LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM112717\
Data File : BM013127.D
Acq On : 28 Nov 2017 00:56
Operator : SJ/JU
Sample : I6514-03DL 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC3DL

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.551	71	79	97	rVB2	83973	267987	5.04%	0.458%
2	4.075	125	168	170	rBV2	765356	5322086	100.00%	9.095%
3	4.675	259	270	275	rBV	172053	395734	7.44%	0.676%
4	4.810	283	293	301	rBV2	142839	288848	5.43%	0.494%
5	5.434	357	399	404	rBV2	710461	5004889	94.04%	8.553%
6	6.816	614	634	638	rBV	360030	1231159	23.13%	2.104%
7	6.916	641	651	659	rVB2	491296	1160780	21.81%	1.984%
8	7.045	667	673	681	rVB	189808	296865	5.58%	0.507%
9	7.245	699	707	714	rBV	255312	409335	7.69%	0.700%
10	7.704	779	785	793	rBV	1029445	1634620	30.71%	2.793%
11	8.416	901	906	911	rBV	325615	516151	9.70%	0.882%
12	8.486	911	918	926	rVB	2335487	4046013	76.02%	6.914%
13	8.857	973	981	988	rVB	261632	424661	7.98%	0.726%
14	9.157	1019	1032	1044	rBV3	232981	608430	11.43%	1.040%
15	9.575	1097	1103	1116	rVB	222880	373518	7.02%	0.638%
16	9.951	1159	1167	1175	rVB2	55598	109627	2.06%	0.187%
17	10.116	1188	1195	1205	rBV	337162	558305	10.49%	0.954%
18	10.486	1250	1258	1265	rBV	1495660	2432642	45.71%	4.157%
19	10.627	1276	1282	1291	rBV	239684	413906	7.78%	0.707%
20	11.051	1344	1354	1363	rBV	266483	539352	10.13%	0.922%
21	11.321	1391	1400	1407	rBV	76428	136736	2.57%	0.234%
22	11.557	1429	1440	1452	rBV	1100676	1909811	35.88%	3.264%
23	12.316	1563	1569	1579	rBV	240895	416092	7.82%	0.711%
24	12.527	1600	1605	1617	rVB2	129820	211814	3.98%	0.362%
25	12.798	1645	1651	1656	rBV4	41223	62857	1.18%	0.107%
26	13.757	1809	1814	1819	rBV	638104	905487	17.01%	1.547%
27	13.810	1819	1823	1831	rVB	92619	135007	2.54%	0.231%
28	14.033	1851	1861	1869	rBV	693530	1094331	20.56%	1.870%
29	14.345	1908	1914	1922	rBV2	2269429	3443155	64.70%	5.884%
30	14.568	1945	1952	1961	rBV	273017	449269	8.44%	0.768%
31	15.339	2076	2083	2089	rBV2	895535	1269338	23.85%	2.169%
32	15.457	2098	2103	2114	rBV2	297736	456144	8.57%	0.780%
33	15.851	2161	2170	2175	rVB8	66349	161144	3.03%	0.275%
34	16.433	2264	2269	2276	rBV	1255245	1744831	32.78%	2.982%

LSC Area Percent Report

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Misc :
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Instrument : BNA_M
ClientSampleId : C0AC3DL

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Title : SVOA CALIBRATION

35	17.092	2372	2381	2386	rBV2	3107418	4413152	82.92%	7.542%
36	17.133	2386	2388	2392	rVV2	136271	179744	3.38%	0.307%
37	17.186	2392	2397	2407	rVB	953390	1455102	27.34%	2.487%
38	17.998	2529	2535	2545	rBV	430321	639204	12.01%	1.092%
39	18.139	2554	2559	2564	rVV2	68974	100133	1.88%	0.171%
40	18.321	2584	2590	2597	rBV4	64504	122910	2.31%	0.210%
41	18.492	2614	2619	2624	rBV	110958	150959	2.84%	0.258%
42	19.280	2749	2753	2761	rBV	422123	583464	10.96%	0.997%
43	19.486	2782	2788	2795	rBV	1175461	1610856	30.27%	2.753%
44	20.180	2903	2906	2910	rVB	76574	92279	1.73%	0.158%
45	20.486	2954	2958	2963	rBV3	66278	105384	1.98%	0.180%
46	20.997	3041	3045	3054	rBV2	254516	365065	6.86%	0.624%
47	21.274	3087	3092	3099	rBV	3890252	4953574	93.08%	8.465%
48	22.338	3270	3273	3276	rBV3	64594	73365	1.38%	0.125%
49	23.356	3441	3446	3452	rBV2	691771	1239343	23.29%	2.118%
50	23.503	3464	3471	3483	rVB	2126138	4000472	75.17%	6.837%

