LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM103017\
Data File : BM012592.D
Acq On : 31 Oct 2017 02:24
Operator : SJ/JU
Sample : I5886-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE9

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-BM102417.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	3.351	41	45	50	rBV	84387	113953	1.14%	0.104%
2	4.993	317	324	334	rVB2	112941	202716	2.03%	0.185%
3	7.022	660	669	683	rBV2	1397196	2537510	25.35%	2.320%
4	7.187	689	697	708	rBV	1131588	1708557	17.07%	1.562%
5	7.392	724	732	740	rBV	1467735	2356106	23.54%	2.154%
6	7.822	798	805	808	rBV	1930569	3042299	30.39%	2.782%
7	7.857	808	811	819	rVB	1326106	1904283	19.02%	1.741%
8	8.557	923	930	940	rBV	1689529	2698323	26.96%	2.467%
9	9.010	999	1007	1016	rBV	1359227	2189317	21.87%	2.002%
10	9.439	1072	1080	1088	rBV2	55257	134813	1.35%	0.123%
11	9.728	1122	1129	1137	rBV	1109829	1895523	18.94%	1.733%
12	10.269	1212	1221	1230	rBV	1786120	2920106	29.17%	2.670%
13	10.375	1230	1239	1255	rBV	2493297	3996134	39.92%	3.654%
14	10.645	1278	1285	1293	rBV	1637031	2732240	27.29%	2.498%
15	10.780	1298	1308	1322	rBV	1087323	1949484	19.47%	1.783%
16	11.957	1504	1508	1516	rVB	108006	170682	1.71%	0.156%
17	12.333	1563	1572	1580	rBV2	87810	158980	1.59%	0.145%
18	12.580	1609	1614	1620	rVB	113091	193204	1.93%	0.177%
19	13.033	1686	1691	1696	rVB4	81390	136664	1.37%	0.125%
20	13.598	1783	1787	1793	rVV2	74560	115930	1.16%	0.106%
21	13.892	1827	1837	1842	rBV	3149488	4370089	43.66%	3.996%
22	13.933	1842	1844	1848	rVV3	251265	364499	3.64%	0.333%
23	13.968	1848	1850	1854	rVB2	112052	125217	1.25%	0.114%
24	14.180	1879	1886	1896	rVB	3315839	5013020	50.08%	4.584%
25	14.486	1931	1938	1946	rBV2	2329657	3536242	35.33%	3.233%
26	14.686	1965	1972	1982	rBV	1059712	1746348	17.45%	1.597%
27	14.833	1993	1997	2003	rVV	152598	230114	2.30%	0.210%
28	15.186	2053	2057	2066	rVB2	62492	104477	1.04%	0.096%
29	15.474	2100	2106	2113	rBV	4136778	5955071	59.49%	5.445%
30	15.598	2121	2127	2135	rBV	1074937	1531456	15.30%	1.400%
31	15.839	2163	2168	2173	rBV	507364	720060	7.19%	0.658%
32	16.204	2225	2230	2231	rBV4	86466	115704	1.16%	0.106%
33	16.221	2231	2233	2237	rVB	119579	144651	1.45%	0.132%
34	16.998	2360	2365	2370	rBV4	78533	191119	1.91%	0.175%

LSC Area Percent Report

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Instrument : BNA_M
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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

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Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Title : SVOA CALIBRATION

35	17.121	2382	2386	2393	rVB7	88999	142997	1.43%	0.131%
36	17.227	2398	2404	2408	rVV2	3004565	4238240	42.34%	3.875%
37	17.268	2408	2411	2415	rVV	305017	410738	4.10%	0.376%
38	17.327	2415	2421	2431	rVB	4463542	6496927	64.90%	5.941%
39	17.798	2497	2501	2507	rVB6	86607	133463	1.33%	0.122%
40	18.115	2549	2555	2559	rBV2	505047	763485	7.63%	0.698%
41	18.227	2571	2574	2579	rVB	74671	101756	1.02%	0.093%
42	18.298	2581	2586	2589	rBV4	96725	175982	1.76%	0.161%
43	18.415	2602	2606	2609	rBV4	95431	123922	1.24%	0.113%
44	18.498	2616	2620	2624	rBV4	175301	278177	2.78%	0.254%
45	19.156	2729	2732	2738	rVB	125768	184001	1.84%	0.168%
46	19.280	2749	2753	2757	rVB	1142429	1368441	13.67%	1.251%
47	19.392	2767	2772	2775	rBV5	479751	774809	7.74%	0.708%
48	19.427	2775	2778	2783	rVB2	648646	811345	8.11%	0.742%
49	19.615	2802	2810	2814	rBV	6335665	10010347	100.00%	9.153%
50	21.109	3062	3064	3071	rVB3	535397	839150	8.38%	0.767%
51	21.397	3107	3113	3117	rBV2	4677752	7211194	72.04%	6.594%
52	21.433	3117	3119	3126	rVB	1041690	1380699	13.79%	1.262%
53	22.156	3238	3242	3253	rVB	2308885	3270550	32.67%	2.991%
54	22.997	3381	3385	3390	rBV3	1295125	2828439	28.26%	2.586%
55	23.550	3474	3479	3485	rBV2	4037560	7412687	74.05%	6.778%
56	23.697	3498	3504	3510	rBV	2793292	5100574	50.95%	4.664%

