LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM101717\
Data File : BM012257.D
Acq On : 17 Oct 2017 20:23
Operator : SJ/JU
Sample : I5664-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0B46

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-BM101217.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	6.957	652	658	675	rBV2	624347	1388614	34.10%	2.707%
2	7.122	679	686	698	rVV	533602	876469	21.52%	1.709%
3	7.316	710	719	733	rBV	760260	1331267	32.69%	2.595%
4	7.786	793	799	808	rBV	738784	1274214	31.29%	2.484%
5	8.504	914	921	937	rBV	815605	1538626	37.78%	3.000%
6	8.957	991	998	1021	rBV	682703	1246475	30.61%	2.430%
7	9.680	1114	1121	1132	rBV	620366	1158880	28.46%	2.259%
8	10.222	1206	1213	1236	rBV	919029	1813442	44.53%	3.536%
9	10.586	1267	1275	1291	rBV	1173780	2048429	50.30%	3.994%
10	10.739	1294	1301	1320	rBV	367618	846956	20.80%	1.651%
11	11.916	1494	1501	1508	rBV	99983	201302	4.94%	0.392%
12	13.851	1822	1830	1834	rBV	1583343	2181572	53.57%	4.253%
13	13.898	1834	1838	1852	rVB	731235	1094661	26.88%	2.134%
14	14.133	1872	1878	1892	rVB	1666581	2540674	62.39%	4.953%
15	14.315	1898	1909	1916	rBV3	37994	100711	2.47%	0.196%
16	14.439	1924	1930	1944	rVB2	1373283	2154910	52.92%	4.201%
17	14.674	1965	1970	1992	rBV	281699	753991	18.51%	1.470%
18	15.439	2093	2100	2116	rBV	2441203	3621671	88.93%	7.061%
19	15.586	2119	2125	2136	rBV	542224	950593	23.34%	1.853%
20	15.680	2137	2141	2145	rVB2	31516	45037	1.11%	0.088%
21	15.798	2156	2161	2171	rBV	668316	979634	24.06%	1.910%
22	16.321	2242	2250	2255	rBV2	41104	67661	1.66%	0.132%
23	17.192	2391	2398	2409	rBV2	1980162	2927723	71.89%	5.708%
24	17.292	2409	2415	2424	rBV	2802578	3985766	97.87%	7.771%
25	17.951	2522	2527	2533	rBV9	20092	44079	1.08%	0.086%
26	18.009	2533	2537	2542	rBV4	37586	68557	1.68%	0.134%
27	18.068	2542	2547	2558	rBV	560353	805732	19.79%	1.571%
28	19.227	2737	2744	2752	rBV4	92386	232550	5.71%	0.453%
29	19.345	2760	2764	2775	rBV	248249	393253	9.66%	0.767%
30	19.586	2799	2805	2819	rBV	3005340	4072347	100.00%	7.940%
31	20.080	2885	2889	2890	rBV4	35609	47609	1.17%	0.093%
32	21.062	3052	3056	3061	rBV	383867	496822	12.20%	0.969%
33	21.374	3104	3109	3115	rBV	1983515	2732471	67.10%	5.327%
34	21.933	3202	3204	3206	rBV2	161597	186660	4.58%	0.364%

LSC Area Percent Report

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Sample : I5664-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0B46

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-BM101217.M
Title : SVOA CALIBRATION

35	22.409	3281	3285	3290	rBV2	438605	658702	16.17%	1.284%
36	22.921	3368	3372	3376	rVB2	323336	469041	11.52%	0.914%
37	23.527	3468	3475	3490	rVB2	1696423	3525161	86.56%	6.873%
38	23.674	3494	3500	3511	rVB	1207629	2429274	59.65%	4.736%

