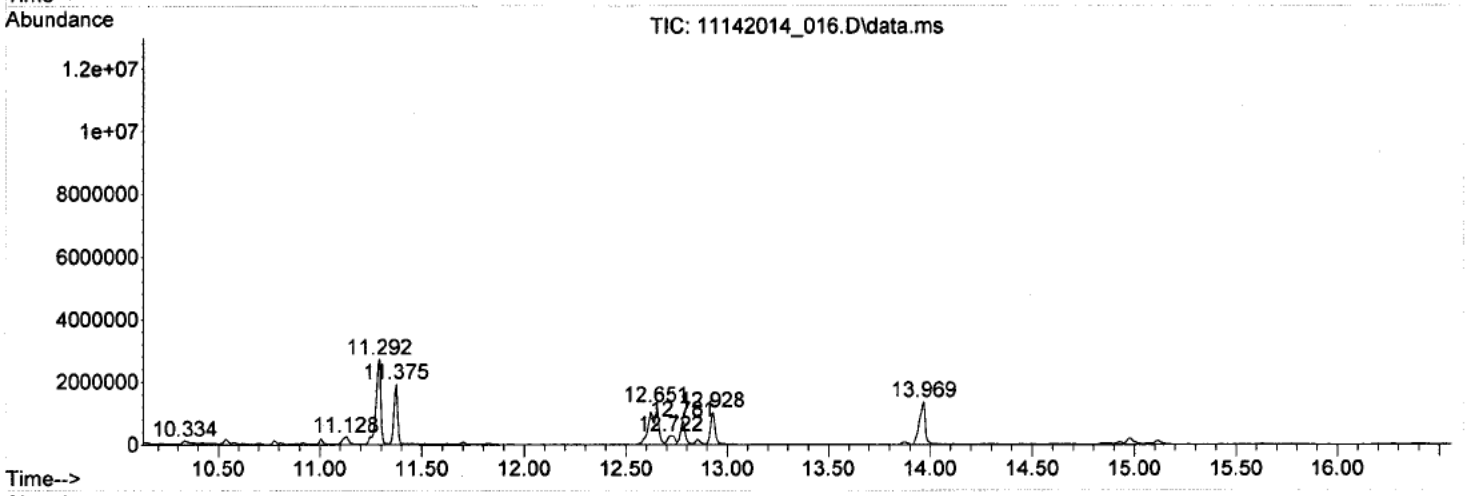
LSC Report - Integrated Chromatogram

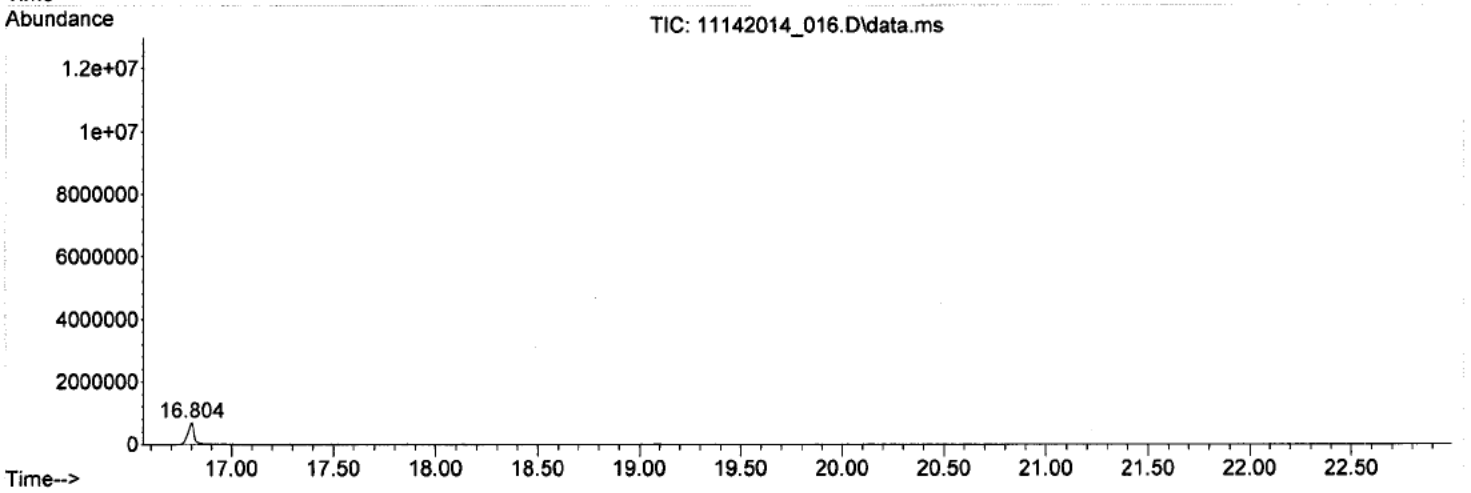
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

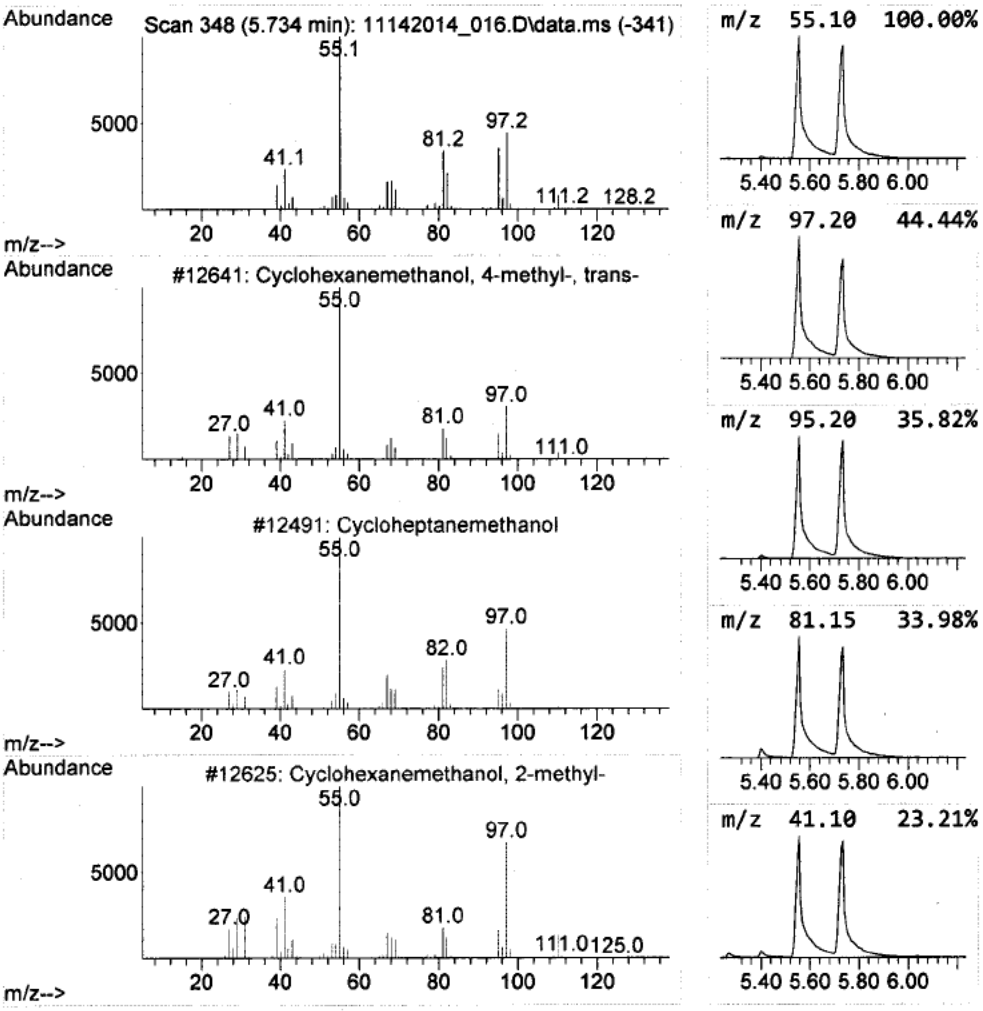
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.734	44.96 ug/mL	6444920	1,4-Dichlorobenzene-d4	5.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	83
2	Cycloheptanemethanol	128	C8H16O	004448-75-3	72
3	Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	64
4	Cycloheptanemethanol	128	C8H16O	004448-75-3	59
5	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	56



Library Search Compound Report

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

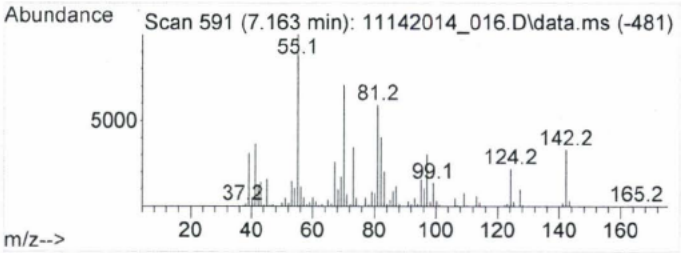
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

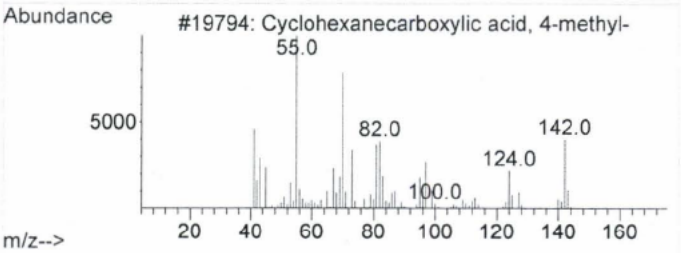
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

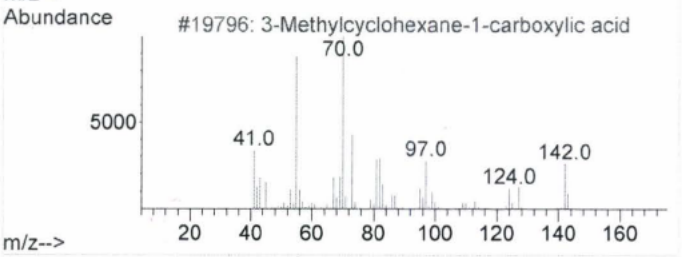
****
Peak Number 2 Cyclohexanecarboxylic acid,... Concentration Rank 1

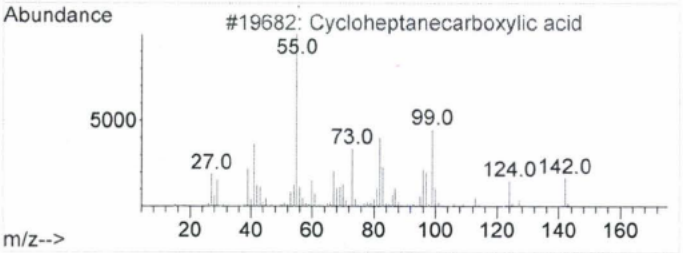
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	516.02 ug/mL	154807000	Naphthalene-d8	6.457

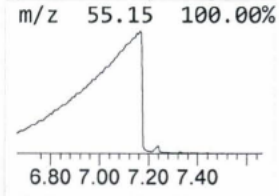
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	95
2	3-Methylcyclohexane-1-carboxylic...	142	C8H14O2	1000132-15-7	60
3	Cycloheptanecarboxylic acid	142	C8H14O2	001460-16-8	46
4	Cyclohexanecarboxylic acid, 2-me...	142	C8H14O2	056586-13-1	37
5	Acrylic acid isoamyl ester	142	C8H14O2	004245-35-6	22