Sum of corrected areas: 109362814

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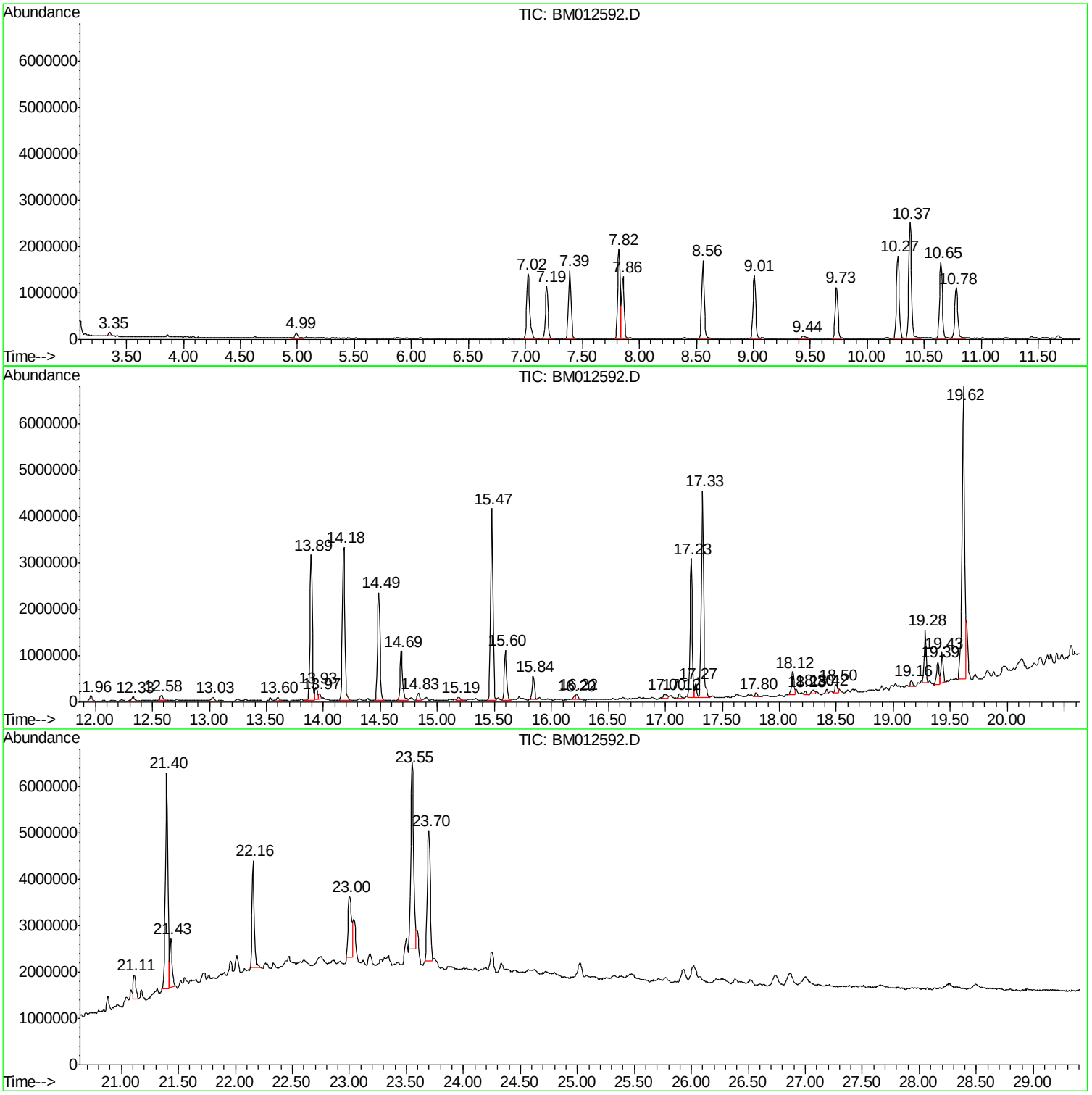
ClientSampleId : ESNE9

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

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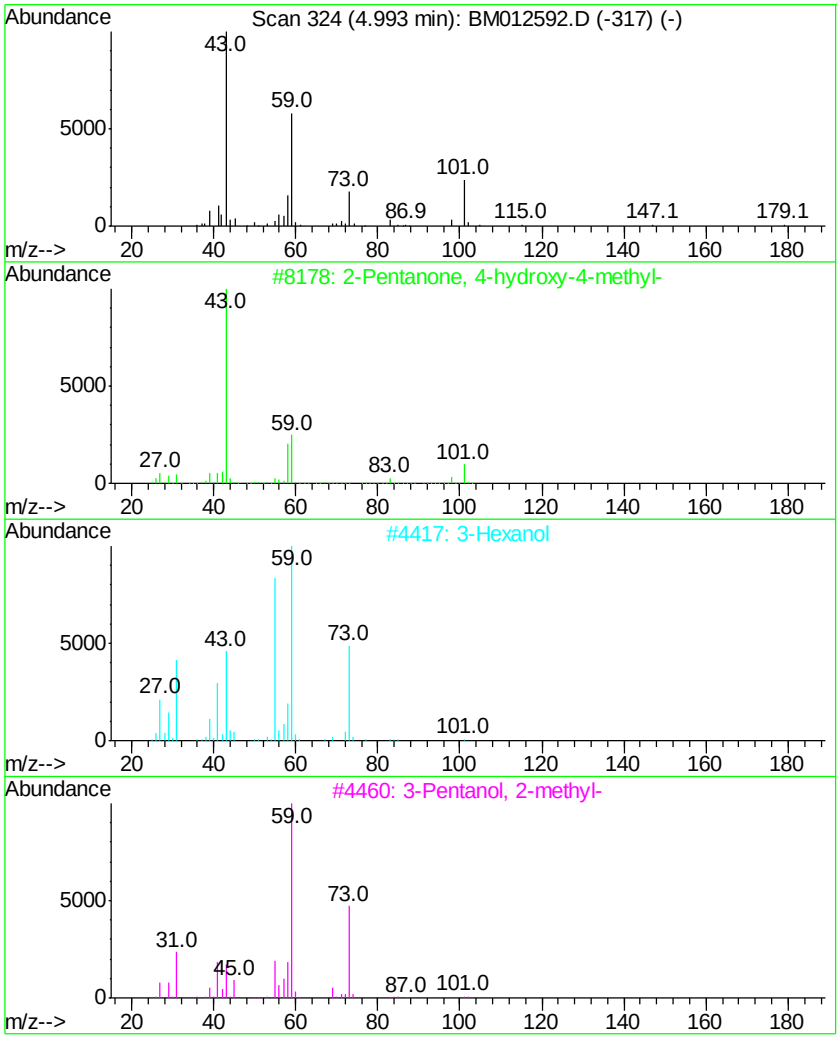
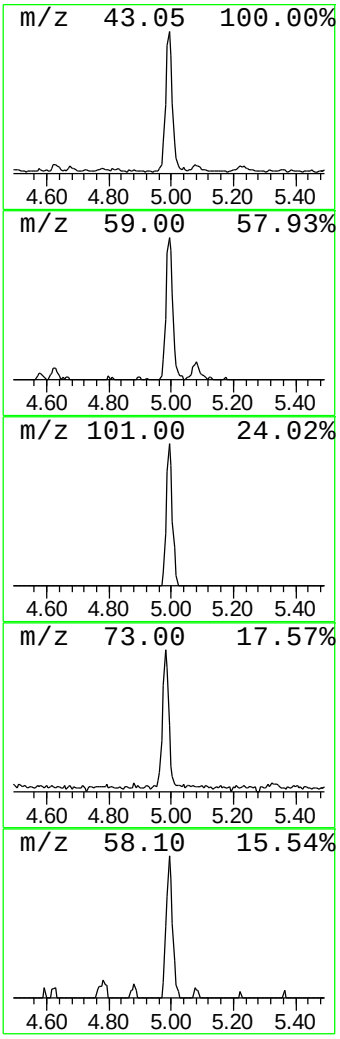
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	2.13 ng/ul	202716	1,4-Dichlorobenzene-d4	7.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	3-Hexanol	102	C6H14O	000623-37-0	38
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	37
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35