Sum of corrected areas: 51291536

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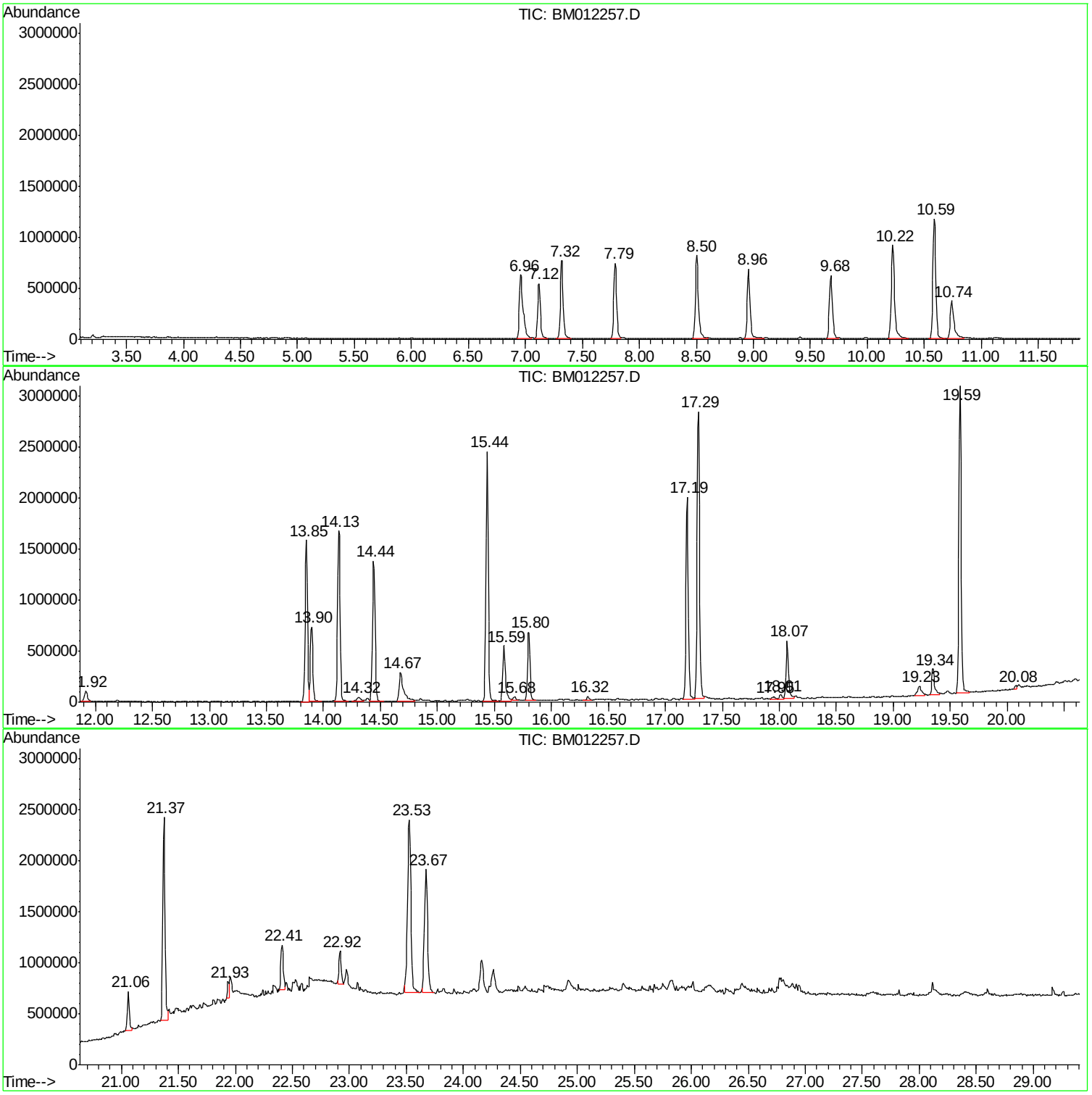
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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



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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