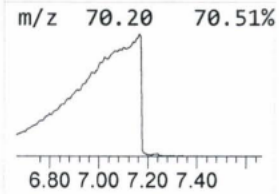


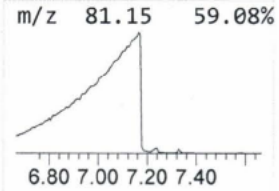


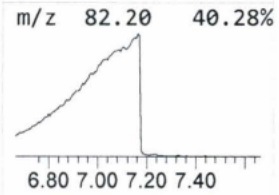


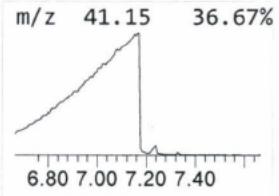












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

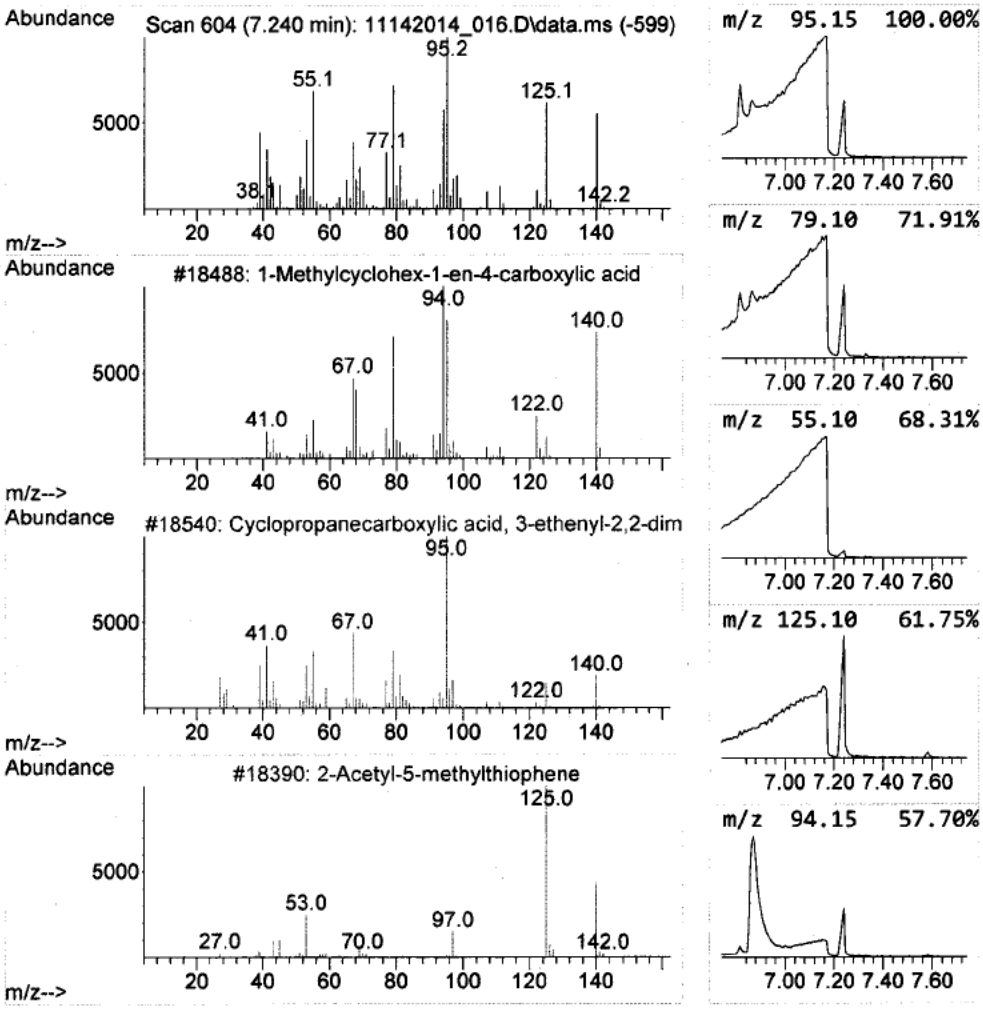
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 3 1-Methylcyclohex-1-en-4-car... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.240	4.20 ug/mL	1259860	Naphthalene-d8	6.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylcyclohex-1-en-4-carboxyl...	140	C8H12O2	004342-60-3	35
2	Cyclopropanecarboxylic acid, 3-e...	140	C8H12O2	067528-58-9	35
3	2-Acetyl-5-methylthiophene	140	C7H8OS	013679-74-8	30
4	1,3-Butadiene-1-carboxylic acid	98	C5H6O2	000626-99-3	30
5	Bicyclo[5.1.0]octane, 8-methylene-	122	C9H14	054211-15-3	30



Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

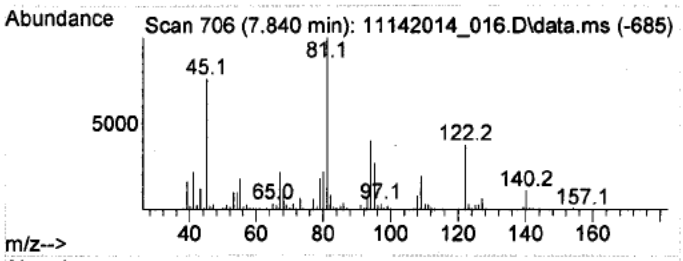
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

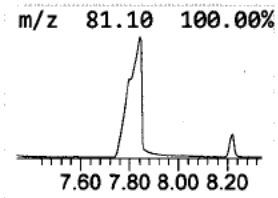
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

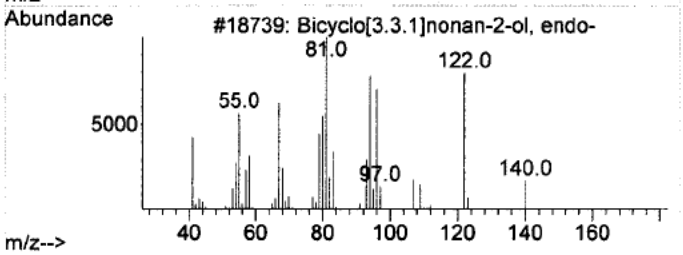
****
Peak Number 4 Bicyclo[3.3.1]nonan-2-ol, e... Concentration Rank 9

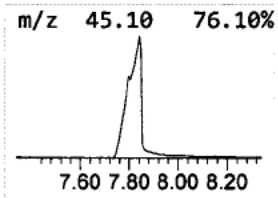
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.840	17.30 ug/mL	4140610	Acenaphthene-d10	8.222

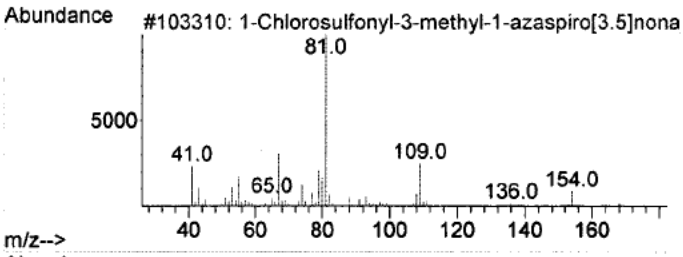
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.3.1]nonan-2-ol, endo-	140	C9H16O	010036-25-6	30
2	1-Chlorosulfonyl-3-methyl-1-azas...	251	C9H14ClNO3S	016933-89-4	27
3	Bicyclo[3.3.1]nonan-2-ol, exo-	140	C9H16O	010036-15-4	22
4	1,5-Hexadiene, 2-methyl-	96	C7H12	004049-81-4	18
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	18

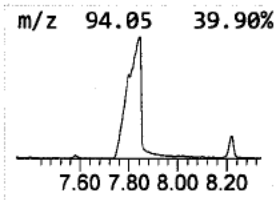


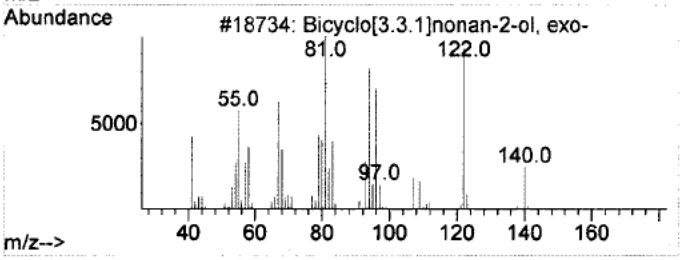


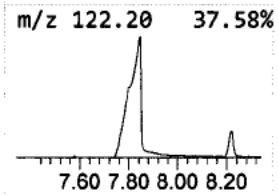


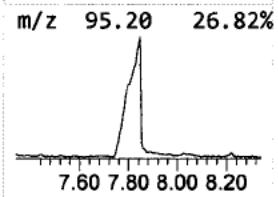












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

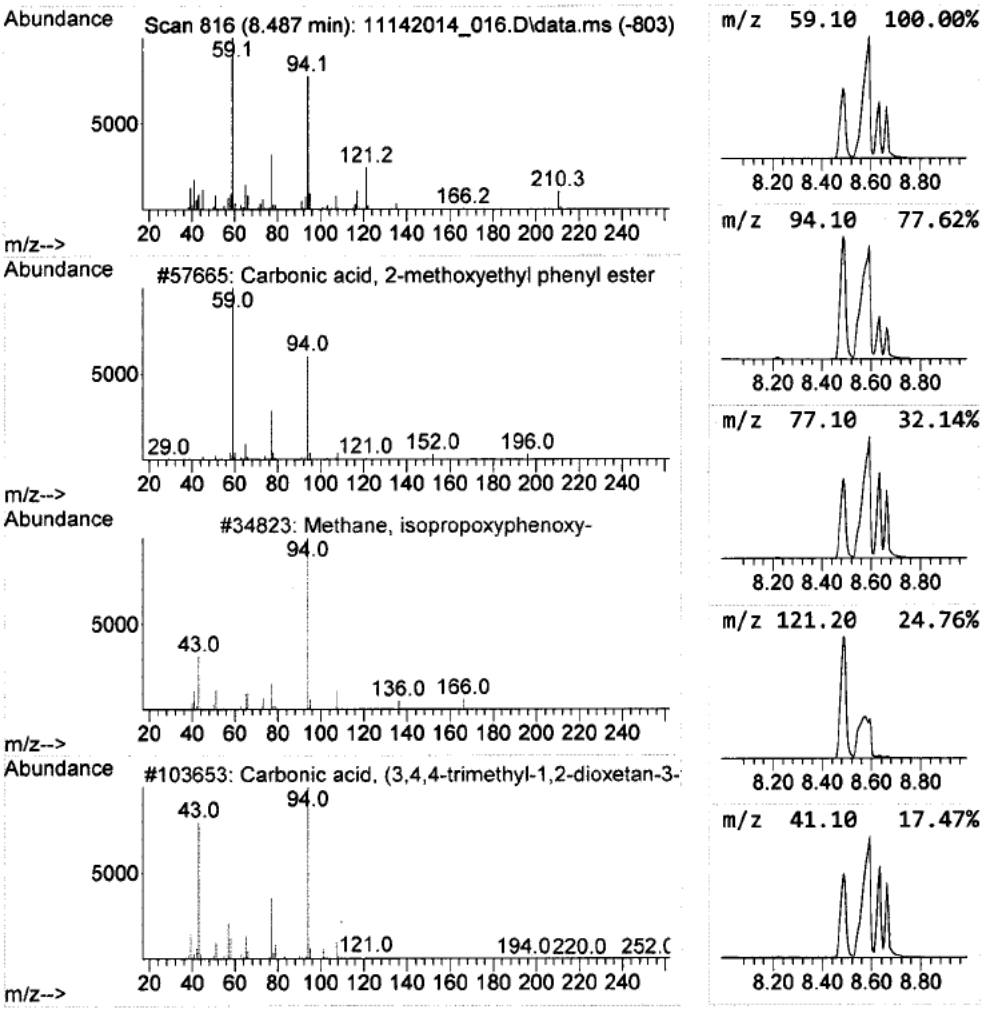
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 5 Carbonic acid, 2-methoxyeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.487	32.75 ug/mL	7839800	Acenaphthene-d10	8.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	56
2	Methane, isopropoxyphenoxy-	166	C10H14O2	000828-12-6	38
3	Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	38
4	3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	35
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	35