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Sample : I5886-11
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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE9

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

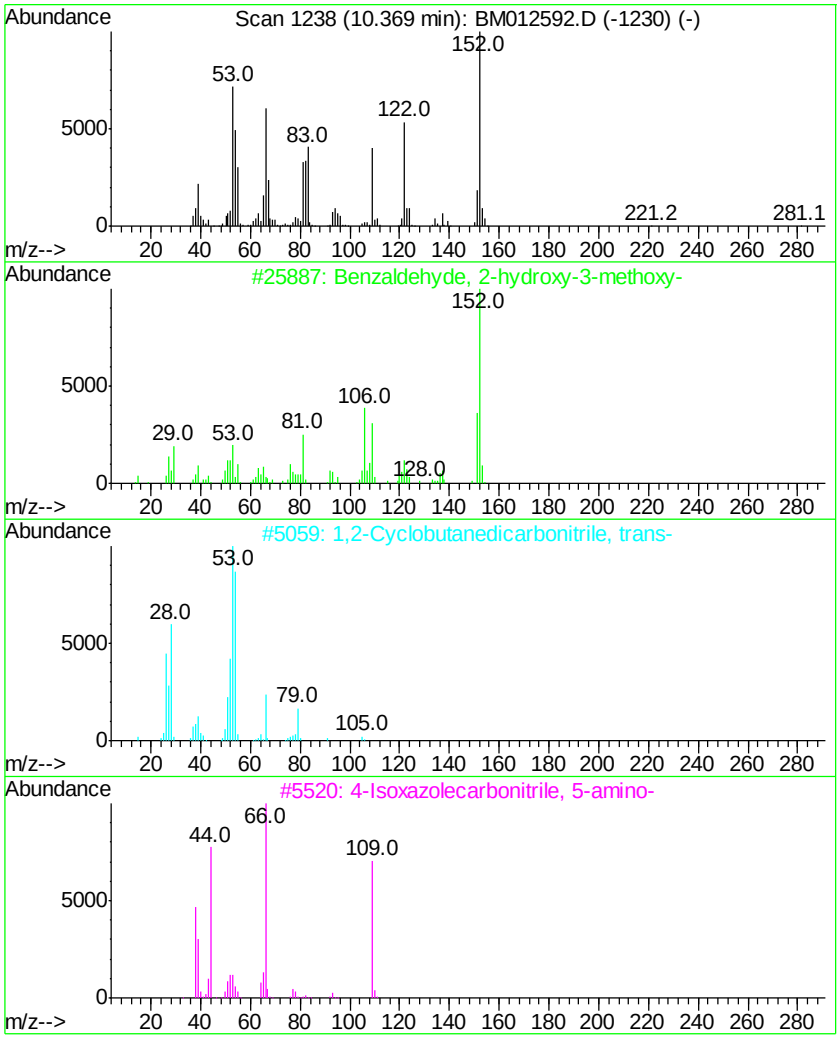
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