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

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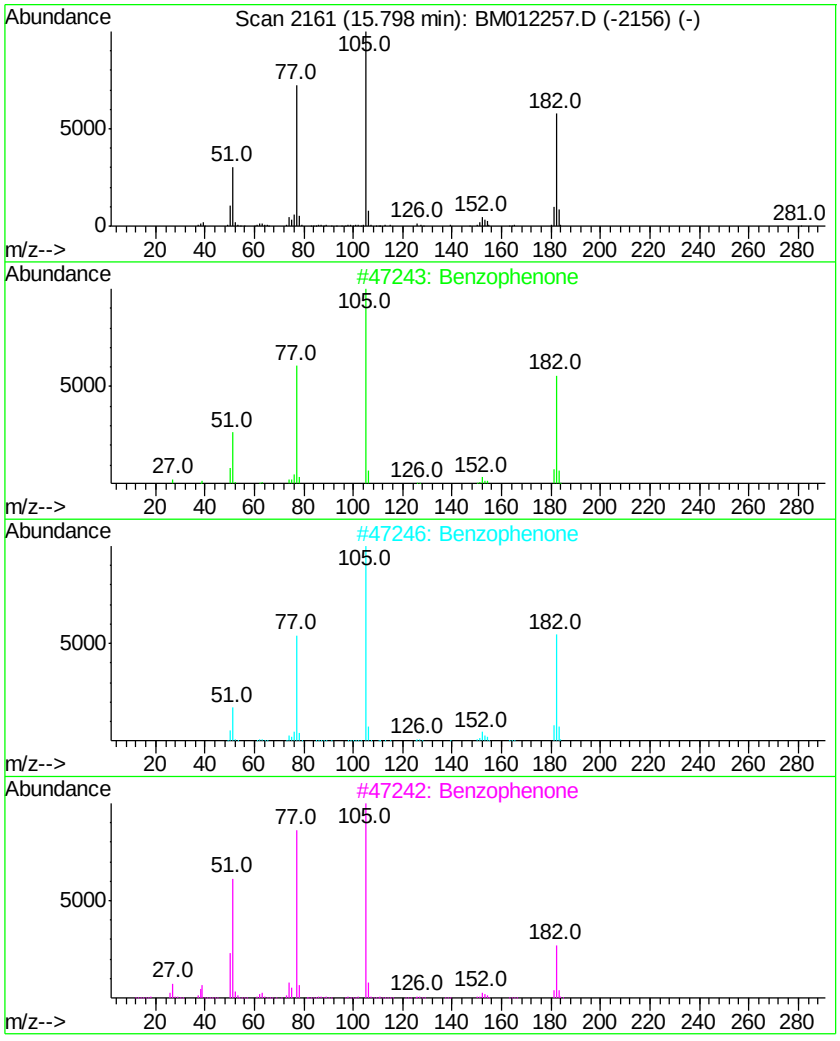
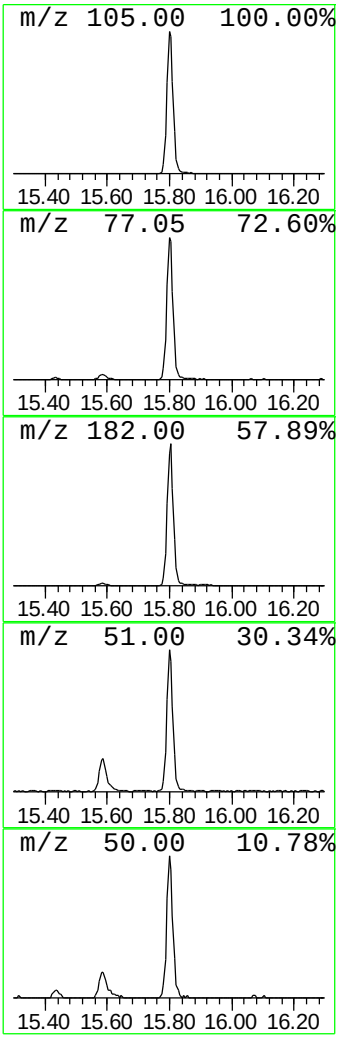
Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	9.09 ng/ul	979634	Acenaphthene-d10	14.44

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





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0B46

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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