Library Search Compound Report

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Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

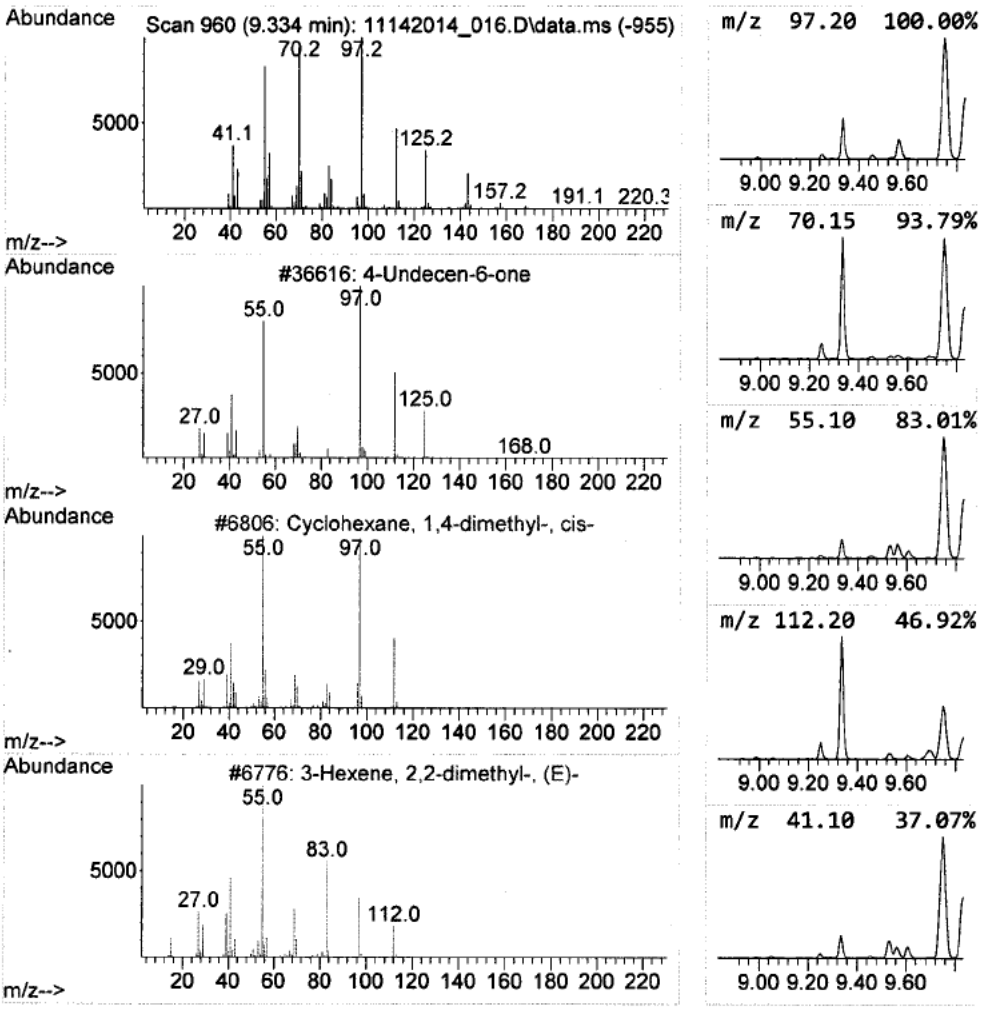
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 6 4-Undecen-6-one Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.334	4.25 ug/mL	943846	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Undecen-6-one	168	C11H20O	032064-74-7	55
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	43
3	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	38
4	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	35
5	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	35



Library Search Compound Report

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

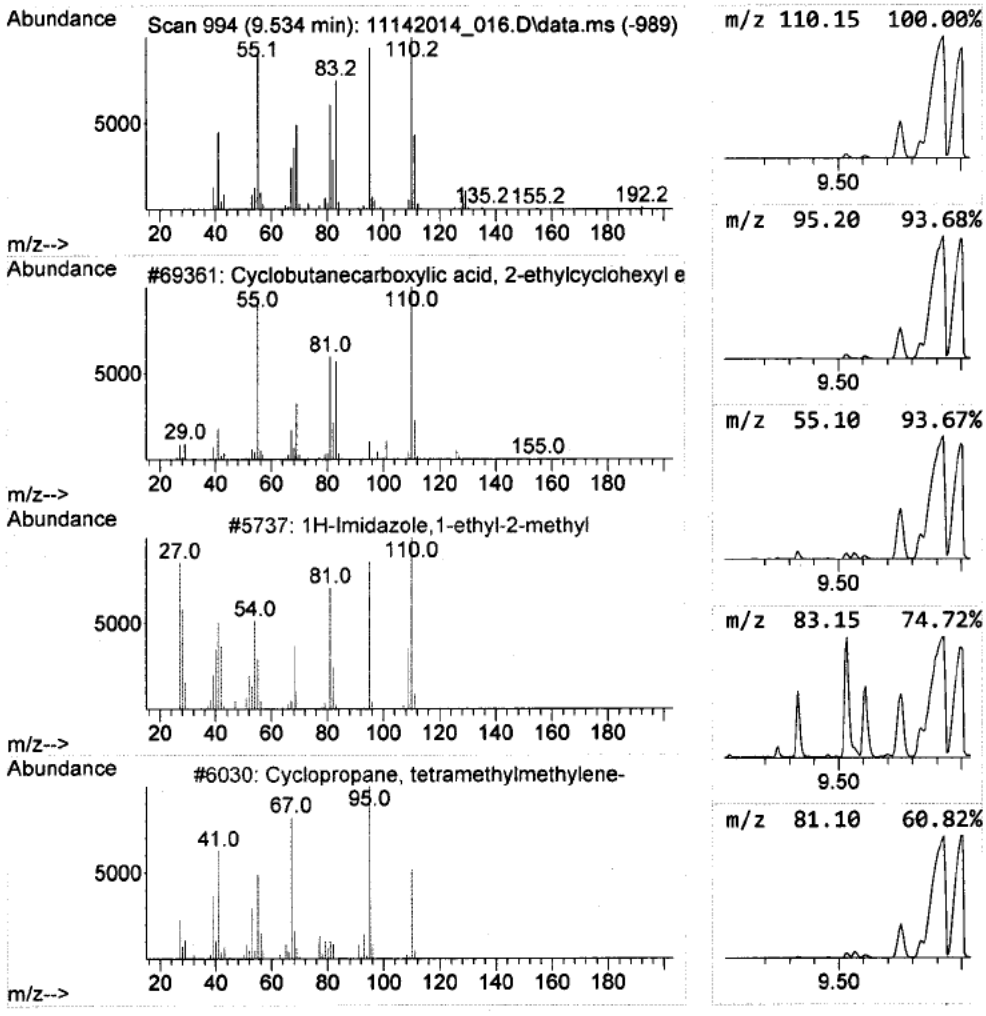
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 7 Cyclobutanecarboxylic acid,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.534	6.05 ug/mL	1342370	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanecarboxylic acid, 2-et...	210	C13H22O2	1000282-61-0	50
2	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	46
3	Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	38
4	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	35
5	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	25



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

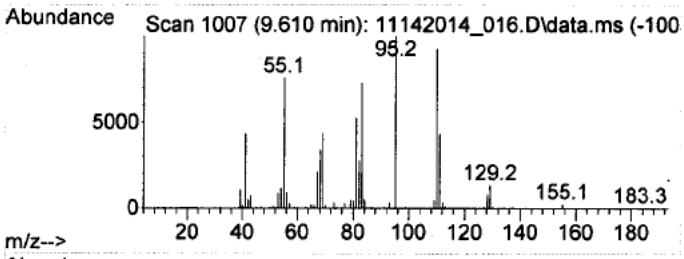
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

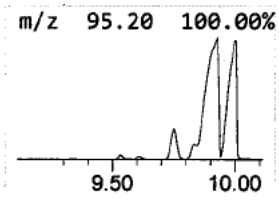
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

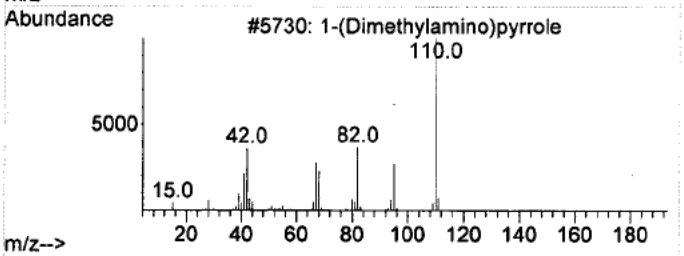
****
Peak Number 8 1-(Dimethylamino)pyrrole Concentration Rank 20

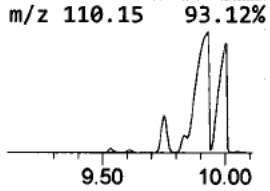
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	2.27 ug/mL	503614	Phenanthrene-d10	9.698

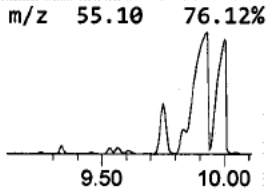
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Dimethylamino)pyrrole	110	C6H10N2	078307-76-3	27
2	1H-Imidazole, 1-(cyclohexylcarbo...	178	C10H14N2O	060718-45-8	27
3	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	22
4	Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	14
5	Cyclohexanecarboxylic acid, (1H-...	195	C8H13N5O	1000310-78-1	14