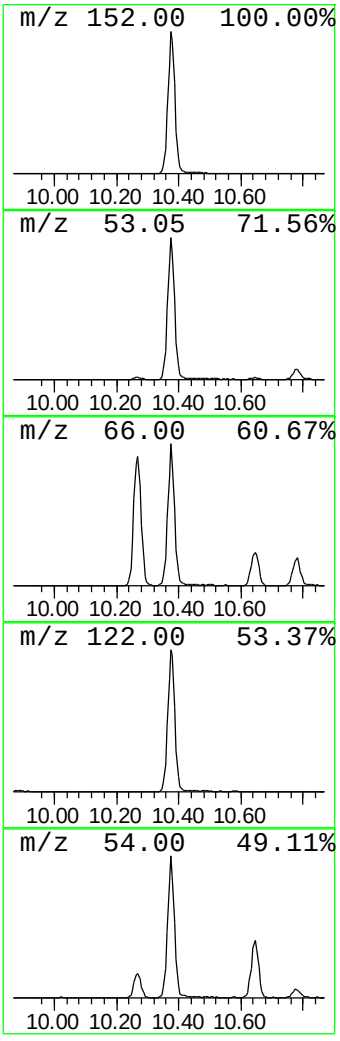
****

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	29.25 ng/ul	3996130	Naphthalene-d8	10.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	25
2	1,2-Cyclobutanedicarbonitrile, t...	106	C6H6N2	003211-20-9	25
3	4-Isoxazolecarbonitrile, 5-amino-	109	C4H3N3O	1000319-36-0	22
4	Diethyl disulfide	122	C4H10S2	000110-81-6	22
5	Propanedinitrile, (ethoxymethyle...	122	C6H6N2O	000123-06-8	18





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Instrument : BNA_M
ClientSampleId : ESNE9

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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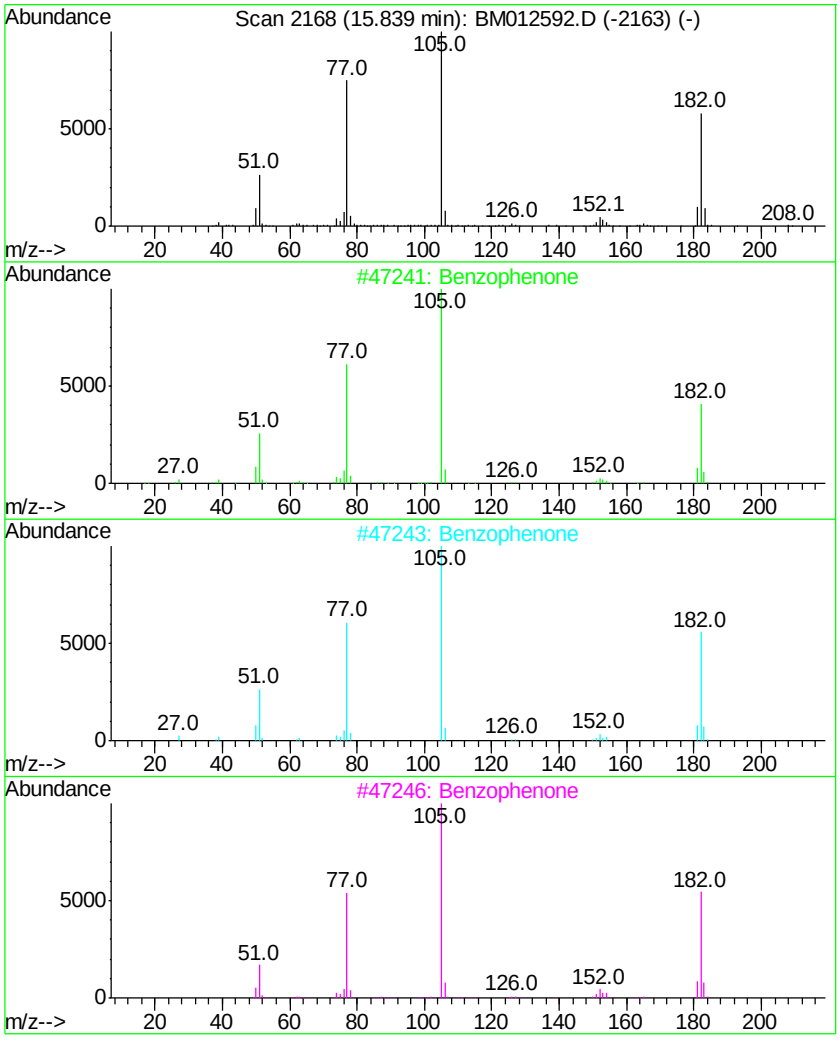
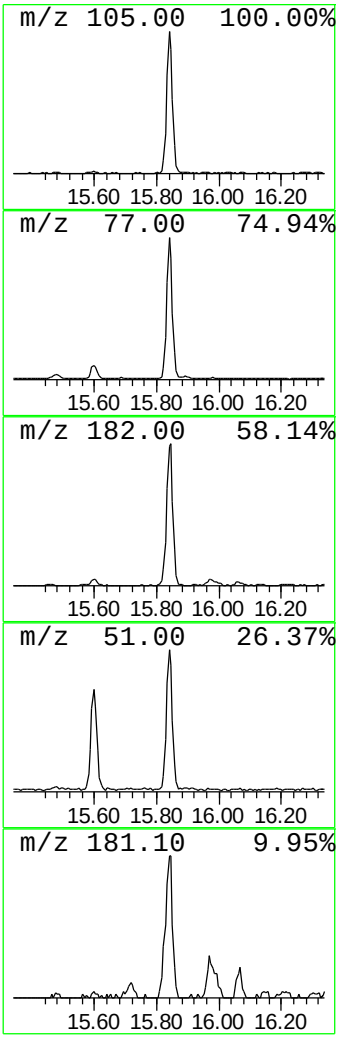
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	4.07 ng/ul	720060	Acenaphthene-d10	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	87





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Instrument : BNA_M
ClientSampleId : ESNE9