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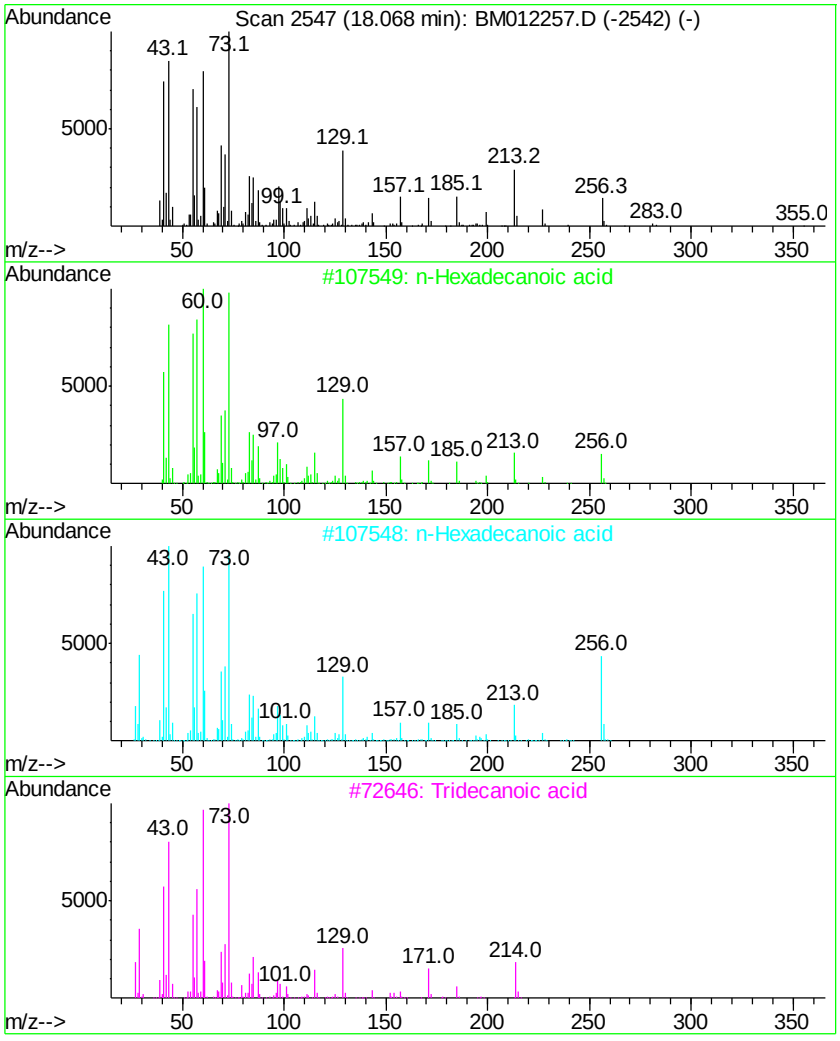
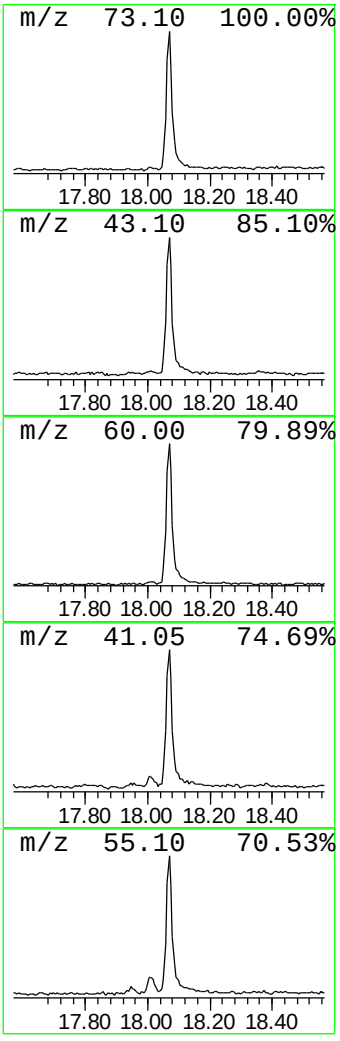
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	5.50 ng/ul	805732	Phenanthrene-d10	17.19

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	98
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





Library Search Compound Report

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Operator : SJ/JU
Sample : I5664-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0B46

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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