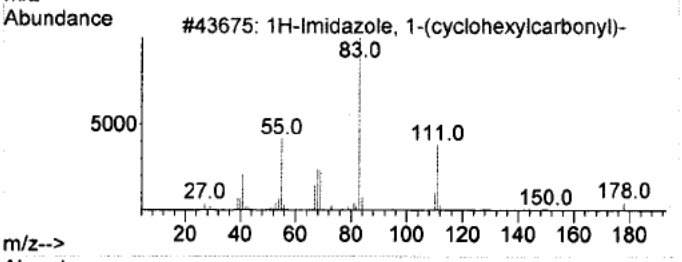


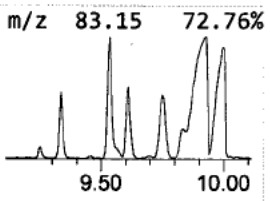


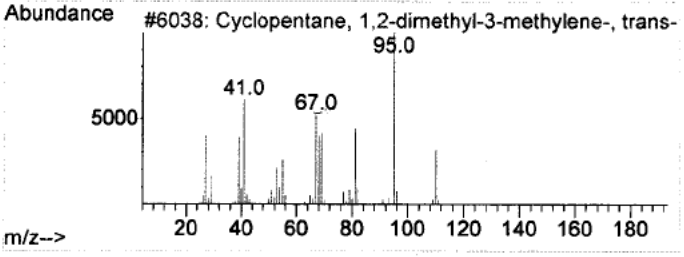


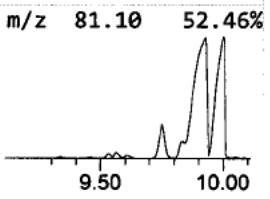












Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

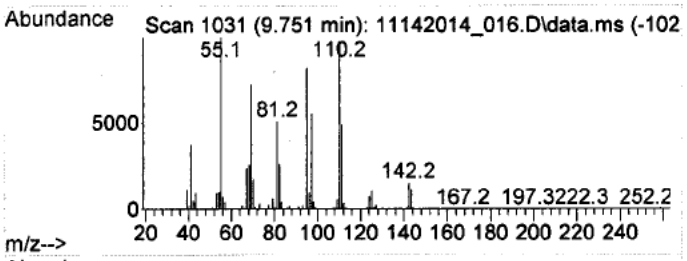
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

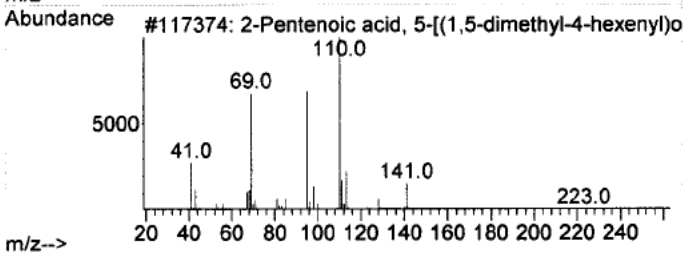
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

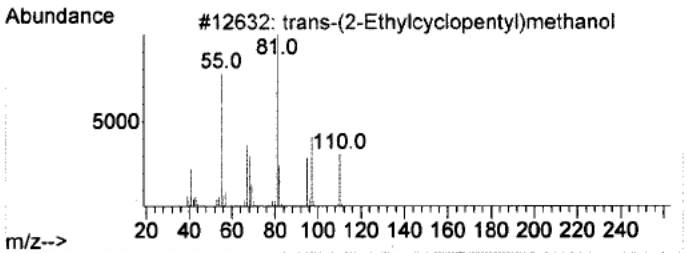
****
Peak Number 9 2-Pentenoic acid, 5-[(1,5-d... Concentration Rank 5

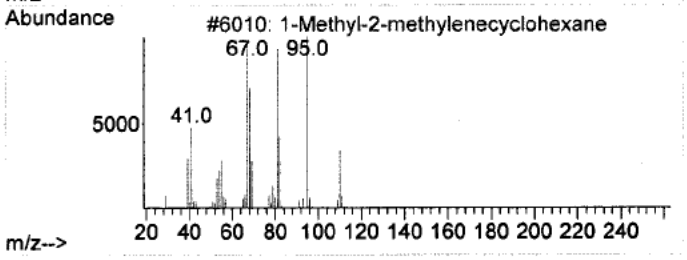
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	36.64 ug/mL	8130680	Phenanthrene-d10	9.698

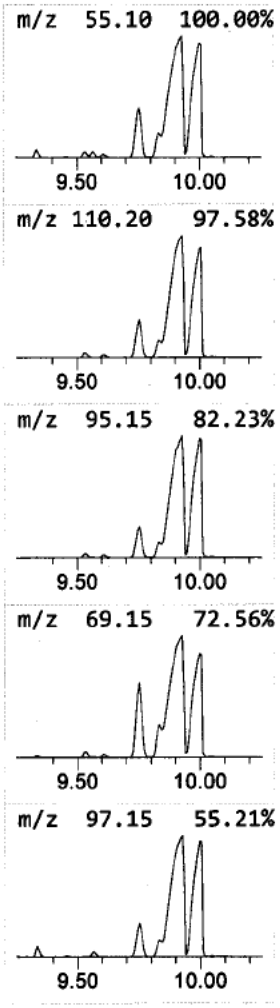
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenoic acid, 5-[(1,5-dimeth...	268	C16H28O3	053311-39-0	47
2	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	43
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	38
4	1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	38
5	Cyclohexanecarboxylic acid, 3,5-...	238	C15H26O2	1000279-52-3	38











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

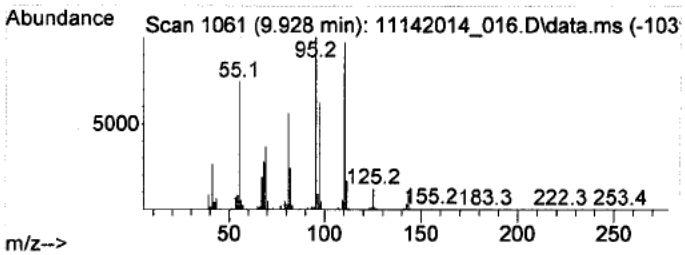
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

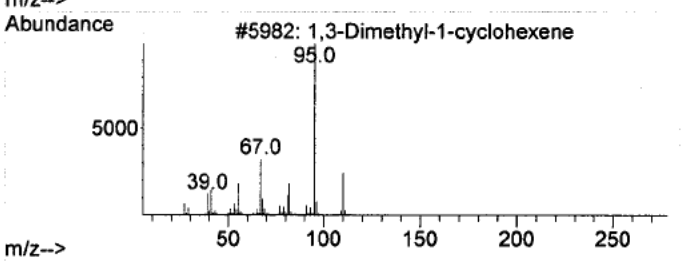
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

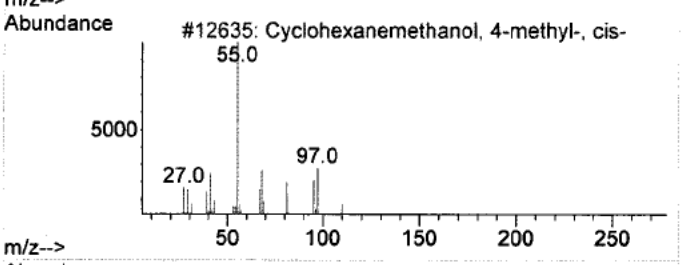
****
Peak Number 10 1,3-Dimethyl-1-cyclohexene Concentration Rank 2

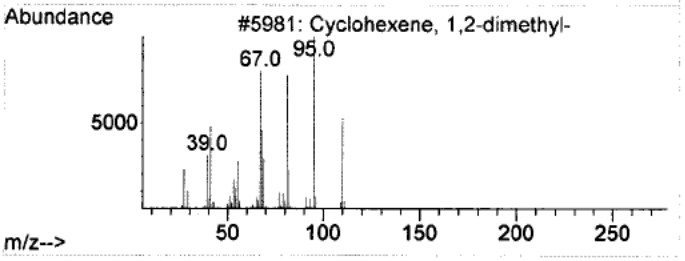
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	230.36 ug/mL	51113300	Phenanthrene-d10	9.698

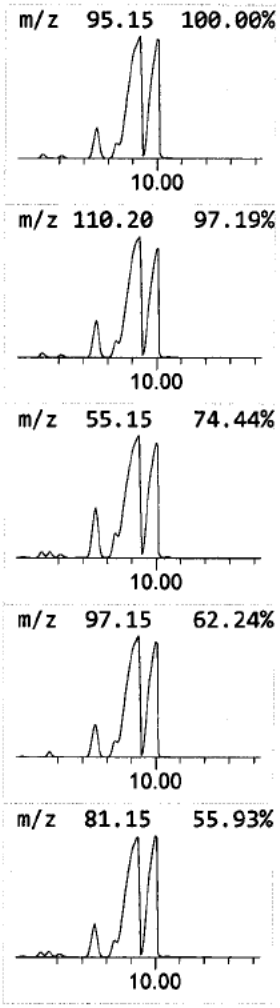
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	47
2	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	43
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	43
4	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	43
5	Methylphosphonic acid, fluoroanh...	208	C9H18FO2P	1000273-29-7	38











Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

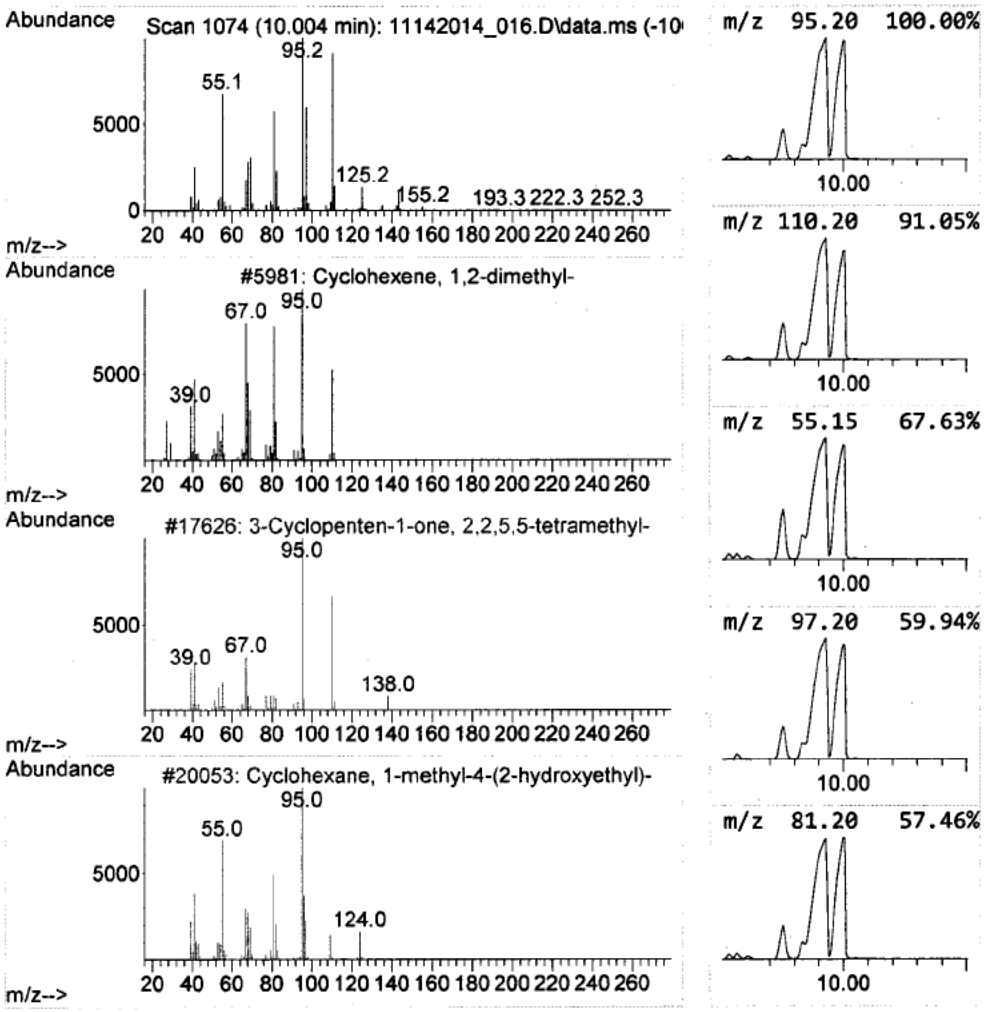
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 11 Cyclohexene, 1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	136.57 ug/mL	30303700	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	64
2	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	47
3	Cyclohexane, 1-methyl-4-(2-hydro...	142	C9H18O	004916-87-4	38
4	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	38
5	3,5-Octadiene, (Z,Z)-	110	C8H14	007348-80-3	35