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

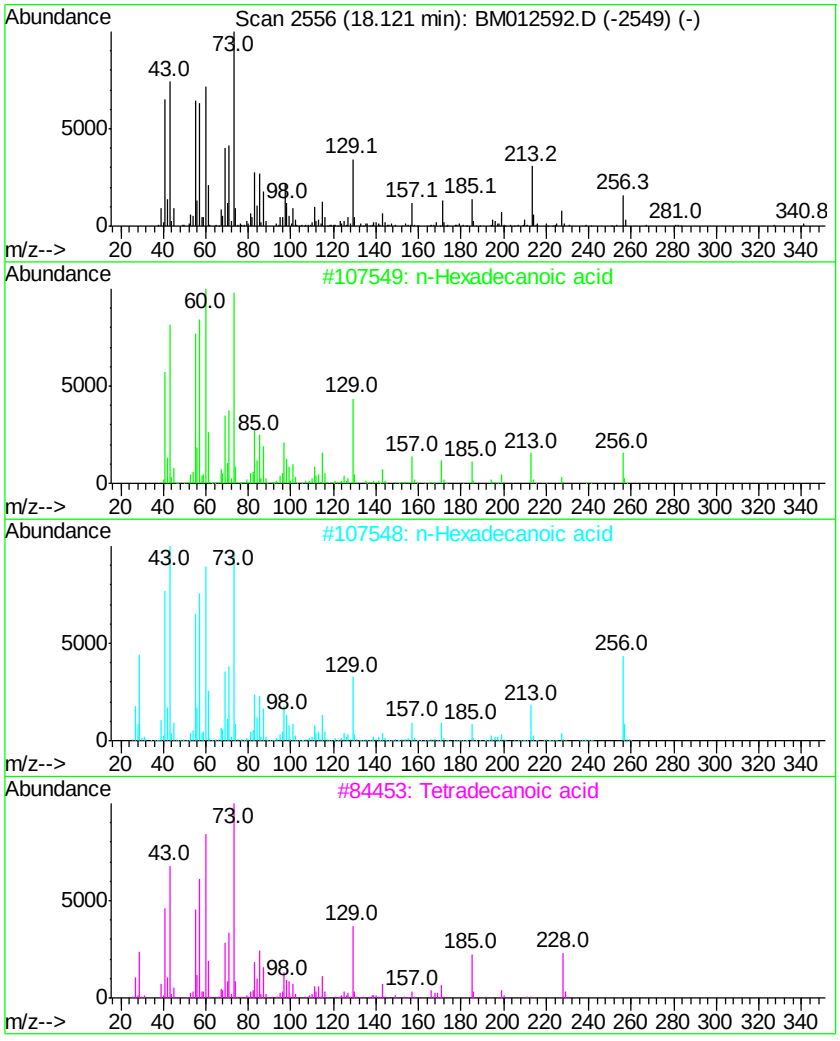
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

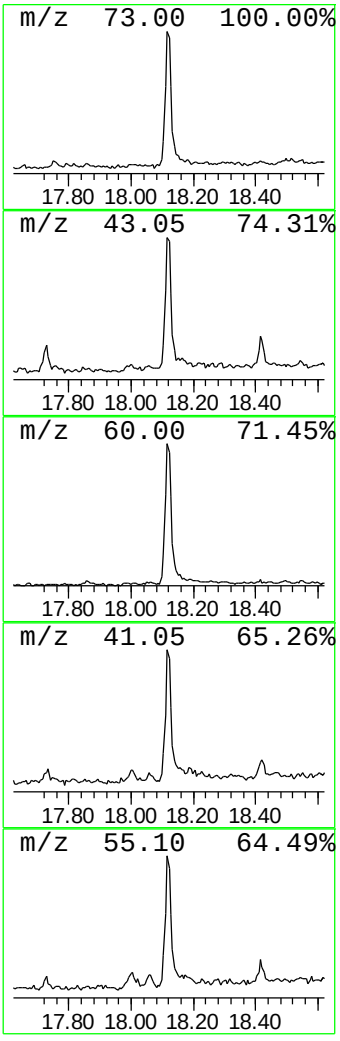
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	3.60 ng/ul	763485	Phenanthrene-d10	17.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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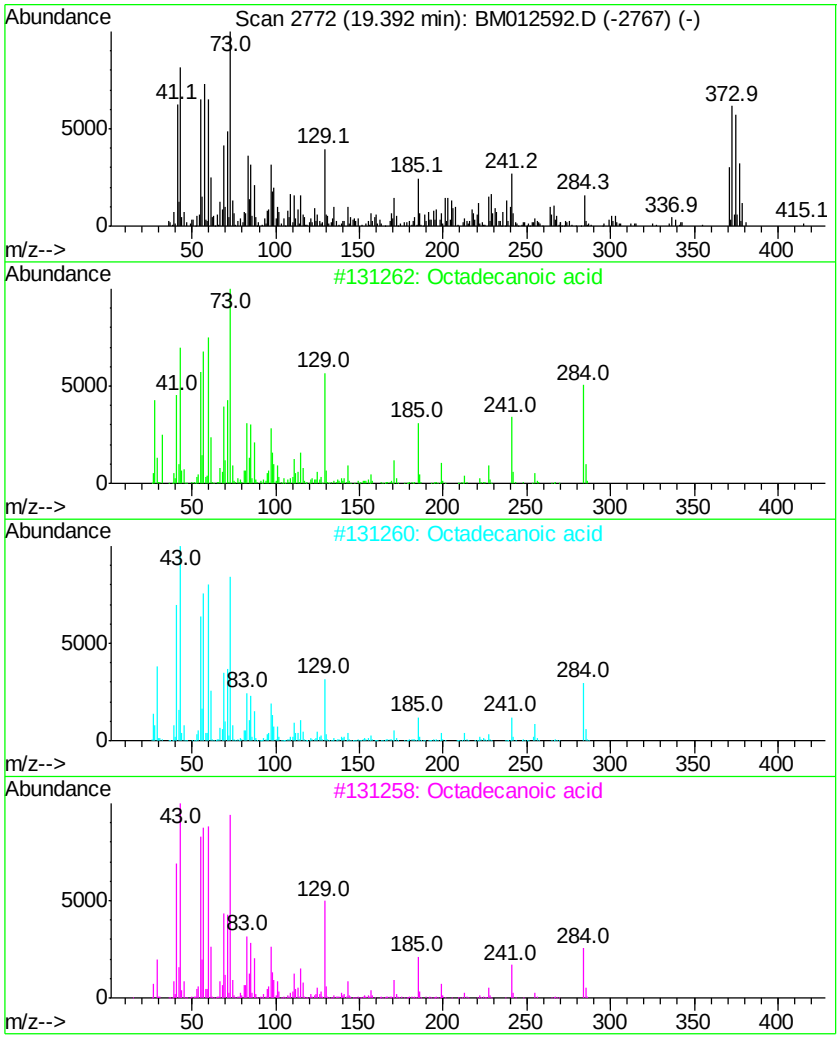
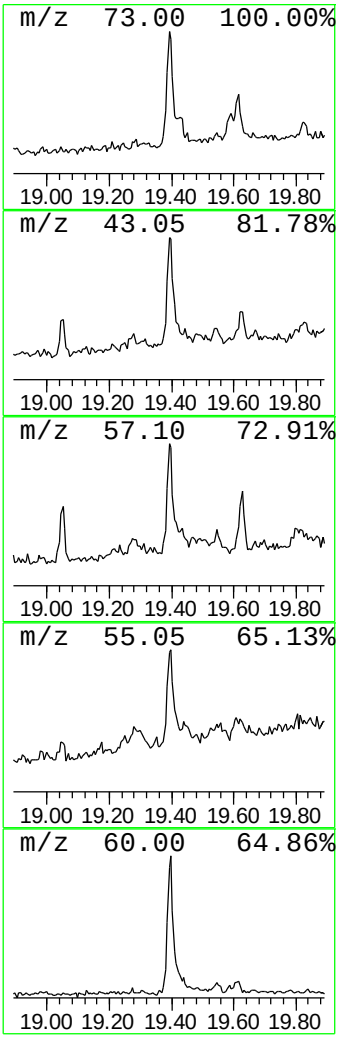
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	2.15 ng/ul	774809	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	74
2	Octadecanoic acid	284	C18H36O2	000057-11-4	74
3	Octadecanoic acid	284	C18H36O2	000057-11-4	70
4	trans-Chlordane	406	C10H6Cl8	005103-74-2	60
5	cis-Chlordane	406	C10H6Cl8	005103-71-9	49