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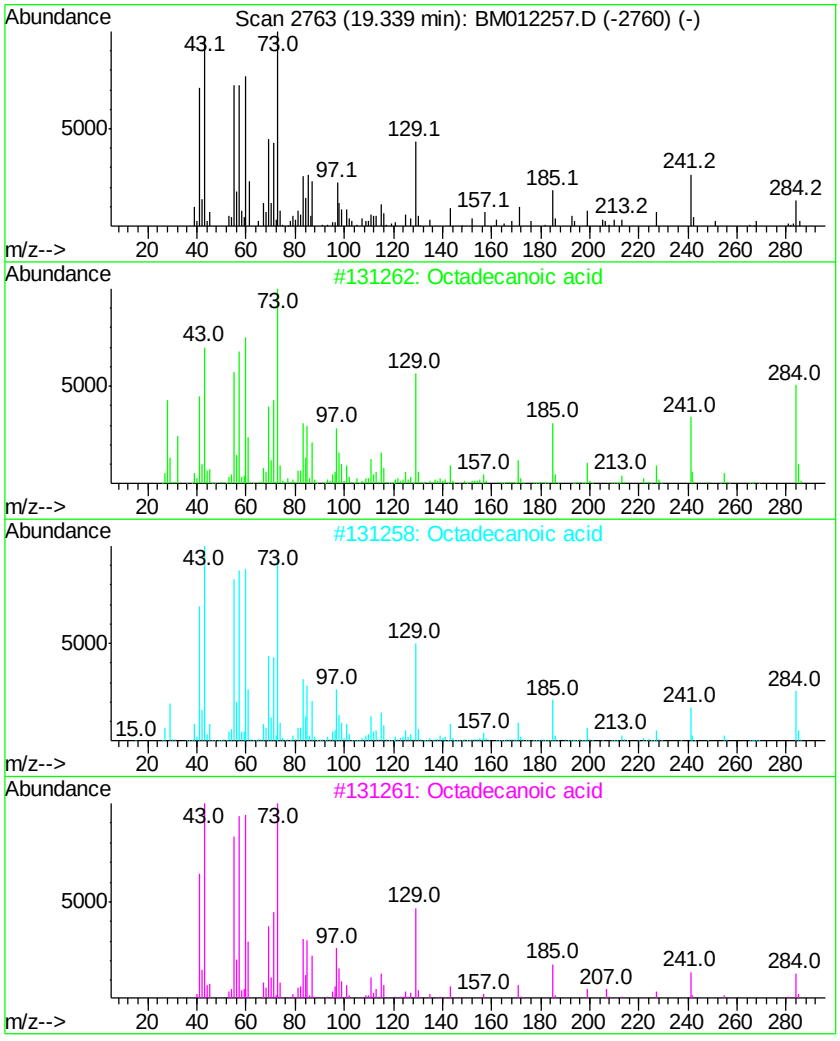
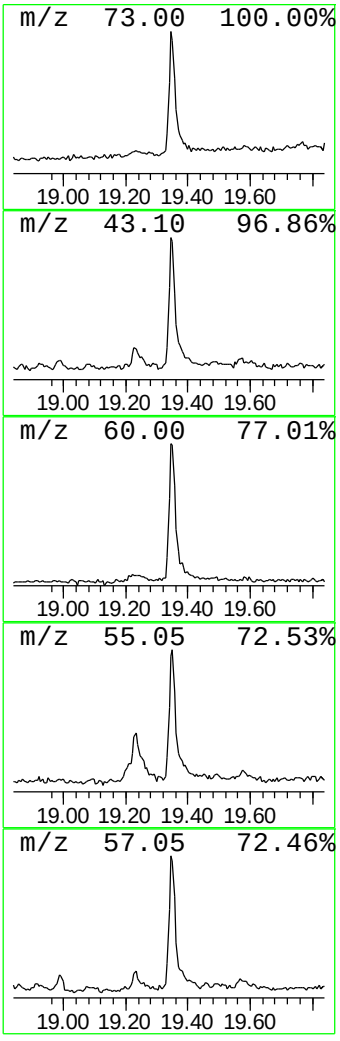
Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.88 ng/ul	393253	Chrysene-d12	21.37

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	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0B46

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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