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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

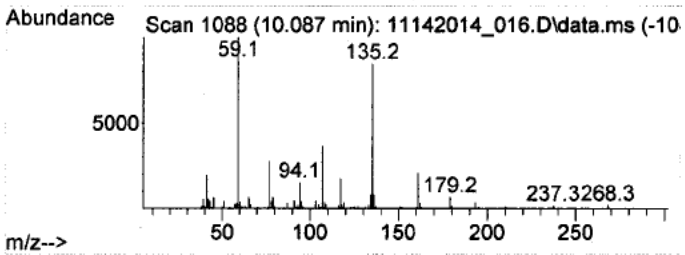
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

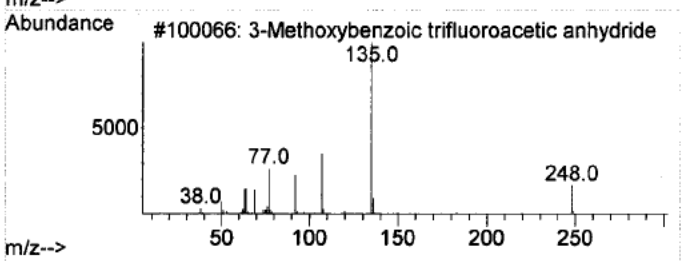
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

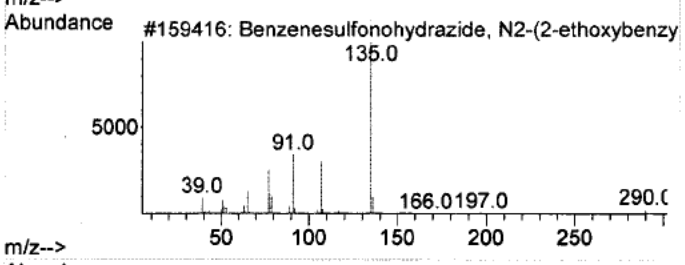
****
Peak Number 12 3-Methoxybenzoic trifluoroa... Concentration Rank 18

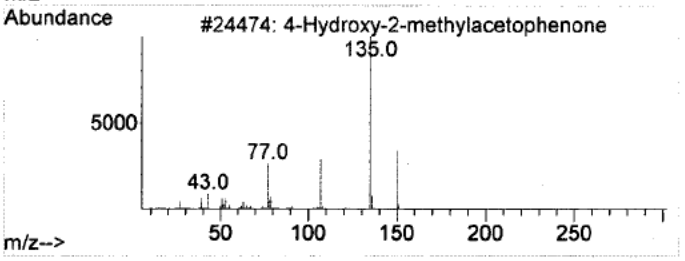
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.087	2.90 ug/mL	643988	Phenanthrene-d10	9.698

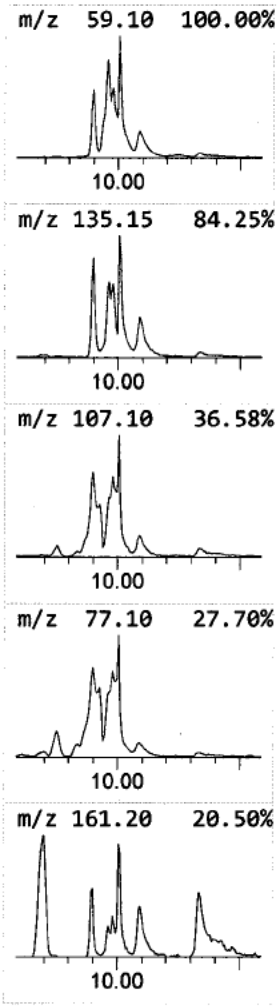
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methoxybenzoic trifluoroacetic...	248	C10H7F3O4	1000375-00-9	35
2	Benzenesulfonohydrazide, N2-(2-e...	318	C16H18N2O3S	065609-76-9	35
3	4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	35
4	4-Methoxyphenylglyoxal, aldoxime	179	C9H9NO3	1000306-61-2	35
5	Glycine, N-(2-methoxybenzoyl)-, ...	223	C11H13NO4	027796-49-2	27











Library Search Compound Report

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

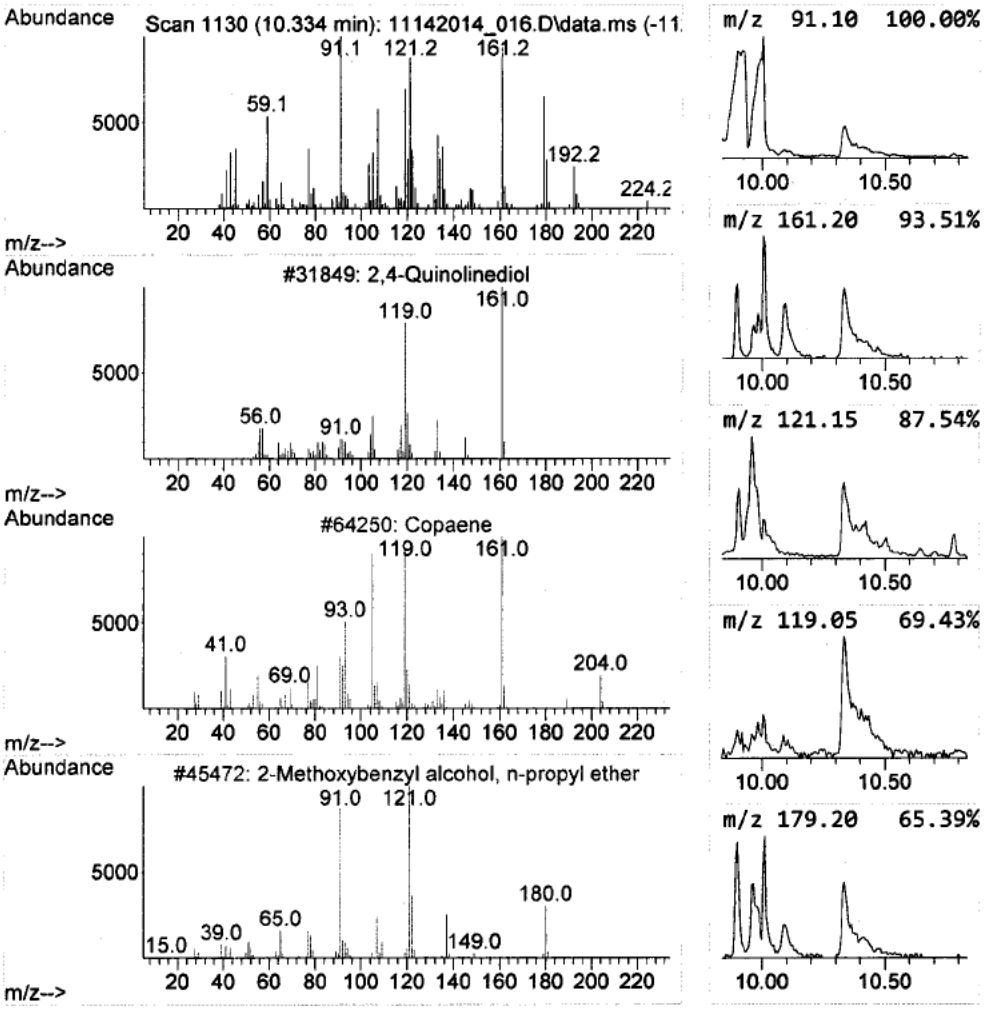
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 13 2,4-Quinolinediol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.334	2.97 ug/mL	658022	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Quinolinediol	161	C9H7NO2	000086-95-3	25
2	Copaene	204	C15H24	003856-25-5	22
3	2-Methoxybenzyl alcohol, n-propy...	180	C11H16O2	1000378-19-2	15
4	1-(4-Ethoxyphenyl)-2-propanol	180	C11H16O2	1000123-12-7	15
5	Benzenemethanol, 4-methoxy-, ace...	180	C10H12O3	000104-21-2	15



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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

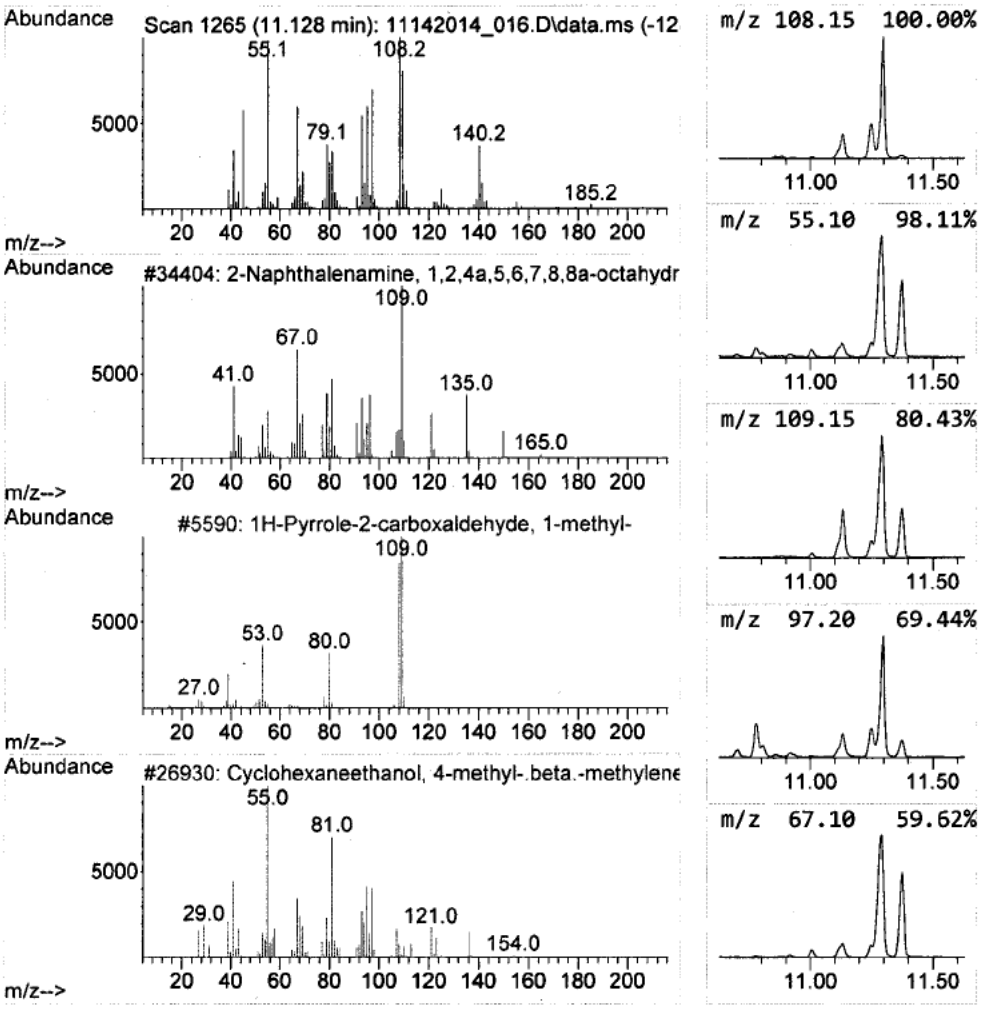
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 14 2-Naphthalenamine, 1,2,4a,5... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.128	2.39 ug/mL	531060	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenamine, 1,2,4a,5,6,7,...	165	C11H19N	056053-03-3	35
2	1H-Pyrrole-2-carboxaldehyde, 1-m...	109	C6H7NO	001192-58-1	25
3	Cyclohexaneethanol, 4-methyl-.be...	154	C10H18O	015714-12-2	16
4	Pyrazole, 4-aminomethyl-3,5-dime...	125	C6H11N3	1000262-42-4	14
5	Bicyclo[2.2.1]heptane-2-carboxal...	138	C9H14O	015780-36-6	14