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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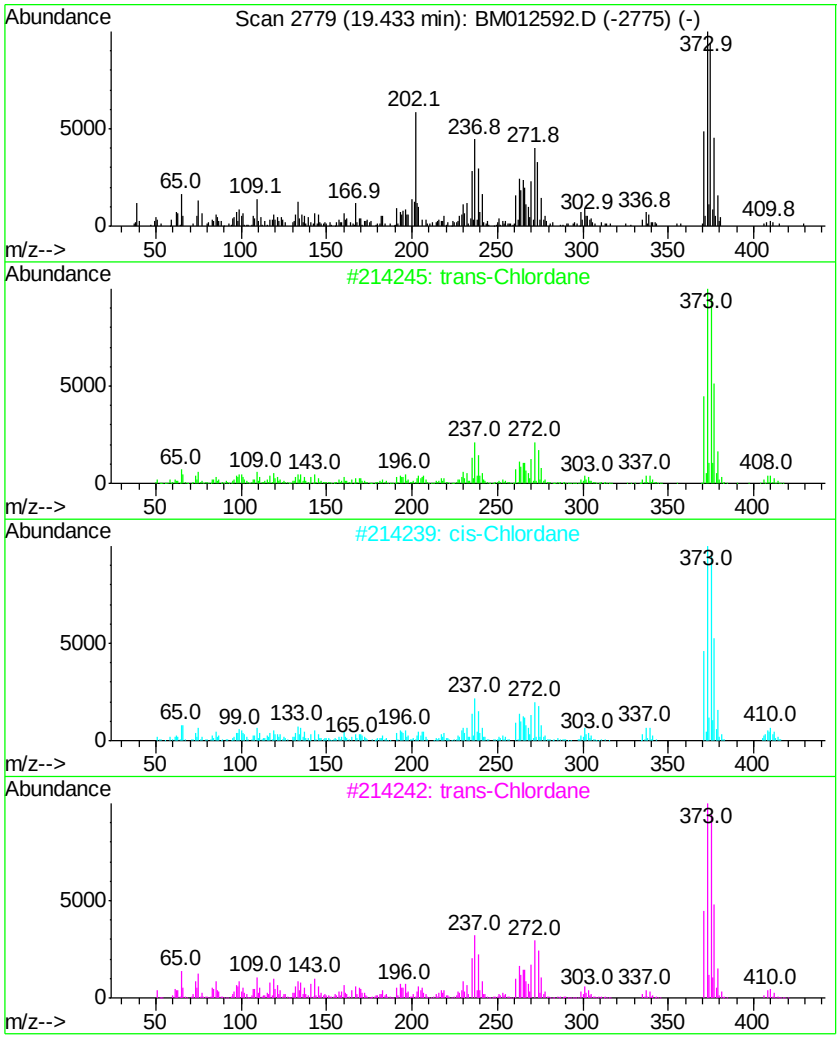
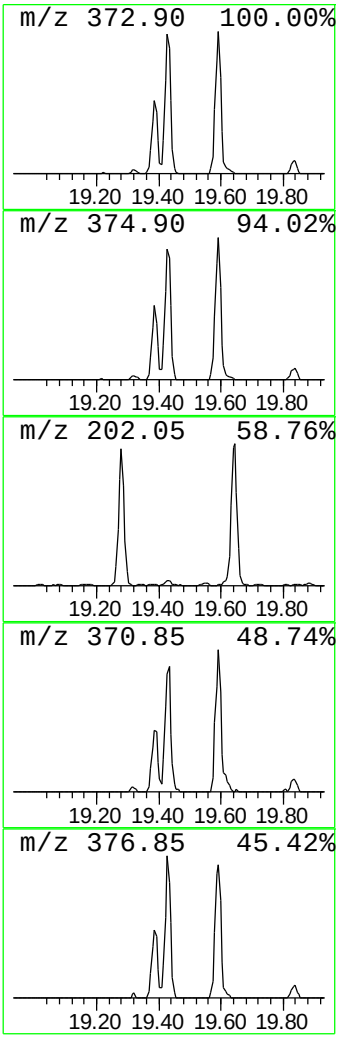
Peak Number 6 trans-Chlordane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	2.25 ng/ul	811345	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Chlordane	406	C10H6Cl8	005103-74-2	99
2	cis-Chlordane	406	C10H6Cl8	005103-71-9	99
3	trans-Chlordane	406	C10H6Cl8	005103-74-2	99
4	Chlordane	406	C10H6Cl8	000057-74-9	92
5	4,7-Methanoindene, 1,2,3,5,6,7,8...	406	C10H6Cl8	1000017-10-9	91