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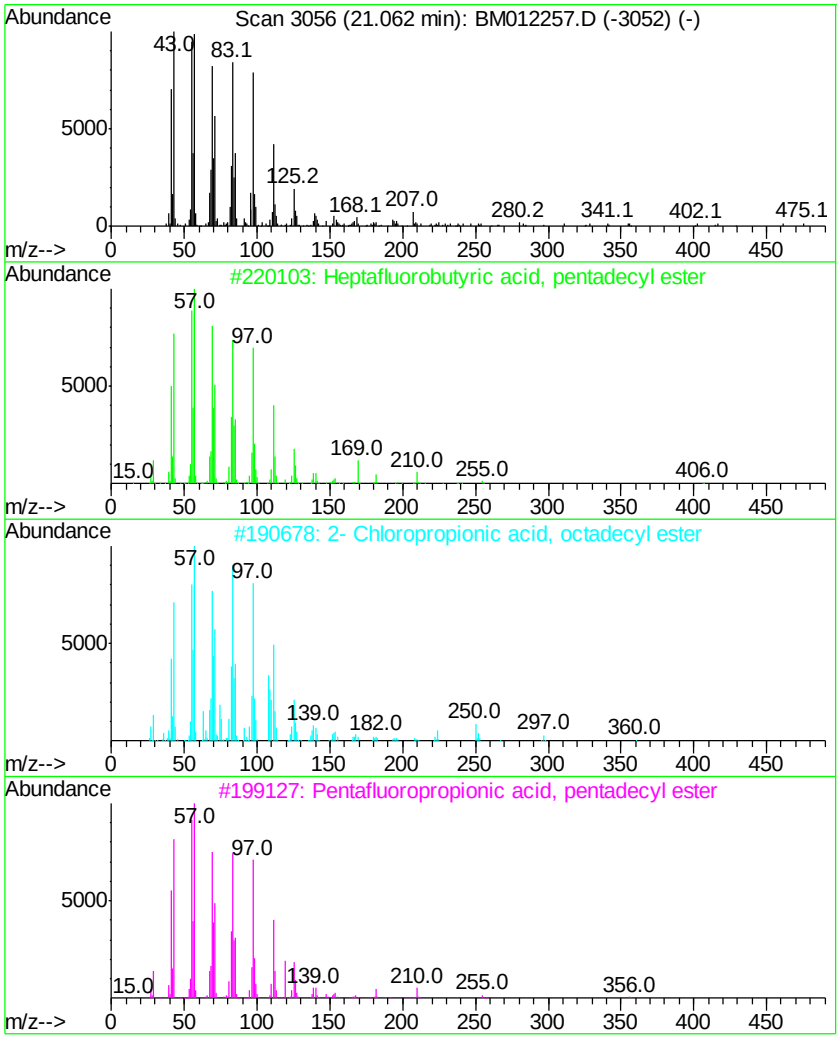
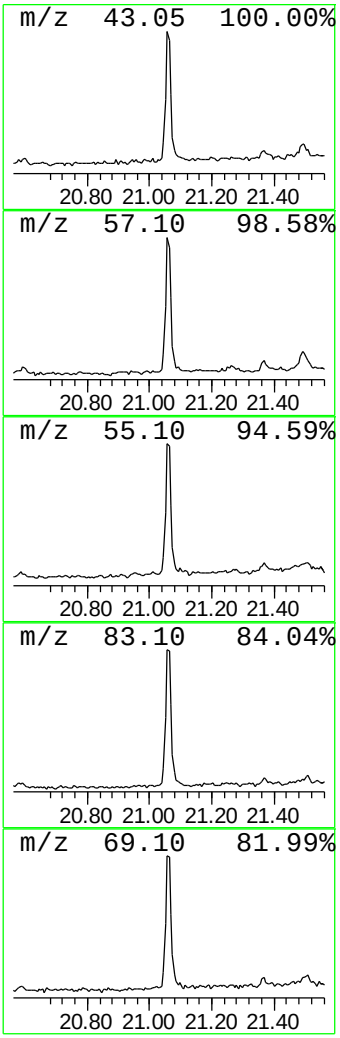
Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	3.64 ng/ul	496822	Chrysene-d12	21.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	1-Nonadecene	266	C19H38	018435-45-5	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





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Instrument : BNA_M
ClientSampleId : C0B46