Sum of corrected areas: 58515930

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ClientSampleId :
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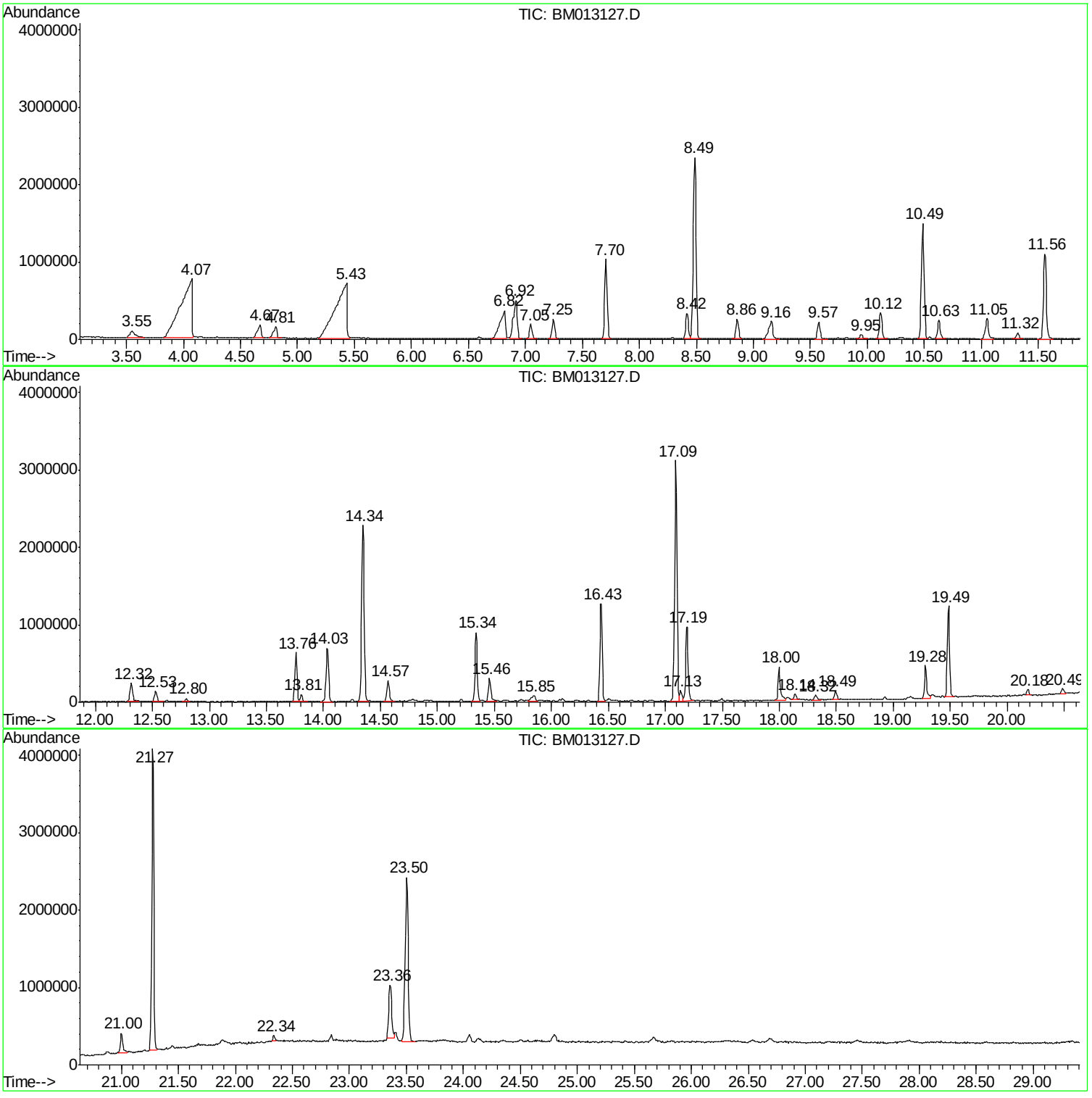
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Sample : I6514-03DL 5X
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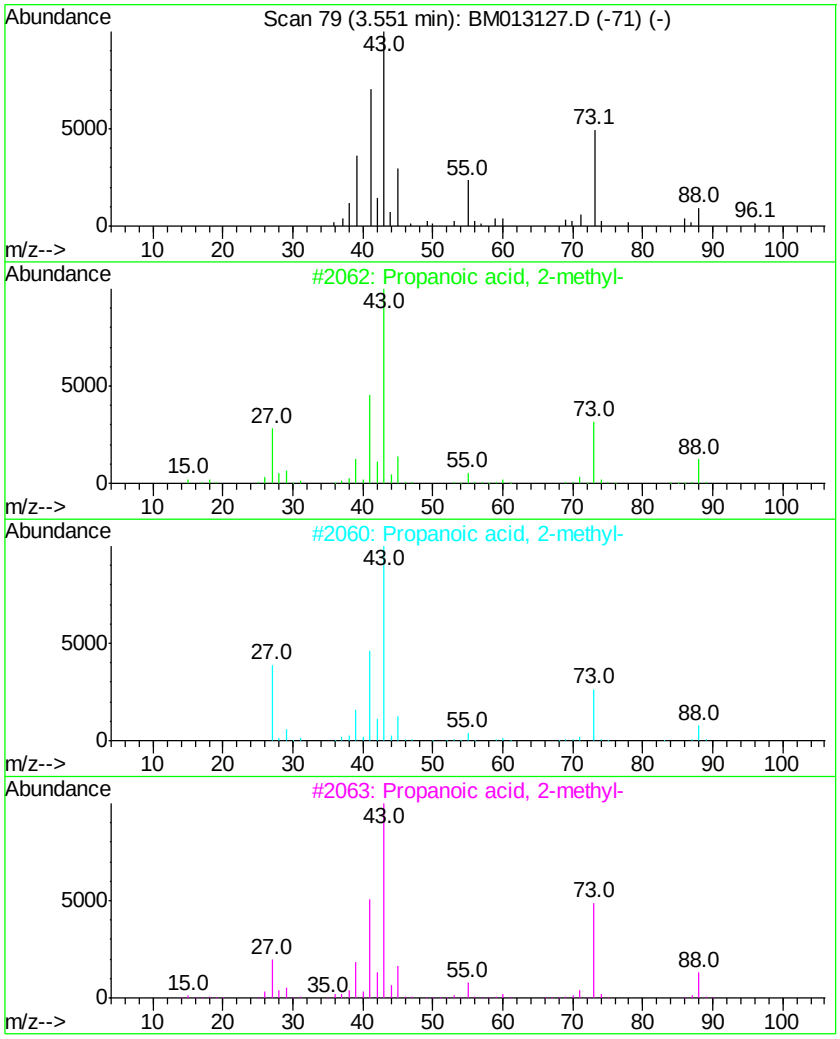
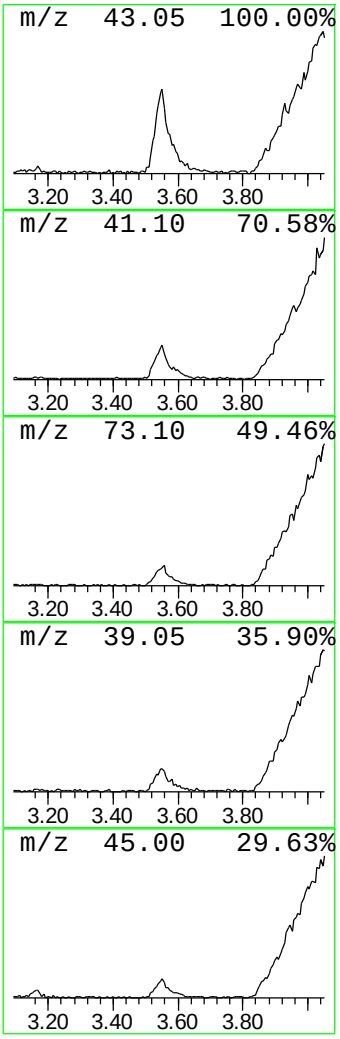
Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.55	3.28 ng/ul	267987	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	59
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	58
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	53
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	52
5	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	47





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Instrument : BNA_M
ClientSampleId : C0AC3DL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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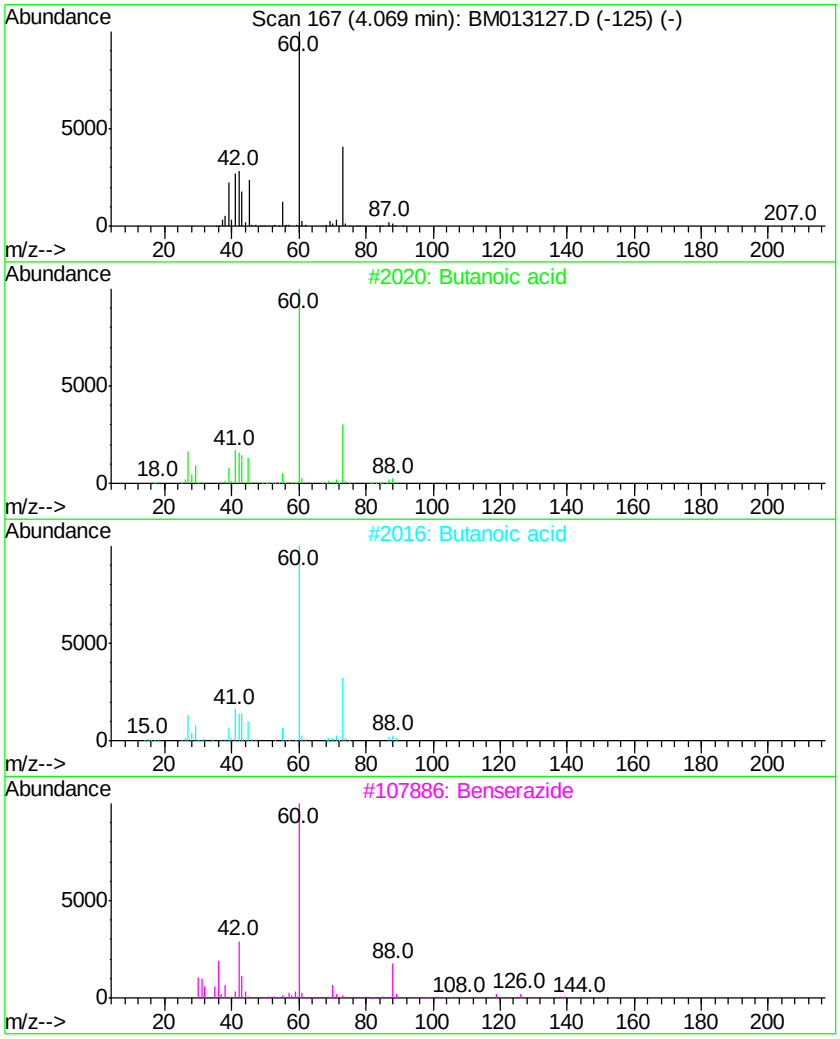
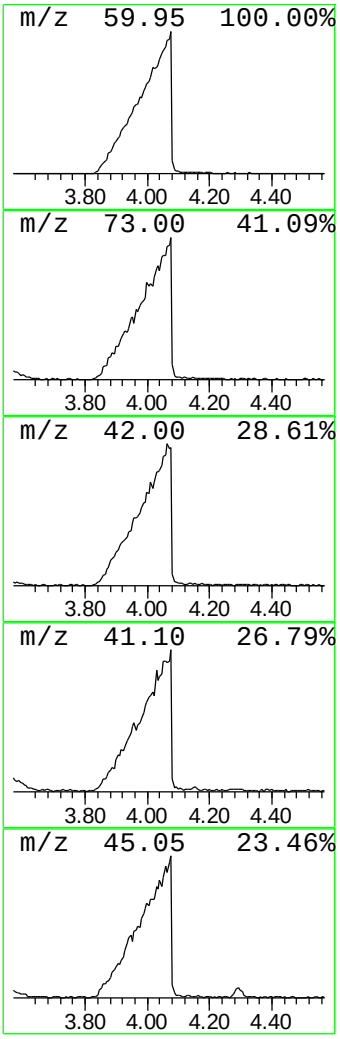
Peak Number 2 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	65.12 ng/ul	5322090	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	64
2	Butanoic acid	88	C4H8O2	000107-92-6	50
3	Benserazide	257	C10H15N3O5	000322-35-0	9
4	5-Hexenoic acid	114	C6H10O2	001577-22-6	9
5	Pentanoic acid	102	C5H10O2	000109-52-4	9