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Quant Title : SVOA CALIBRATION

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

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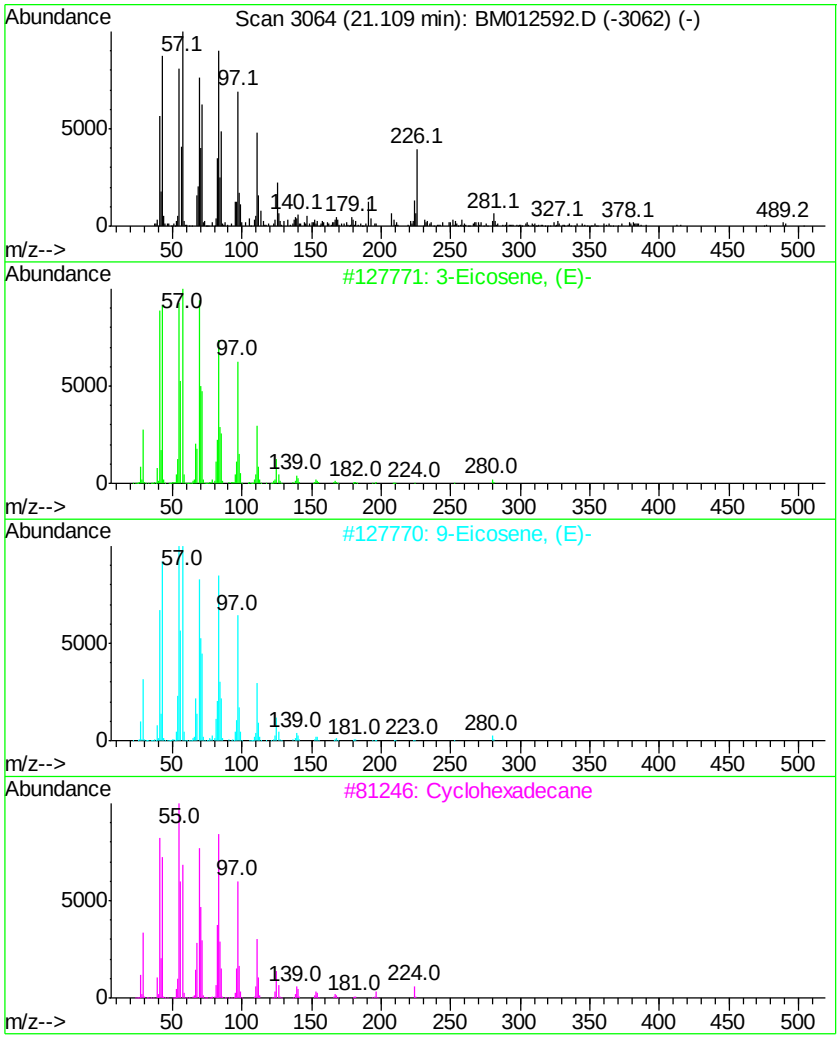
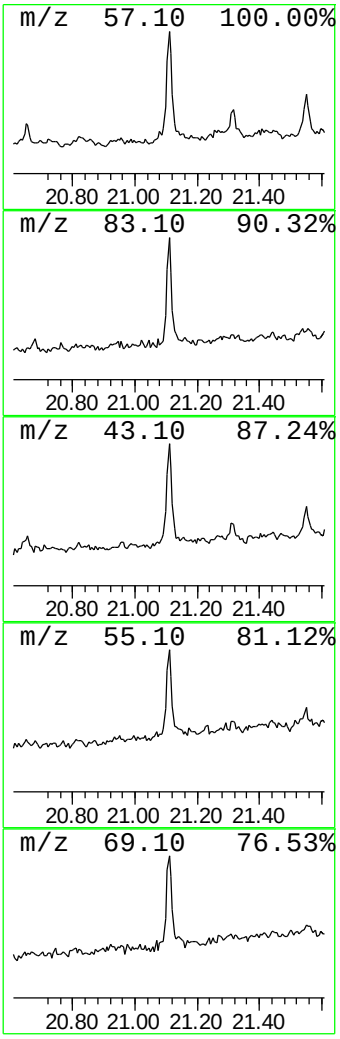
Peak Number 7 (DEL) Alkane: Cyclic21.11 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.11	2.33 ng/ul	839150	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	Cyclohexadecane	224	C16H32	000295-65-8	86
4	1-Nonadecene	266	C19H38	018435-45-5	83
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	83