Library Search Compound Report

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

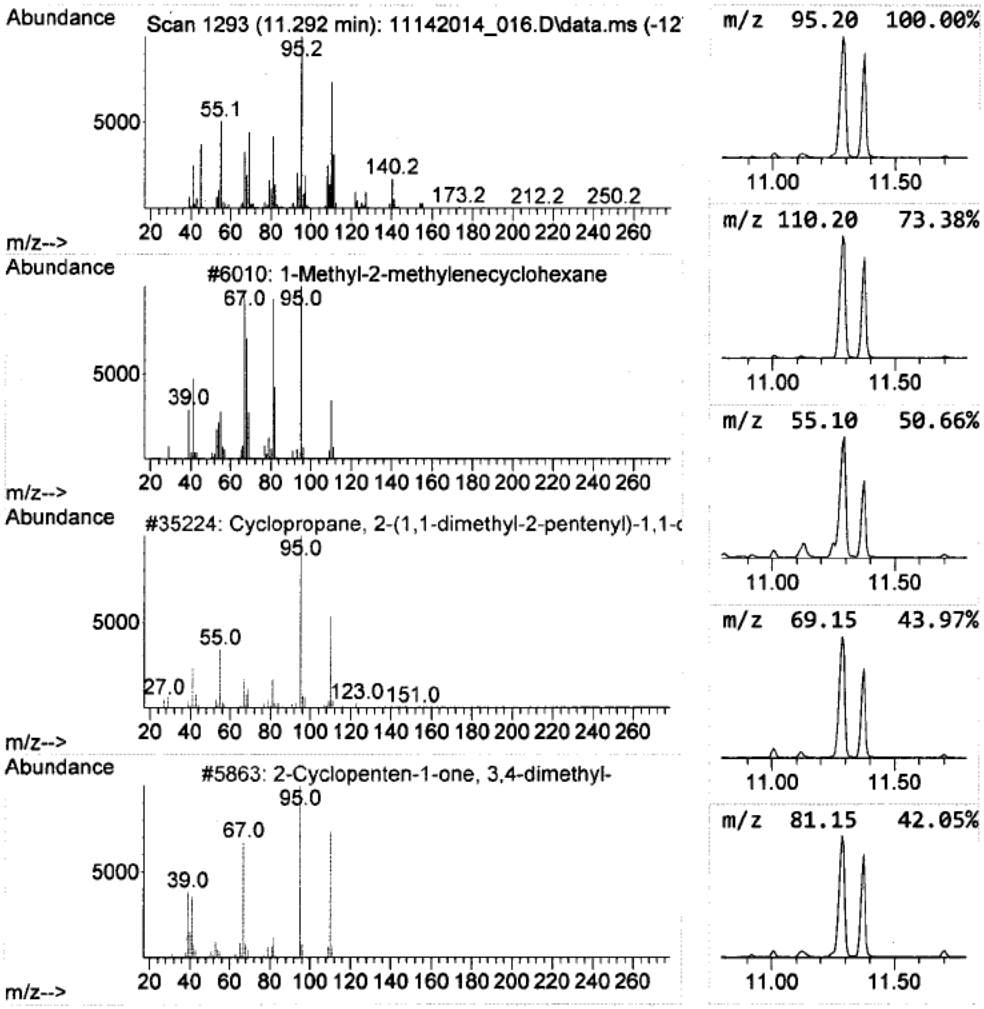
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 15 1-Methyl-2-methylenecyclohe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.292	21.09 ug/mL	4680650	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	58
2	Cyclopropane, 2-(1,1-dimethyl-2-...	166	C12H22	074663-76-6	50
3	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	50
4	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	50
5	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	47



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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

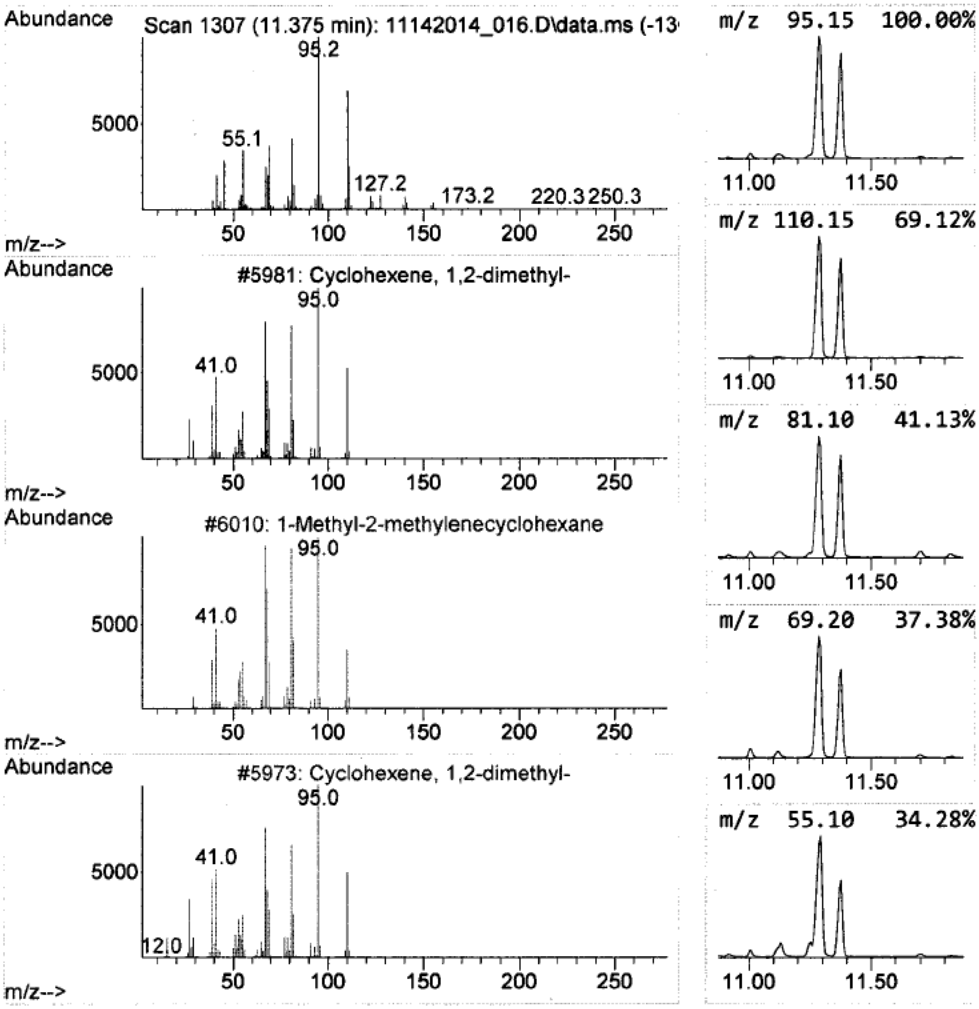
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 16 Cyclohexene, 1,2-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.375	11.00 ug/mL	2440800	Phenanthrene-d10	9.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	68
2	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	62
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	62
4	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	50
5	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	50



Library Search Compound Report

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Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

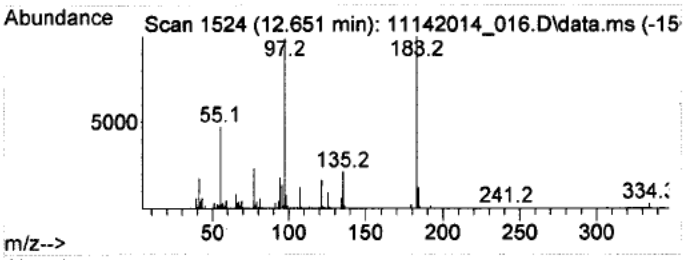
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

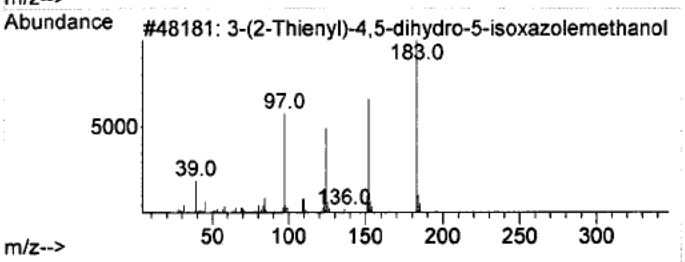
****

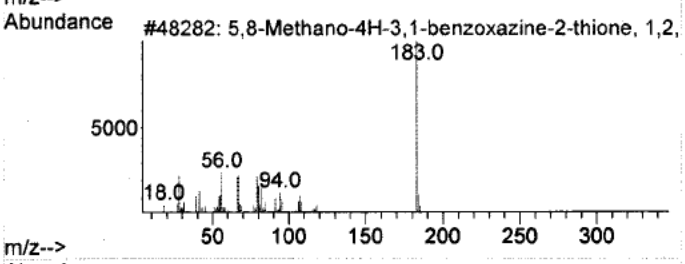
Peak Number 17 3-(2-Thienyl)-4,5-dihydro-5... Concentration Rank 7

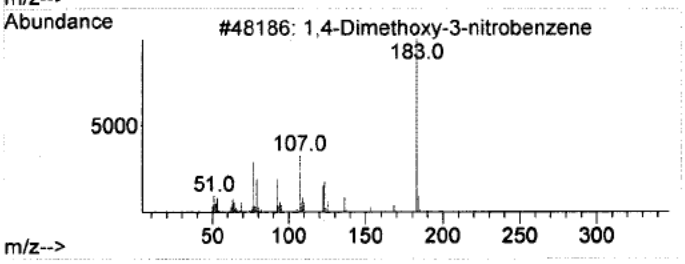
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	27.66 ug/mL	3715970	Chrysene-d12	13.969