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC3DL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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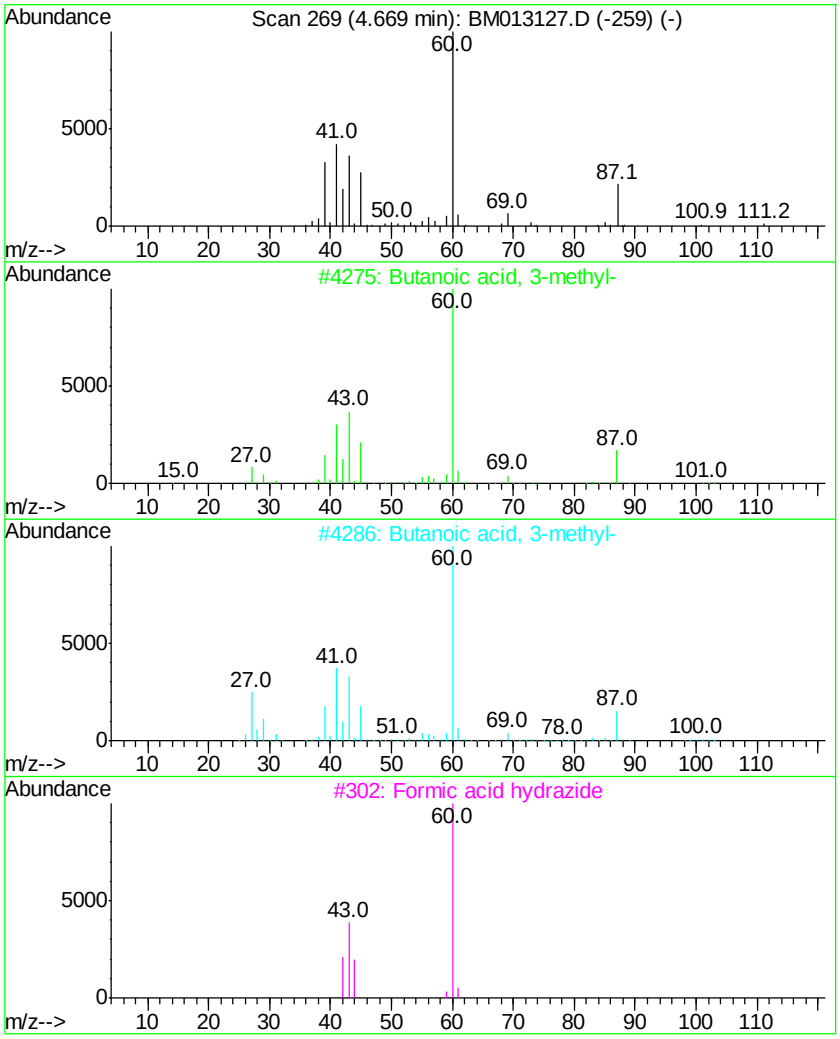
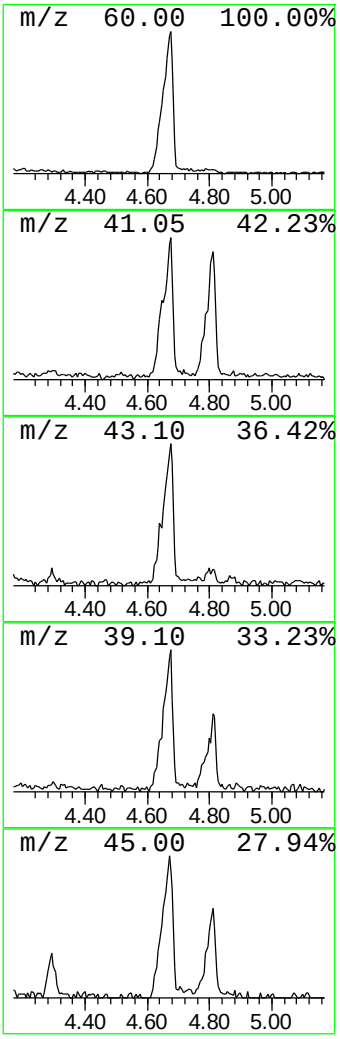
Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	4.84 ng/ul	395734	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	50
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	45
5	Benserazide	257	C10H15N3O5	000322-35-0	42





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC3DL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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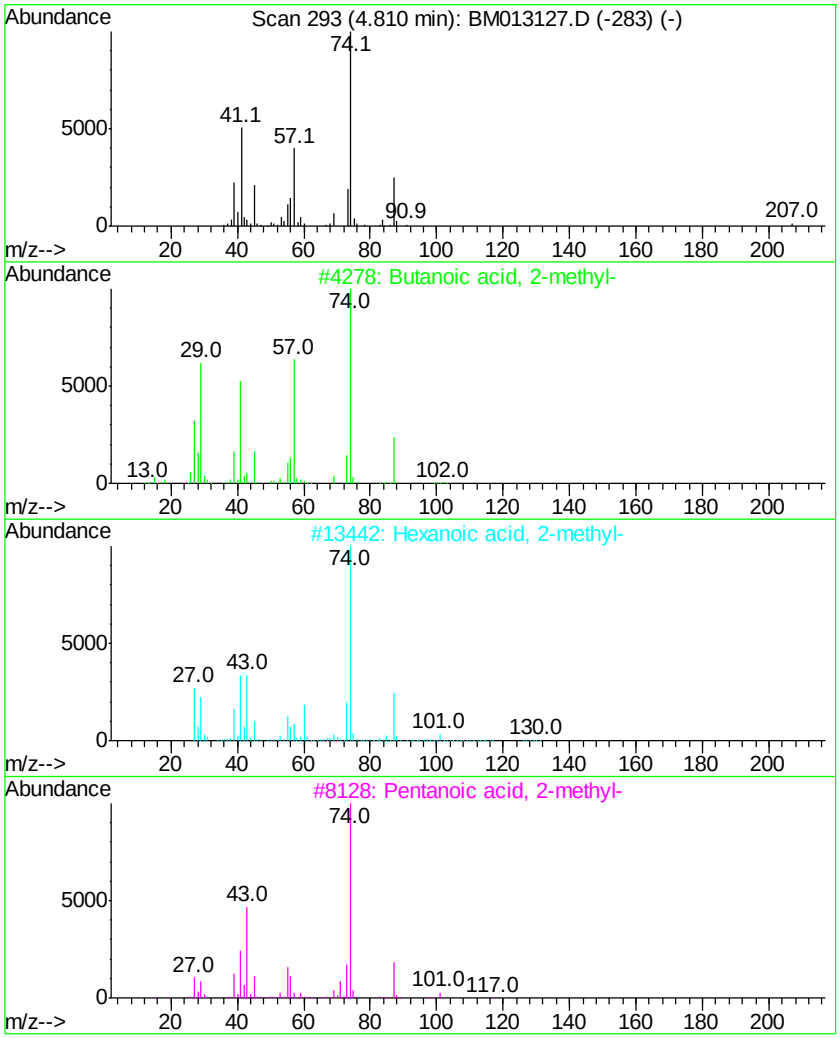
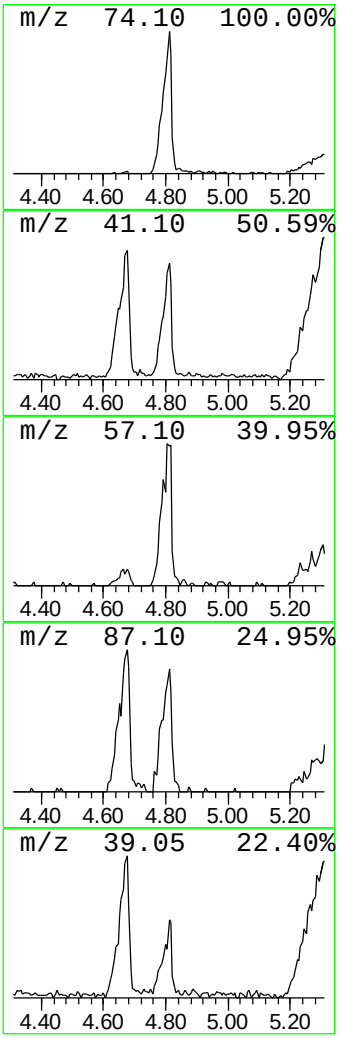
Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	3.53 ng/ul	288848	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	64
3	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64
4	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	50
5	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	50