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Quant Title : SVOA CALIBRATION

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

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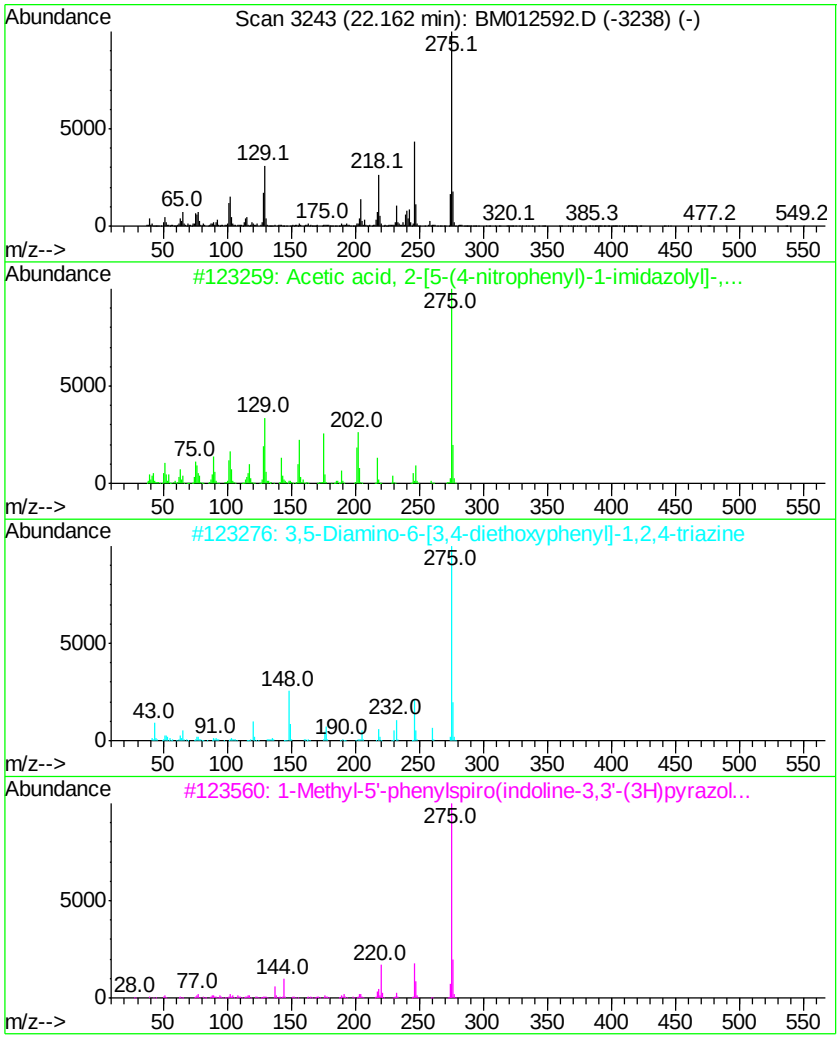
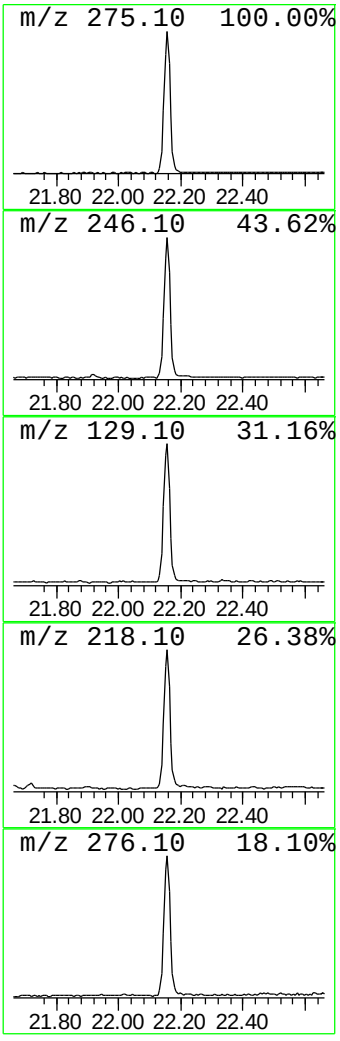
Peak Number 8 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	9.07 ng/ul	3270550	Chrysene-d12	21.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	55
2	3,5-Diamino-6-[3,4-diethoxypheny...	275	C13H17N5O2	058848-69-4	47
3	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	46
4	5H-[1]Benzopyrano[4,3-d]pyrimidi...	275	C16H9N3O2	1000337-49-1	46
5	1H-Indole, 2-cyclohexyl-3-phenyl-	275	C20H21N	1000163-87-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM103017\
Data File : BM012592.D
Acq On : 31 Oct 2017 02:24
Operator : SJ/JU
Sample : I5886-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : ESNE9

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
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
2-Pentanone, 4-hy...	4.99	2.1	ng/ul	202716	1	7.86	1904280	20.0
unknown-01	10.37	29.3	ng/ul	3996130	2	10.65	2732240	20.0
Benzophenone	15.84	4.1	ng/ul	720060	3	14.49	3536240	20.0
n-Hexadecanoic acid	18.12	3.6	ng/ul	763485	4	17.23	4238240	20.0
Octadecanoic acid	19.39	2.1	ng/ul	774809	5	21.40	7211190	20.0
trans-Chlordane	19.43	2.3	ng/ul	811345	5	21.40	7211190	20.0
(DEL) Alkane: Cyc...	21.11	2.3	ng/ul	839150	5	21.40	7211190	20.0
Acetic acid, 2-[5...	22.16	9.1	ng/ul	3270550	5	21.40	7211190	20.0