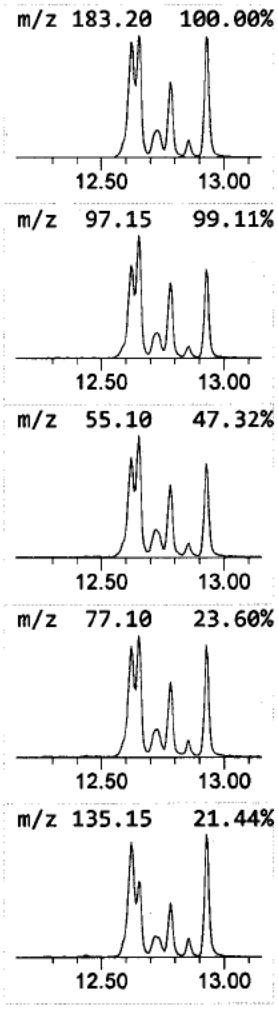
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Thienyl)-4,5-dihydro-5-isox...	183	C8H9NO2S	022353-85-1	52
2	5,8-Methano-4H-3,1-benzoxazine-2...	183	C9H13NOS	1000142-76-8	25
3	1,4-Dimethoxy-3-nitrobenzene	183	C8H9NO4	000089-39-4	23
4	Benzene, 1,3-dimethoxy-2-nitro-	183	C8H9NO4	006665-97-0	23
5	Benzenamine, 2,4-dinitro-	183	C6H5N3O4	000097-02-9	22











Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

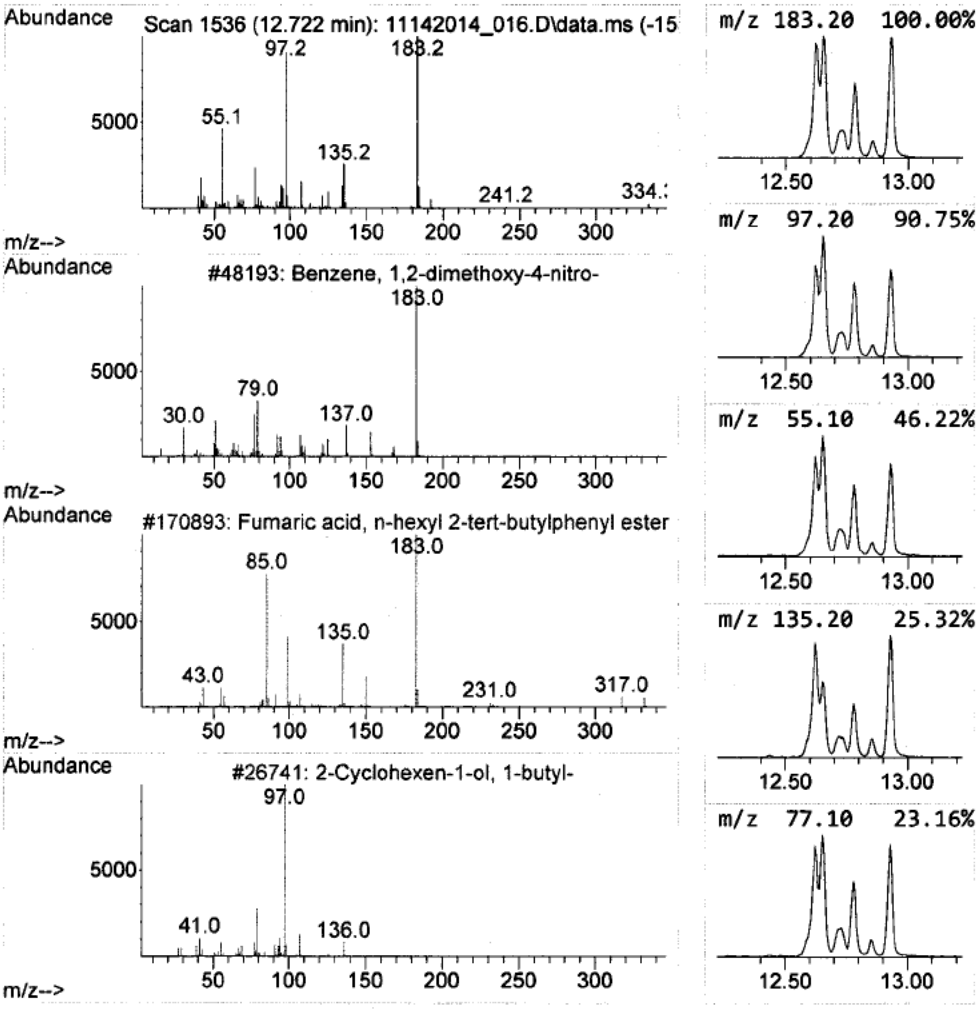
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

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

****
Peak Number 18 Benzene, 1,2-dimethoxy-4-ni... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	5.07 ug/mL	681715	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	38
2	Fumaric acid, n-hexyl 2-tert-but...	332	C20H28O4	1000344-94-2	35
3	2-Cyclohexen-1-ol, 1-butyl-	154	C10H18O	088116-46-5	27
4	1,4-Dimethoxy-3-nitrobenzene	183	C8H9NO4	000089-39-4	27
5	5,8-Methano-4H-3,1-benzoxazine-2...	183	C9H13NOS	1000142-76-8	25



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

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

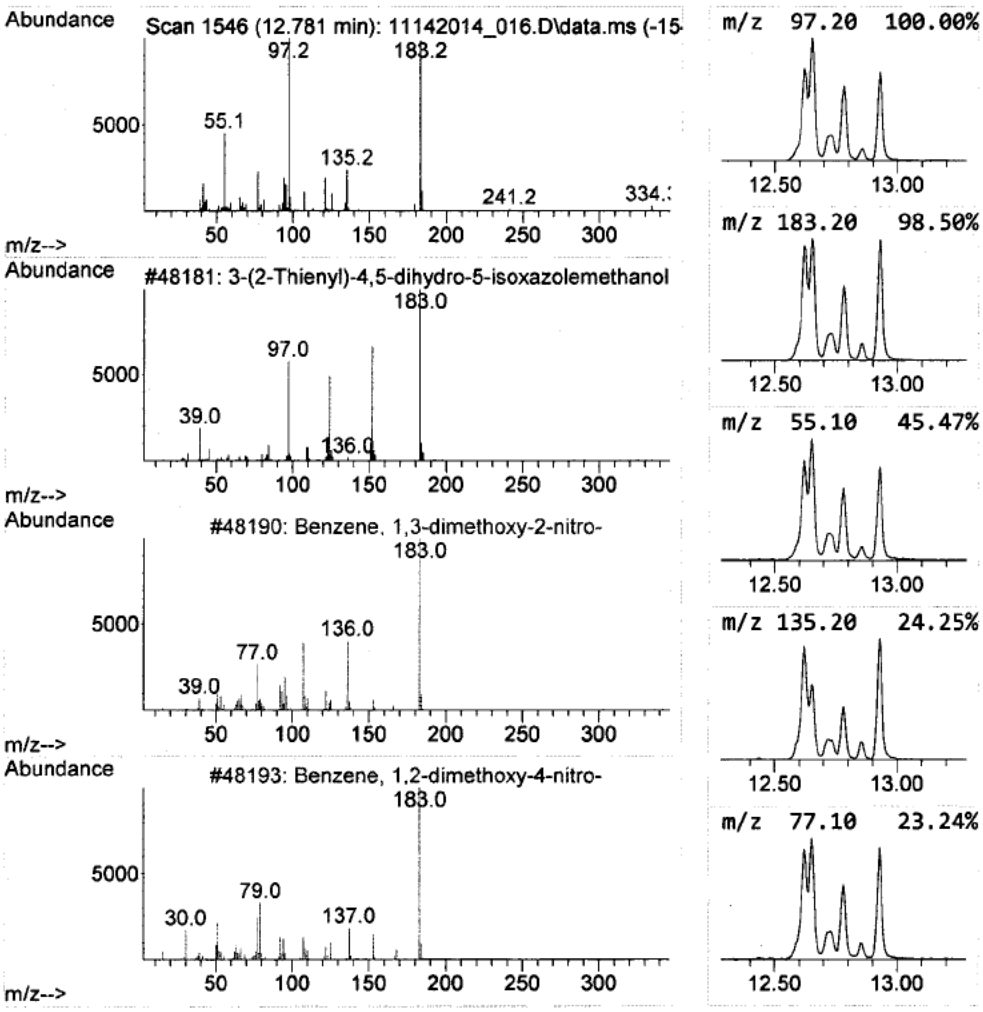
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****

Peak Number 19 3-(2-Thienyl)-4,5-dihydro-5... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.781	8.55 ug/mL	1148980	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Thienyl)-4,5-dihydro-5-isox...	183	C8H9NO2S	022353-85-1	52
2	Benzene, 1,3-dimethoxy-2-nitro-	183	C8H9NO4	006665-97-0	38
3	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	37
4	2-Thiopheneacetic acid, propyl e...	184	C9H12O2S	153850-63-6	22
5	Benzenamine, 2,4-dinitro-	183	C6H5N3O4	000097-02-9	22



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

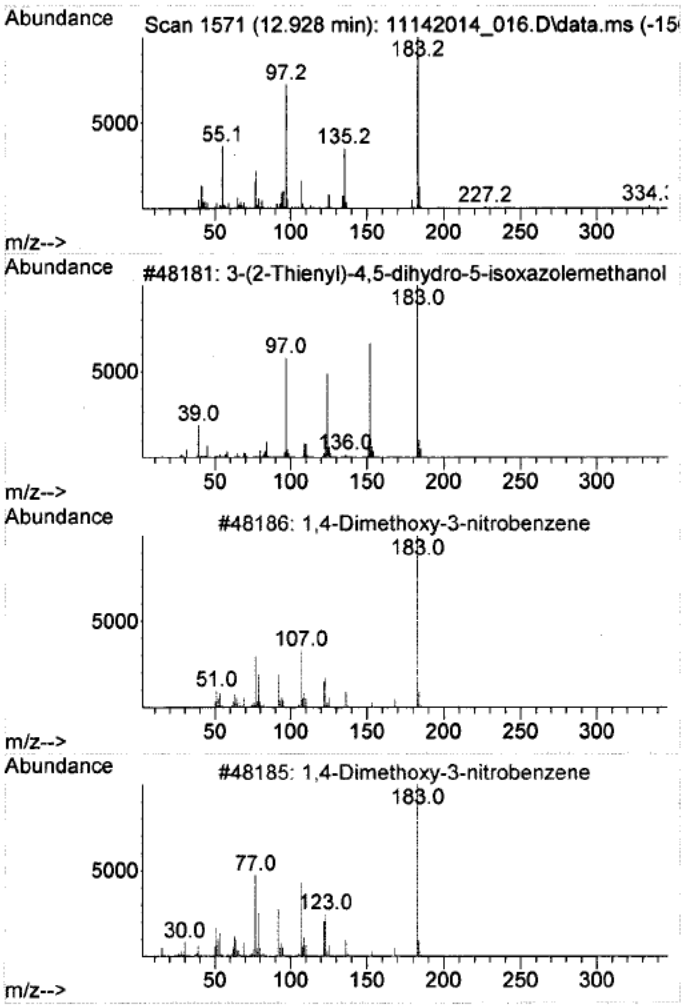
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

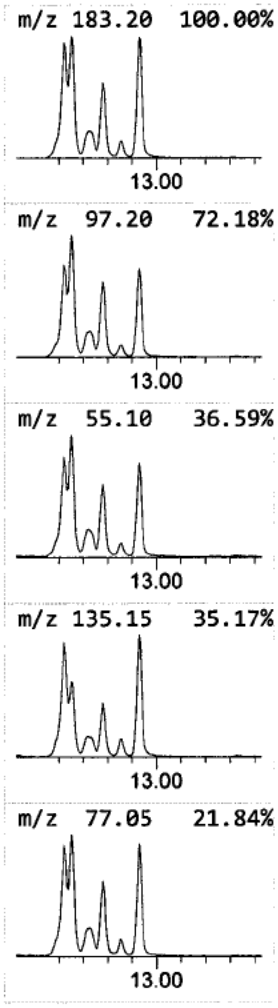
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