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Instrument : BNA_M
ClientSampleId : C0AC3DL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

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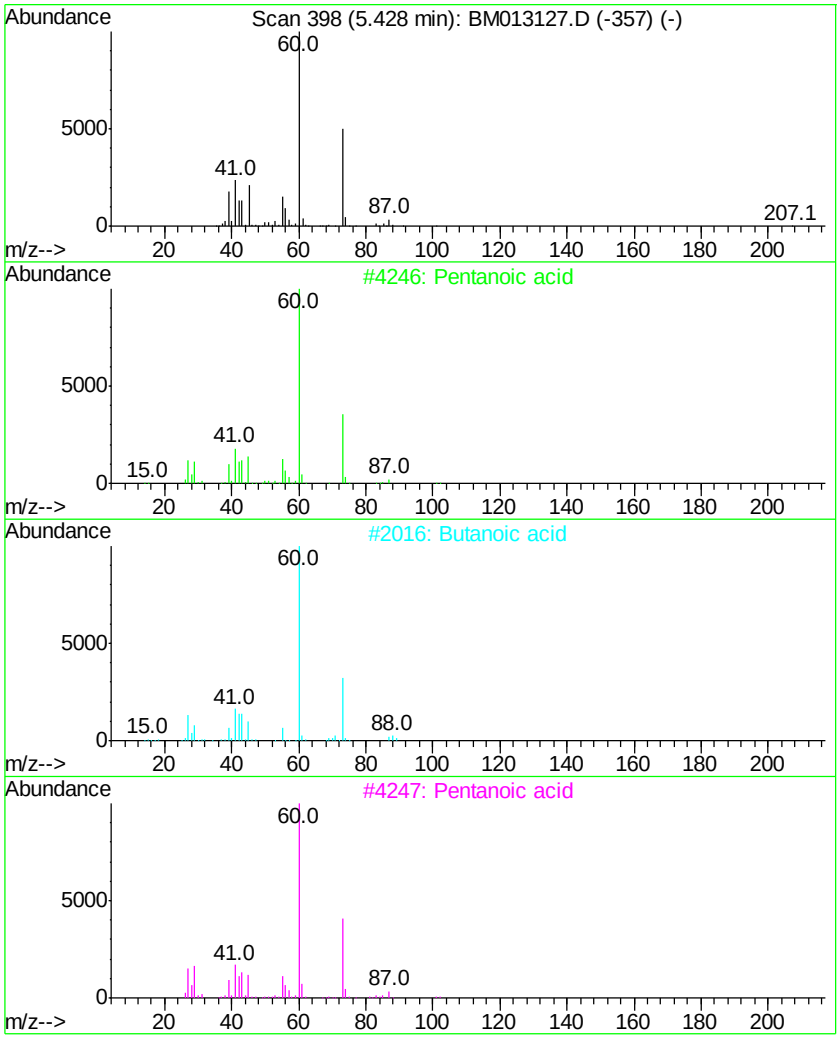
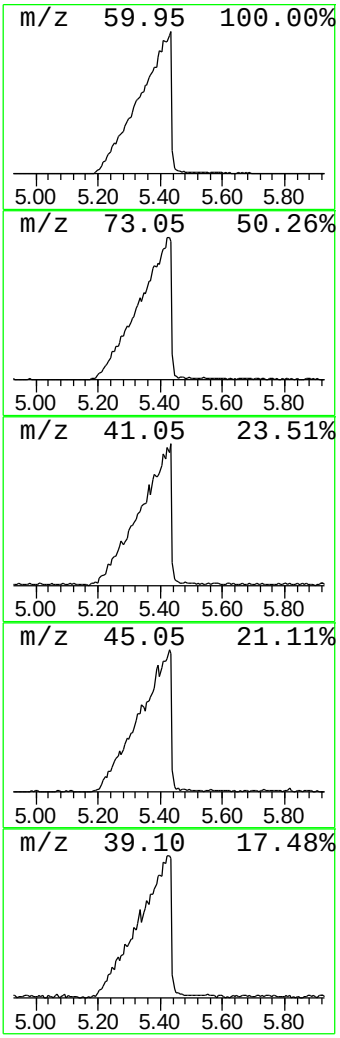
Peak Number 5 Pentanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.43	61.24 ng/ul	5004890	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	78
2	Butanoic acid	88	C4H8O2	000107-92-6	72
3	Pentanoic acid	102	C5H10O2	000109-52-4	64
4	Hexanoic acid	116	C6H12O2	000142-62-1	56
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





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Quant Title : SVOA CALIBRATION

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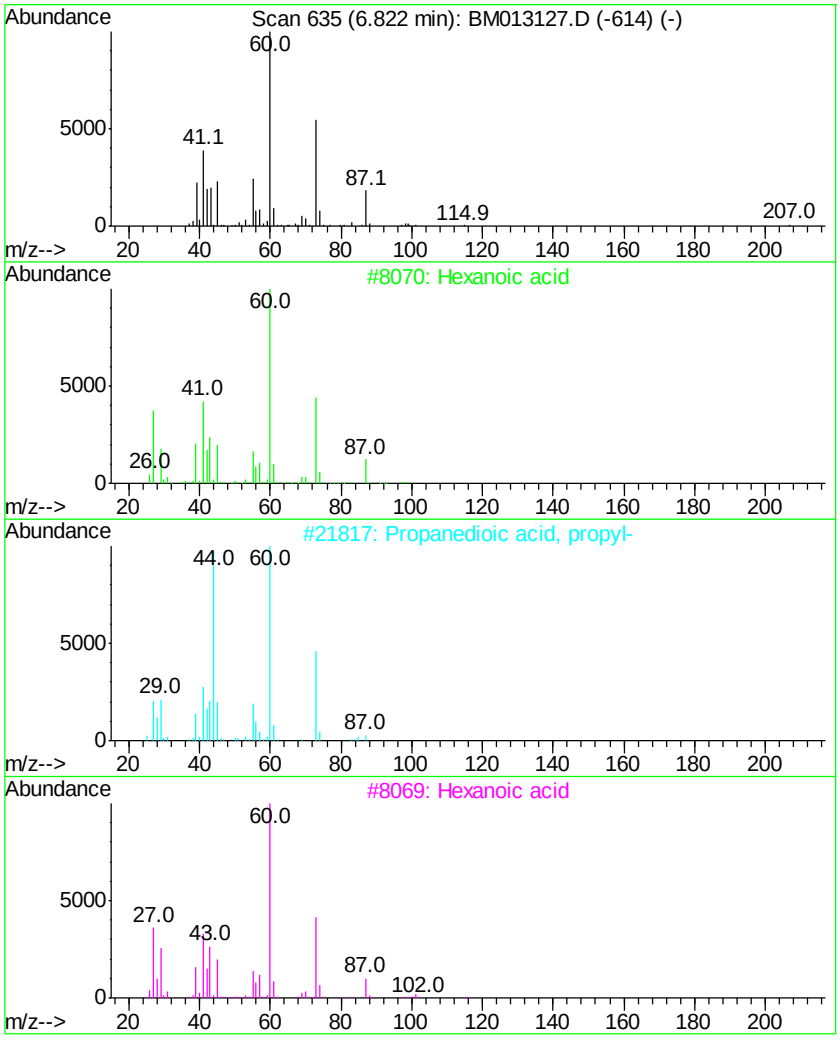
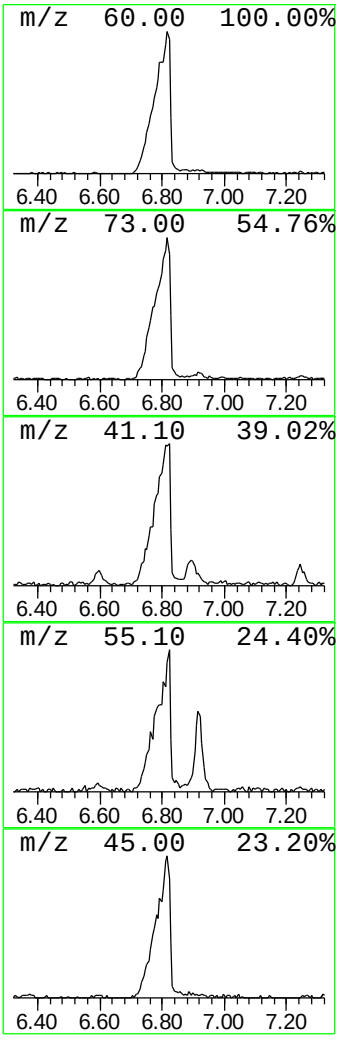
Peak Number 6 Hexanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	15.06 ng/ul	1231160	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	78
3	Hexanoic acid	116	C6H12O2	000142-62-1	74
4	Pentanoic acid	102	C5H10O2	000109-52-4	72
5	Hexanoic acid	116	C6H12O2	000142-62-1	72