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

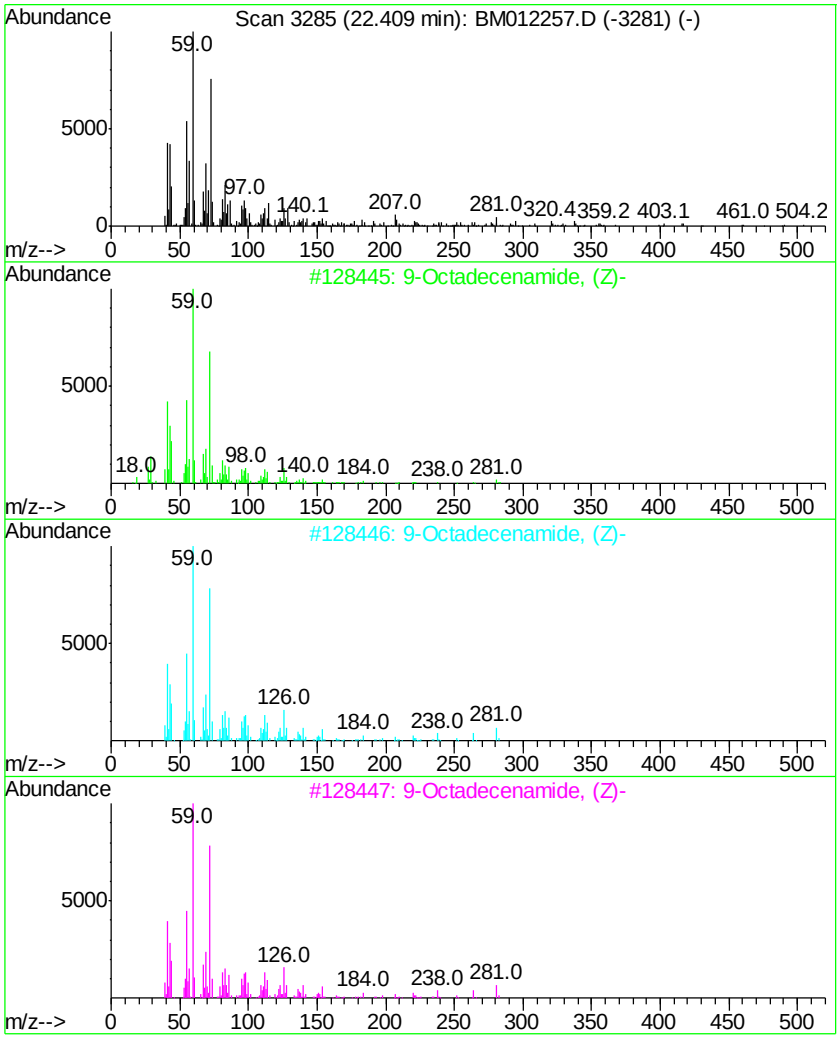
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

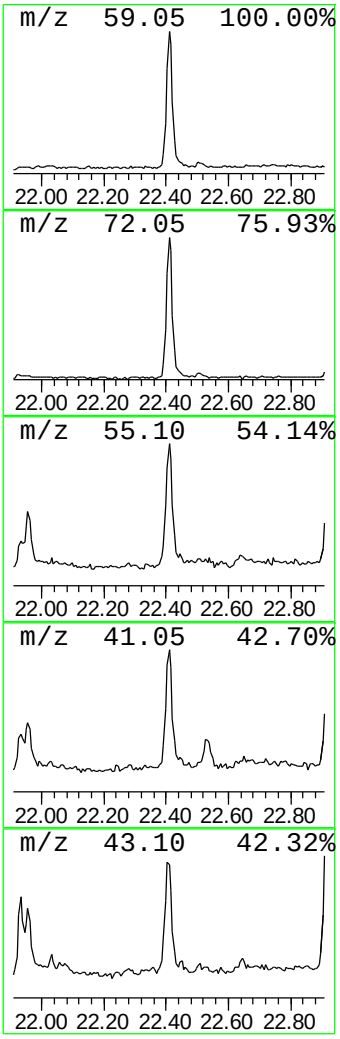
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	4.82 ng/ul	658702	Chrysene-d12	21.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64





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Quant Title : SVOA CALIBRATION