****
Peak Number 20 3-(2-Thienyl)-4,5-dihydro-5... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.928	12.20 ug/mL	1639570	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Thienyl)-4,5-dihydro-5-isox...	183	C8H9NO2S	022353-85-1	49
2	1,4-Dimethoxy-3-nitrobenzene	183	C8H9NO4	000089-39-4	47
3	1,4-Dimethoxy-3-nitrobenzene	183	C8H9NO4	000089-39-4	47
4	Benzene, 1,2-dimethoxy-4-nitro-	183	C8H9NO4	000709-09-1	38
5	5,8-Methano-4H-3,1-benzoxazine-2...	183	C9H13NOS	1000142-76-8	38





Tentatively Identified Compound (LSC) summary

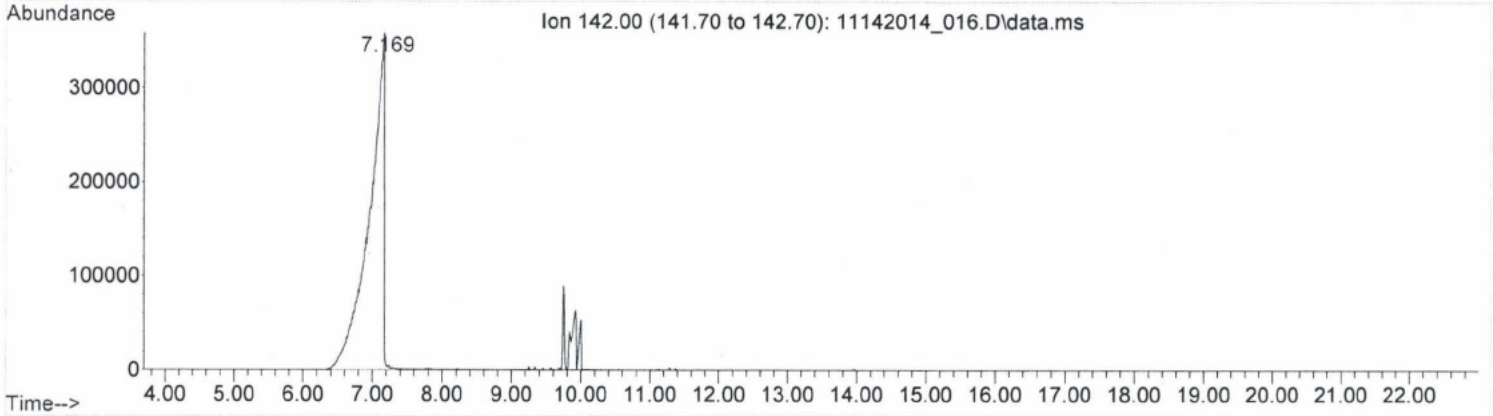
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_016.D
Acq On : 14 Nov 2014 05:13 pm
Operator : [redacted]
Sample : NE36691
Misc : Tag # NE36691, 10X
ALS Vial : 15 Sample Multiplier: 1

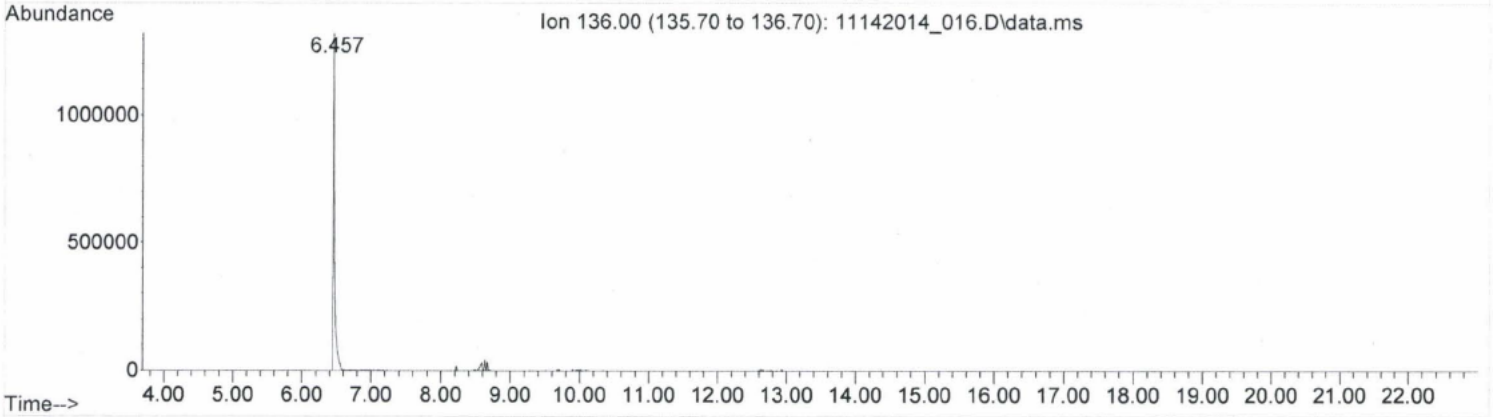
Quant Method : D:\MassHunter\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

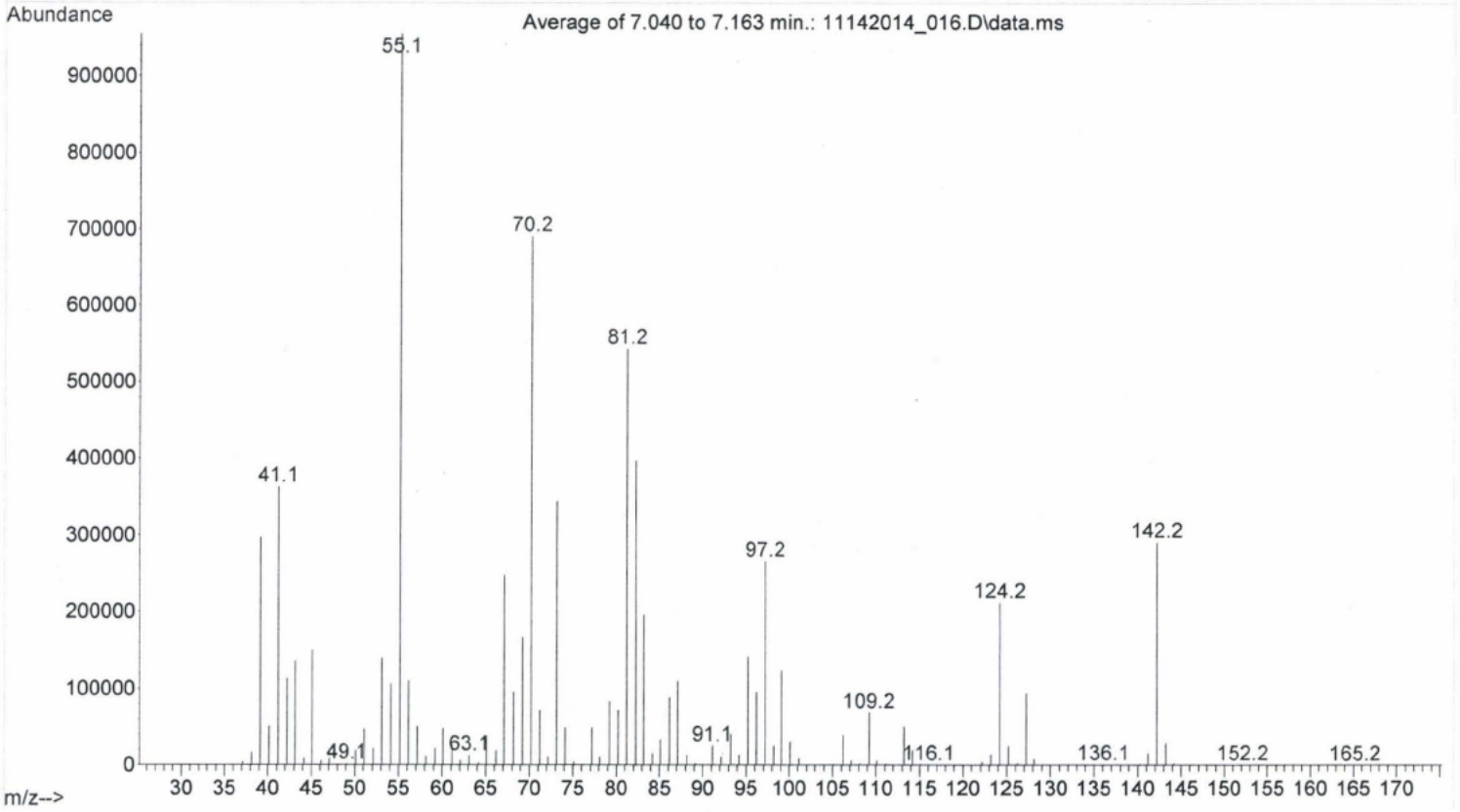
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Cyclohexanemeth...	5.734	45.0	ug/mL	6444920	1	5.081	2866890	20.0
Cyclohexanecarb...	7.163	516.0	ug/mL	154807000	2	6.457	6000020	20.0
1-Methylcyclohe...	7.240	4.2	ug/mL	1259860	2	6.457	6000020	20.0
Bicyclo[3.3.1]n...	7.840	17.3	ug/mL	4140610	3	8.222	4787260	20.0
Carbonic acid, ...	8.487	32.8	ug/mL	7839800	3	8.222	4787260	20.0
4-Undecen-6-one	9.334	4.3	ug/mL	943846	4	9.698	4437730	20.0
Cyclobutanecarb...	9.534	6.0	ug/mL	1342370	4	9.698	4437730	20.0
1-(Dimethylamin...	9.610	2.3	ug/mL	503614	4	9.698	4437730	20.0
2-Pentenoic aci...	9.751	36.6	ug/mL	8130680	4	9.698	4437730	20.0
1,3-Dimethyl-1-...	9.928	230.4	ug/mL	51113300	4	9.698	4437730	20.0
Cyclohexene, 1,...	10.004	136.6	ug/mL	30303700	4	9.698	4437730	20.0
3-Methoxybenzoi...	10.087	2.9	ug/mL	643988	4	9.698	4437730	20.0
2,4-Quinolinediol	10.334	3.0	ug/mL	658022	4	9.698	4437730	20.0
2-Naphthalenami...	11.128	2.4	ug/mL	531060	4	9.698	4437730	20.0
1-Methyl-2-meth...	11.292	21.1	ug/mL	4680650	4	9.698	4437730	20.0
Cyclohexene, 1,...	11.375	11.0	ug/mL	2440800	4	9.698	4437730	20.0
3-(2-Thienyl)-4...	12.651	27.7	ug/mL	3715970	5	13.969	2687180	20.0
Benzene, 1,2-di...	12.722	5.1	ug/mL	681715	5	13.969	2687180	20.0
3-(2-Thienyl)-4...	12.781	8.6	ug/mL	1148980	5	13.969	2687180	20.0
3-(2-Thienyl)-4...	12.928	12.2	ug/mL	1639570	5	13.969	2687180	20.0

File :D:[redacted]\RP1616\11142014_Run\11142014_016.D
Operator : [redacted]
Acquired : 14 Nov 2014 05:13 pm using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36691
Misc Info : Tag # NE36691, 10X
Vial Number: 15







[redacted] RP1616 12/17/14