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TIC Library : C:\DATABASE\NIST11.L
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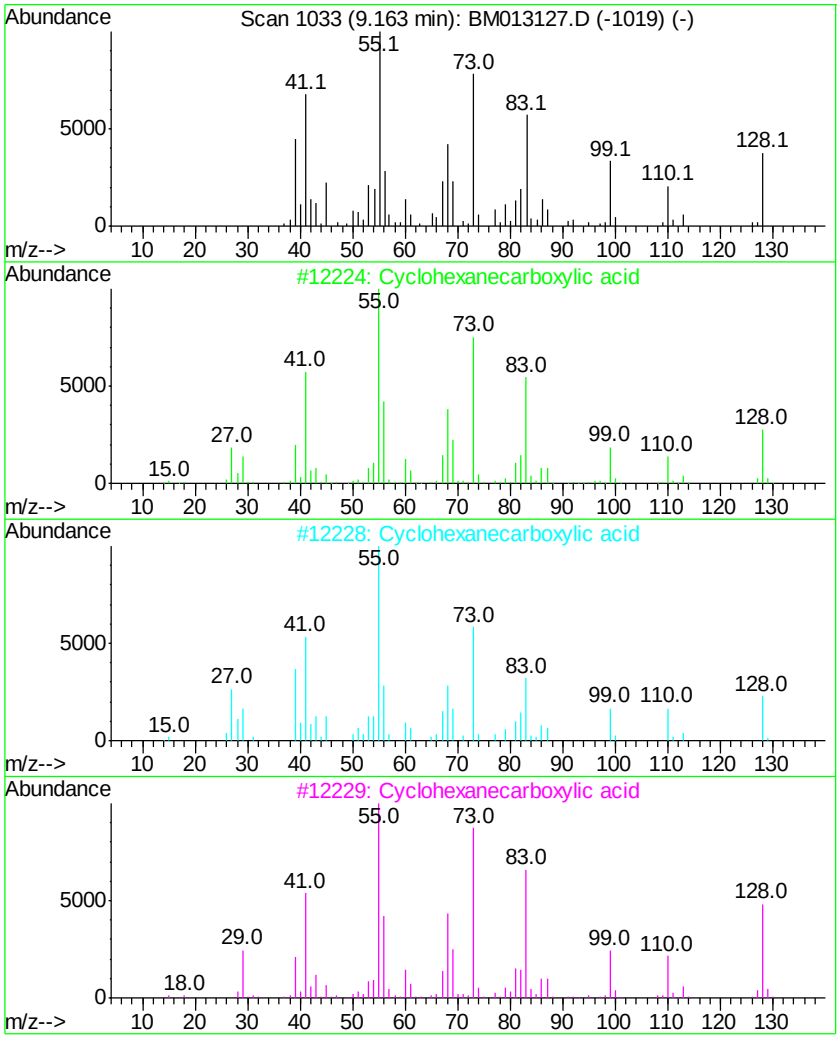
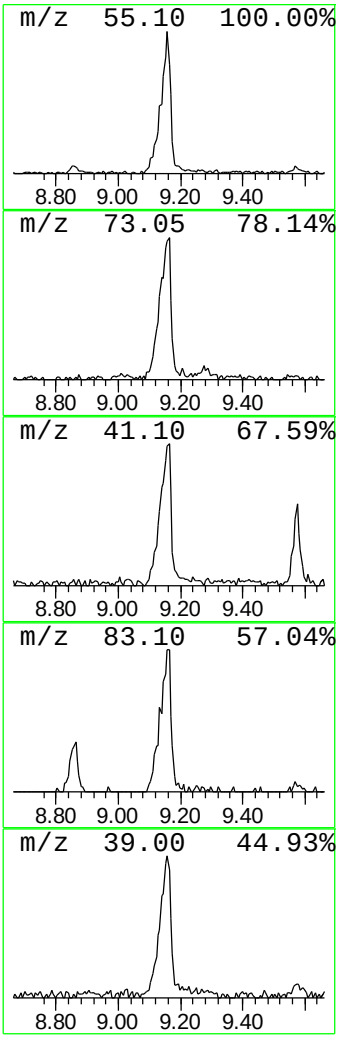
Peak Number 7 Cyclohexanecarboxylic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	5.00 ng/ul	608430	Naphthalene-d8	10.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	92
2	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	92
3	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	70
4	1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	35
5	2-Hexenoic acid	114	C6H10O2	001191-04-4	25





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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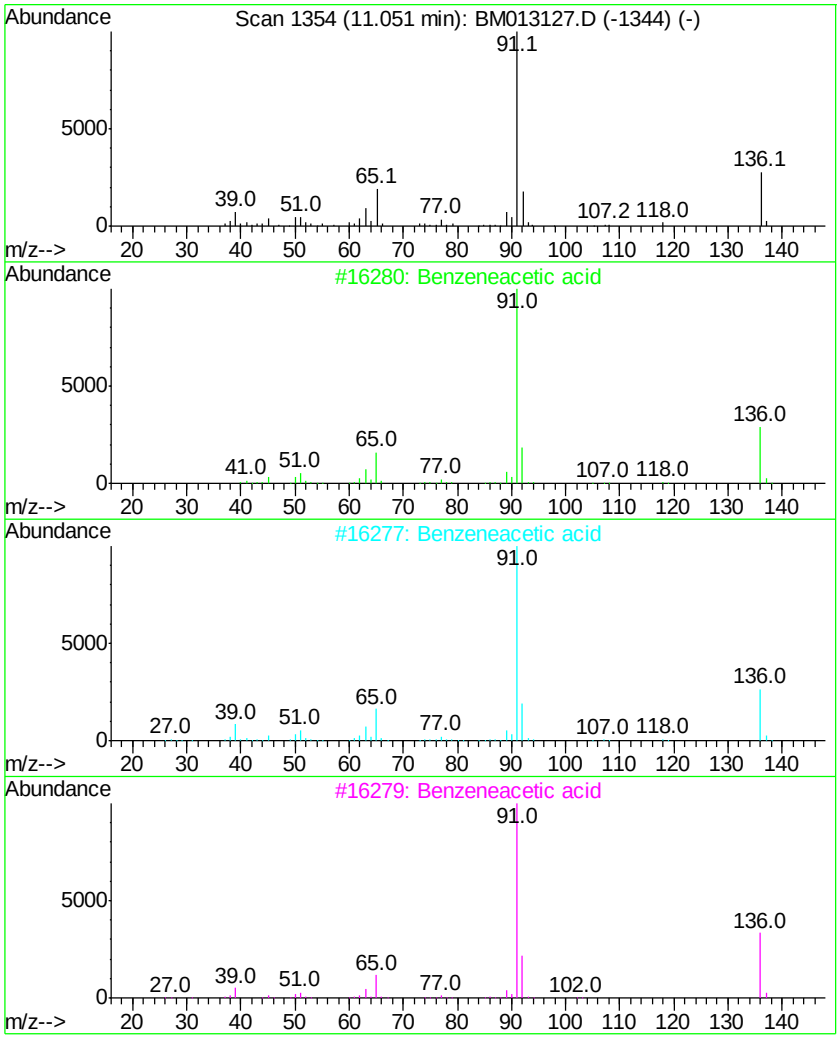
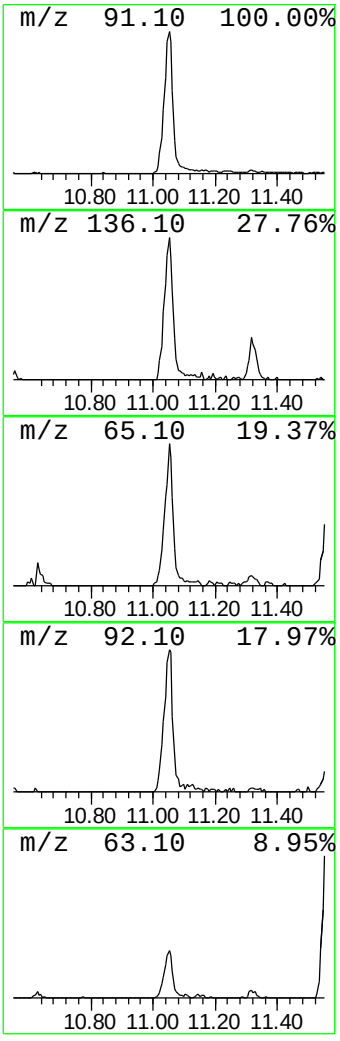
Peak Number 8 Benzeneacetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	4.43 ng/ul	539352	Naphthalene-d8	10.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	94
2	Benzeneacetic acid	136	C8H8O2	000103-82-2	91
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	87
4	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	59
5	Benzeneacetic acid	136	C8H8O2	000103-82-2	53