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

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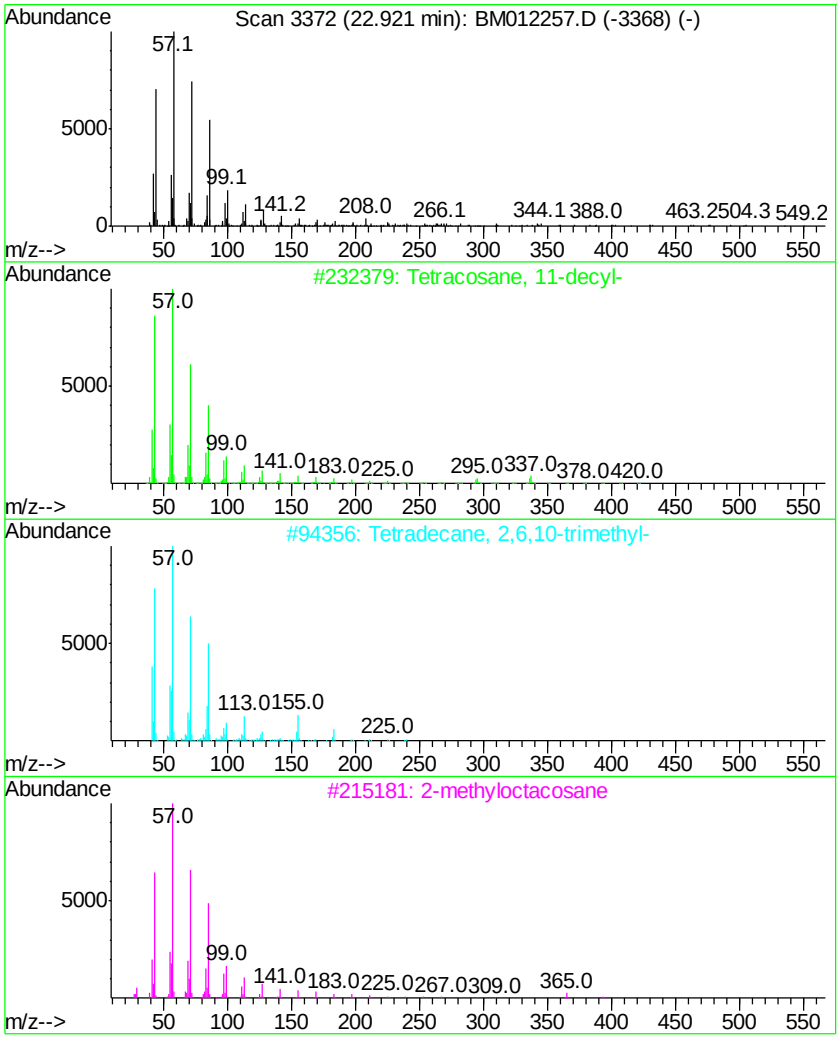
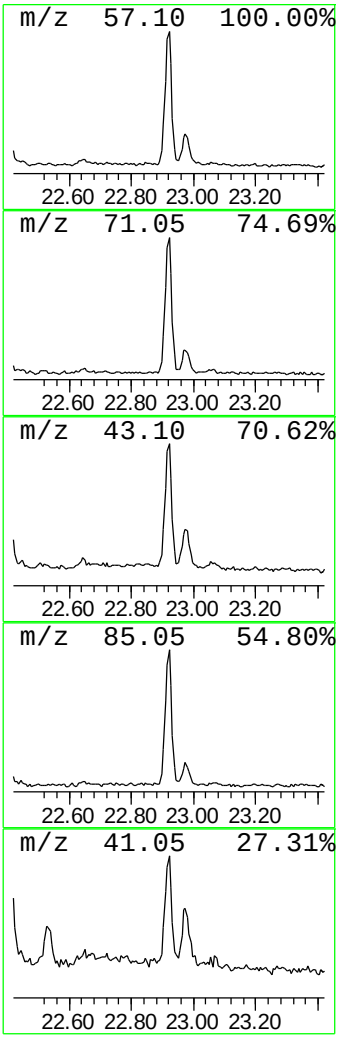
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.92	3.86 ng/ul	469041	Perylene-d12	23.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Tentatively Identified Compound (LSC) summary

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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
Benzophenone	15.80	9.1	ng/ul	979634	3	14.44	2154910	20.0
n-Hexadecanoic acid	18.07	5.5	ng/ul	805732	4	17.19	2927720	20.0
Octadecanoic acid	19.34	2.9	ng/ul	393253	5	21.37	2732470	20.0
Heptafluorobutyri...	21.06	3.6	ng/ul	496822	5	21.37	2732470	20.0
9-Octadecenamide,...	22.41	4.8	ng/ul	658702	5	21.37	2732470	20.0
(DEL) Alkane: Str...	22.92	3.9	ng/ul	469041	6	23.67	2429270	20.0