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Data File : BM013127.D
Acq On : 28 Nov 2017 00:56
Operator : SJ/JU
Sample : I6514-03DL 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC3DL

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111617.M
Quant Title : SVOA CALIBRATION

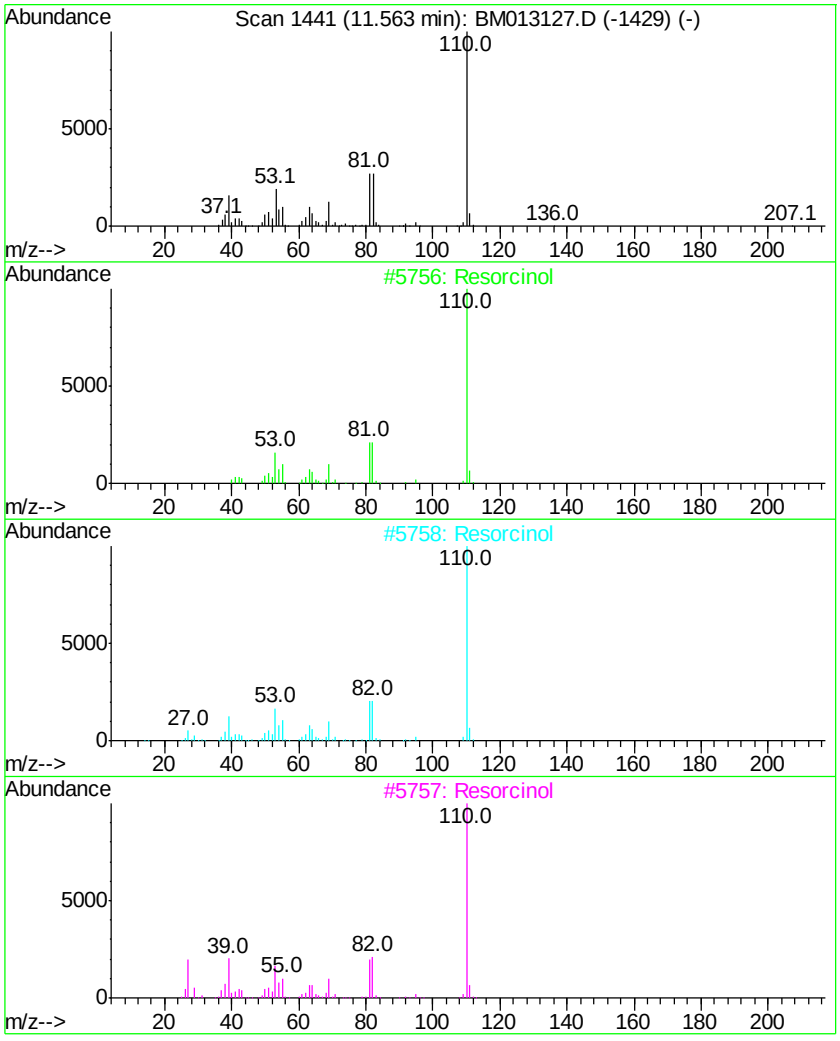
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

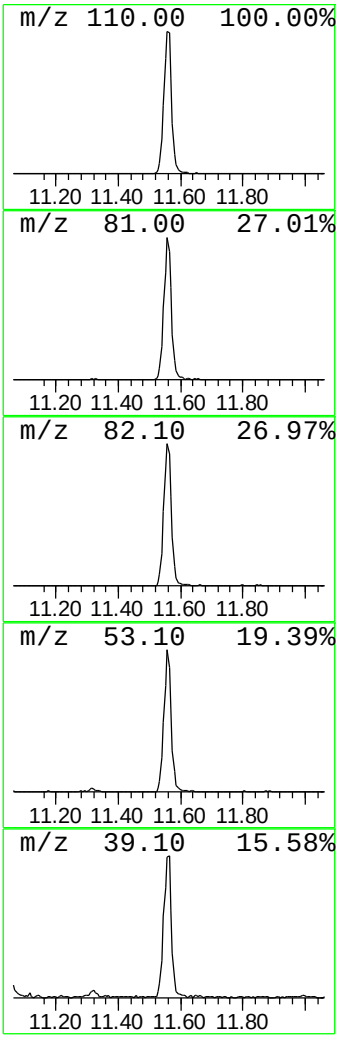
****

Peak Number 9 Resorcinol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	15.70 ng/ul	1909810	Naphthalene-d8	10.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Resorcinol	110	C6H6O2	000108-46-3	97
2	Resorcinol	110	C6H6O2	000108-46-3	97
3	Resorcinol	110	C6H6O2	000108-46-3	94
4	Hydroquinone	110	C6H6O2	000123-31-9	80
5	Resorcinol	110	C6H6O2	000108-46-3	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM112717\
Data File : BM013127.D
Acq On : 28 Nov 2017 00:56
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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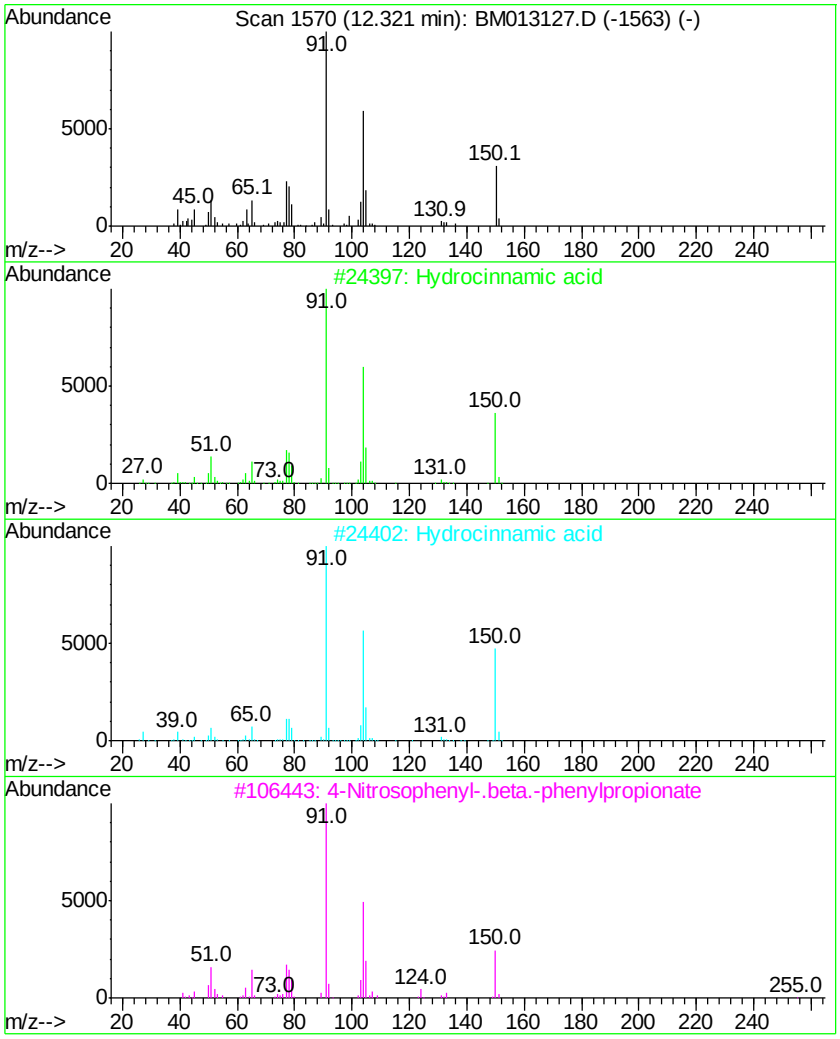
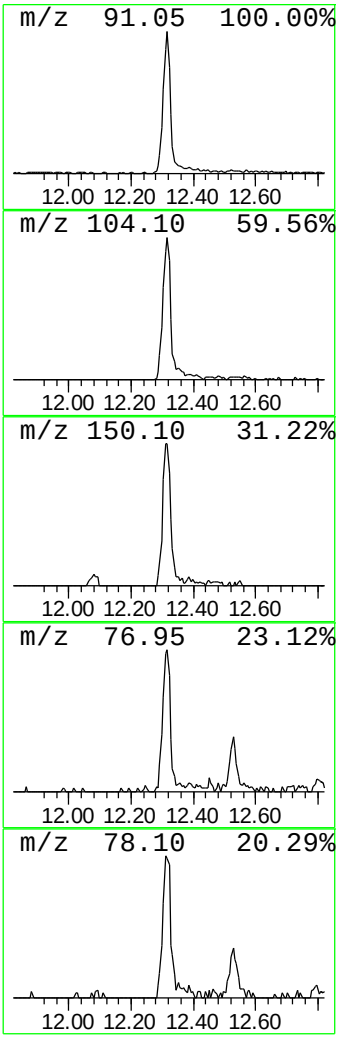
Peak Number 10 Hydrocinnamic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	3.42 ng/ul	416092	Naphthalene-d8	10.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
2	Hydrocinnamic acid	150	C9H10O2	000501-52-0	87
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
4	Hydrocinnamic acid	150	C9H10O2	000501-52-0	81
5	Hydrocinnamic acid	150	C9H10O2	000501-52-0	80





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Sample : I6514-03DL 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC3DL

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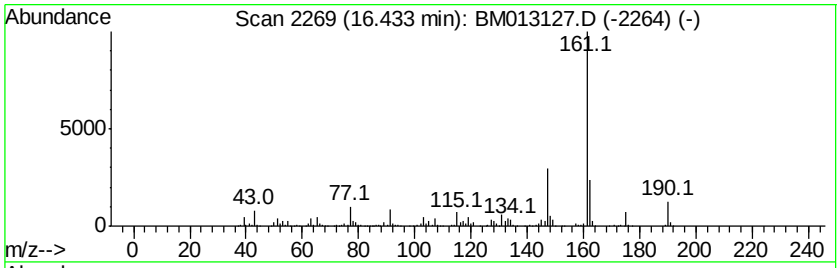
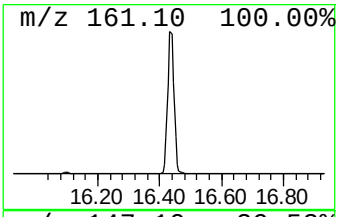
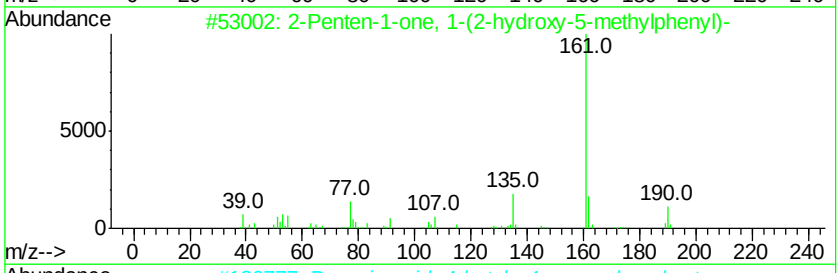
Peak Number 11 2-Penten-1-one, 1-(2-hydrox... Concentration Rank 5

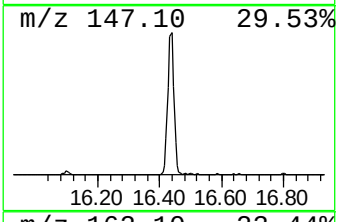
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	7.91 ng/ul	1744830	Phenanthrene-d10	17.09

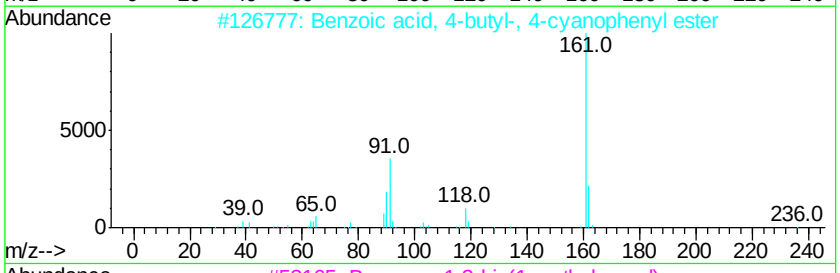
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Penten-1-one, 1-(2-hydroxy-5-m...	190	C12H14O2	051956-78-6	58
2	Benzoic acid, 4-butyl-, 4-cyanop...	279	C18H17NO2	038690-77-6	47
3	Benzene, 1,3-bis(1-methylpropyl)-	190	C14H22	001079-96-5	45
4	Benzeneacetaldehyde, .alpha.-met...	190	C13H18O	051407-46-6	45
5	Benzene, ethylpentamethyl-	176	C13H20	002388-04-7	42

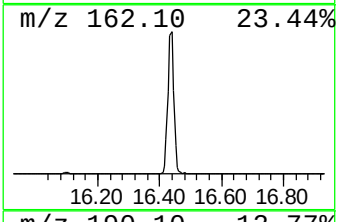


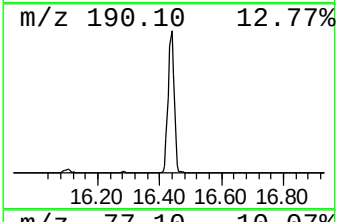


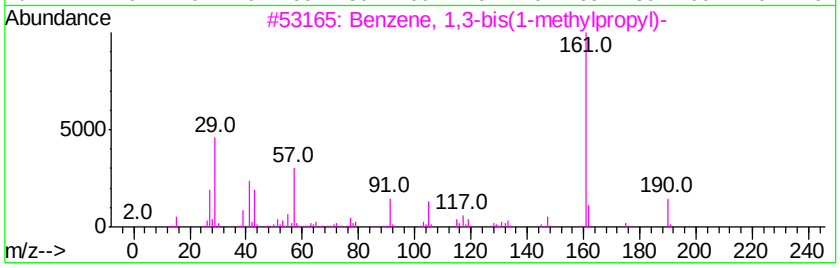


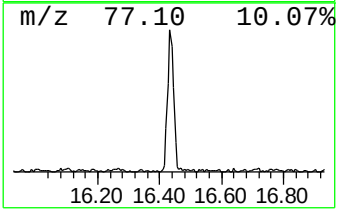












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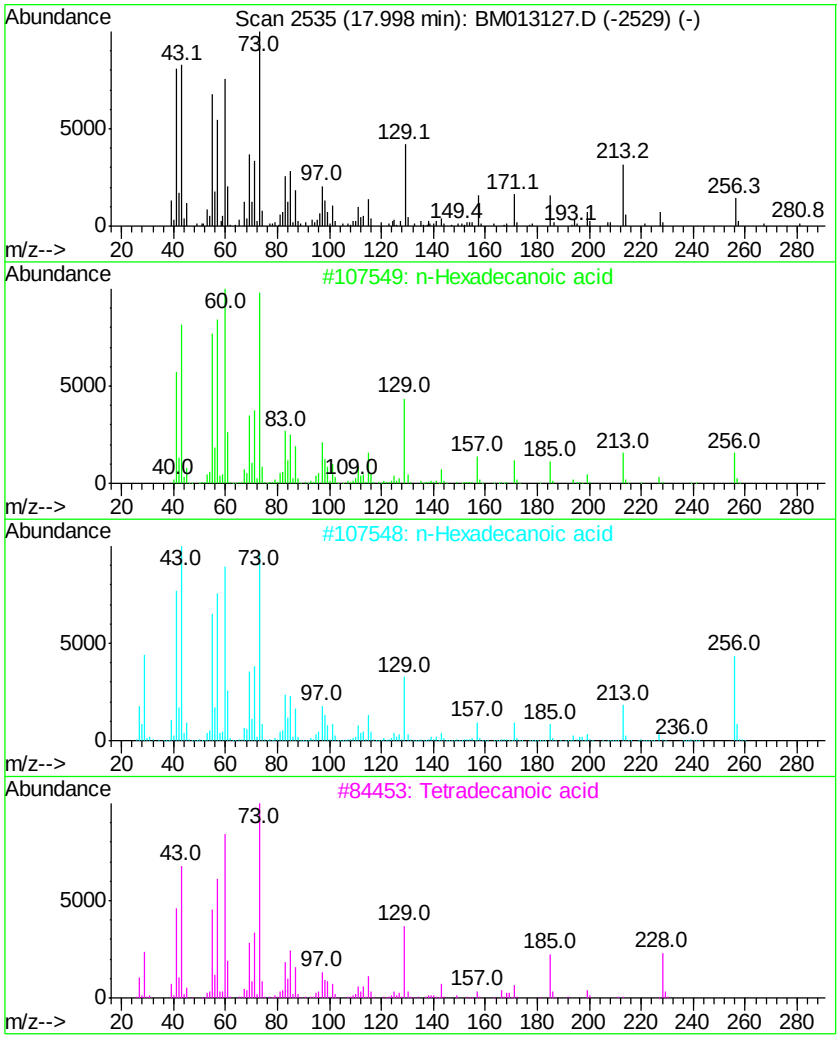
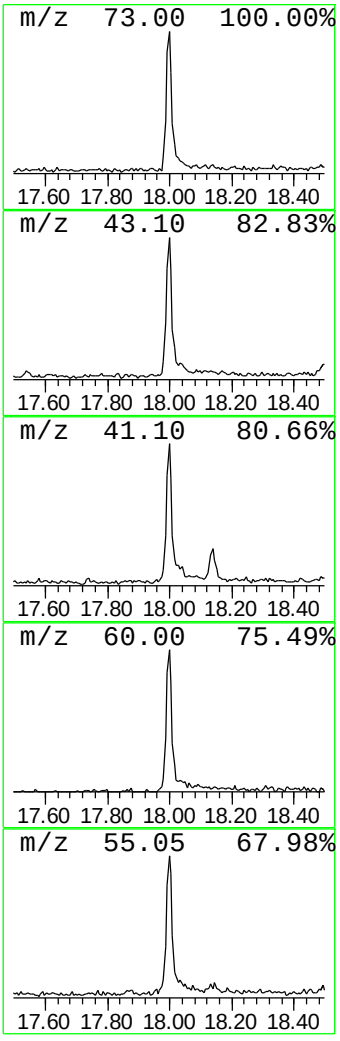
Peak Number 12 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	2.90 ng/ul	639204	Phenanthrene-d10	17.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	89





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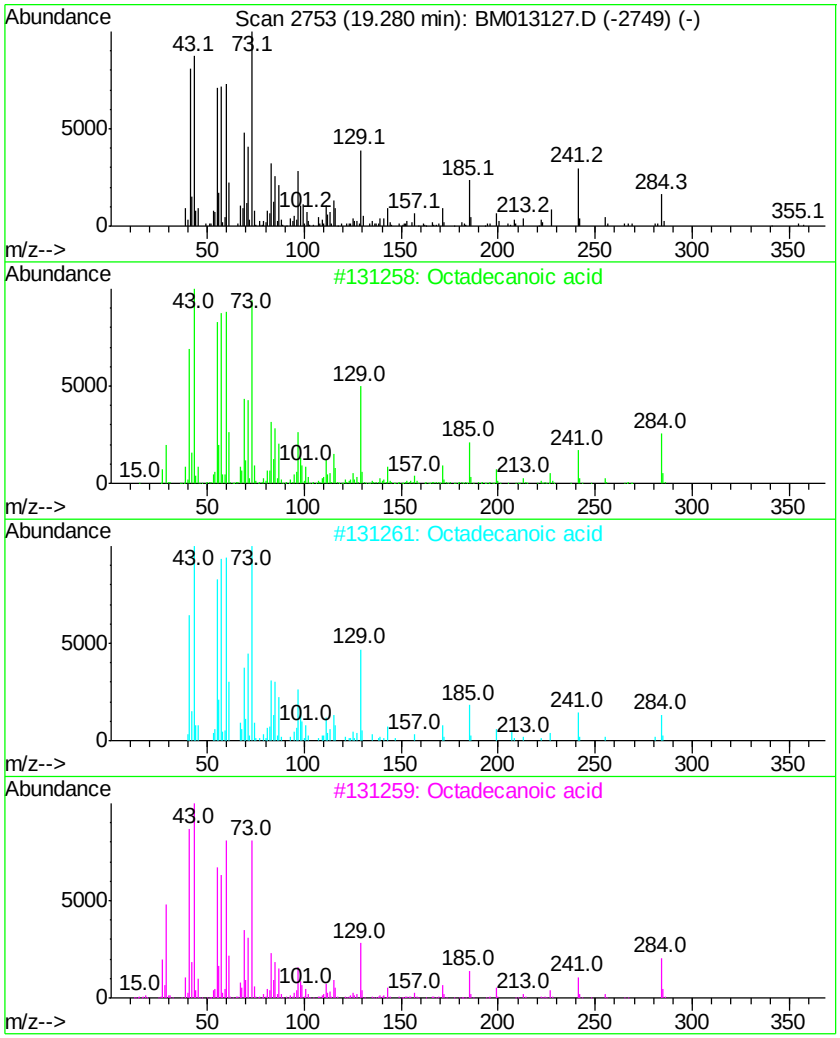
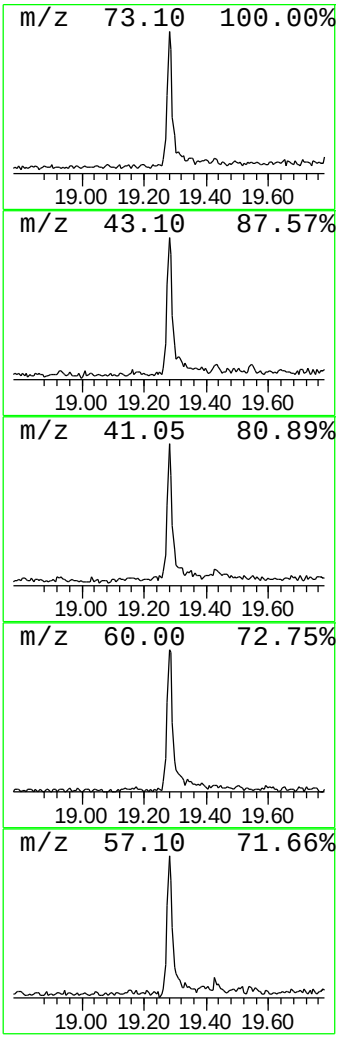
Peak Number 13 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	2.36 ng/ul	583464	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	95
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_M
ClientSampleId : C0AC3DL

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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid, 2...	3.55	3.3	ng/ul	267987	1	7.70	1634620	20.0
Butanoic acid	4.07	65.1	ng/ul	5322090	1	7.70	1634620	20.0
Butanoic acid, 3-...	4.67	4.8	ng/ul	395734	1	7.70	1634620	20.0
Butanoic acid, 2-...	4.81	3.5	ng/ul	288848	1	7.70	1634620	20.0
Pentanoic acid	5.43	61.2	ng/ul	5004890	1	7.70	1634620	20.0
Hexanoic acid	6.82	15.1	ng/ul	1231160	1	7.70	1634620	20.0
Cyclohexanecarbox...	9.16	5.0	ng/ul	608430	2	10.49	2432640	20.0
Benzeneacetic acid	11.05	4.4	ng/ul	539352	2	10.49	2432640	20.0
Resorcinol	11.56	15.7	ng/ul	1909810	2	10.49	2432640	20.0
Hydrocinnamic acid	12.32	3.4	ng/ul	416092	2	10.49	2432640	20.0
2-Penten-1-one, 1...	16.43	7.9	ng/ul	1744830	4	17.09	4413150	20.0
n-Hexadecanoic acid	18.00	2.9	ng/ul	639204	4	17.09	4413150	20.0
Octadecanoic acid	19.28	2.4	ng/ul	583464	5	21.27	4953570	20.0