

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
 Data File : BM010635.D
 Acq On : 21 Jun 2017 22:28
 Operator : SJ/JU
 Sample : I3627-14
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F5E25

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 1 % of largest Peak
 Max Peaks: 100
 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-BM062017.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	6.646	632	639	650	rVB	244718	397058	16.96%	1.462%
2	6.816	661	668	675	rBV	183317	268858	11.49%	0.990%
3	6.998	693	699	706	rVB	257156	391708	16.74%	1.442%
4	7.463	772	778	785	rBV	338127	501310	21.42%	1.846%
5	8.169	892	898	906	rVB	335388	510886	21.83%	1.881%
6	8.604	966	972	980	rVB	262766	419392	17.92%	1.544%
7	9.322	1088	1094	1102	rVB	255455	395563	16.90%	1.456%
8	9.851	1178	1184	1191	rBB	384955	610208	26.07%	2.247%
9	10.228	1241	1248	1253	rBV	480004	778438	33.26%	2.866%
10	10.281	1253	1257	1262	rVB2	18932	27954	1.19%	0.103%
11	10.369	1265	1272	1279	rBV	337556	538641	23.01%	1.983%
12	13.533	1804	1810	1815	rBV	796556	1136068	48.54%	4.183%
13	13.580	1815	1818	1824	rVB	389826	534601	22.84%	1.968%
14	13.804	1849	1856	1865	rBV	812645	1181082	50.46%	4.348%
15	14.116	1900	1909	1917	rVB2	793952	1225324	52.35%	4.511%
16	14.322	1939	1944	1951	rBV	311959	408982	17.47%	1.506%
17	15.116	2073	2079	2085	rBV	1131322	1534083	65.54%	5.648%
18	15.239	2094	2100	2109	rBV	326526	435265	18.60%	1.603%
19	15.486	2137	2142	2151	rBV	303322	422633	18.06%	1.556%
20	15.868	2202	2207	2211	rBV3	18099	25945	1.11%	0.096%
21	16.868	2371	2377	2383	rBV2	1112378	1568469	67.01%	5.775%
22	16.968	2388	2394	2406	rVB2	1255930	1751320	74.82%	6.448%
23	17.727	2518	2523	2530	rBV5	23818	39327	1.68%	0.145%
24	17.792	2530	2534	2543	rBV	234659	309107	13.21%	1.138%
25	18.286	2615	2618	2622	rVB4	20441	27446	1.17%	0.101%
26	18.674	2678	2684	2688	rBV4	35820	49946	2.13%	0.184%
27	18.939	2725	2729	2736	rVB	225197	307389	13.13%	1.132%
28	19.092	2750	2755	2762	rBV	140350	189987	8.12%	0.699%
29	19.280	2778	2787	2791	rBV	1609381	2340613	100.00%	8.618%
30	19.392	2800	2806	2811	rVB8	15618	35779	1.53%	0.132%
31	19.645	2841	2849	2853	rBV4	36603	81703	3.49%	0.301%
32	19.768	2866	2870	2873	rBV3	29869	47601	2.03%	0.175%
33	19.968	2898	2904	2909	rBV3	51096	85290	3.64%	0.314%
34	20.109	2924	2928	2932	rBV	32790	42493	1.82%	0.156%

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Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	20.151	2932	2935	2939	rBV3	27741	39460	1.69%	0.145%
36	20.562	3001	3005	3009	rVB	42512	51340	2.19%	0.189%
37	20.651	3016	3020	3025	rBV	163848	185450	7.92%	0.683%
38	20.727	3027	3033	3036	rVV4	45154	83194	3.55%	0.306%
39	20.774	3037	3041	3043	rVV3	48106	67593	2.89%	0.249%
40	20.821	3043	3049	3053	rVV2	247437	338168	14.45%	1.245%
41	20.856	3053	3055	3062	rVB2	48786	63832	2.73%	0.235%
42	21.033	3082	3085	3087	rBV3	21232	26910	1.15%	0.099%
43	21.086	3087	3094	3098	rVV	1670525	2337349	99.86%	8.606%
44	21.121	3098	3100	3107	rVB	156741	196222	8.38%	0.722%
45	21.386	3142	3145	3152	rBV4	25092	47068	2.01%	0.173%
46	21.621	3182	3185	3189	rVB2	53462	67178	2.87%	0.247%
47	21.686	3191	3196	3203	rVV2	41190	105685	4.52%	0.389%
48	22.133	3269	3272	3276	rVB4	53363	62114	2.65%	0.229%
49	22.592	3344	3350	3352	rBV2	192967	341036	14.57%	1.256%
50	22.750	3374	3377	3383	rBV4	34051	71183	3.04%	0.262%
51	23.044	3421	3427	3429	rBV	92364	149912	6.40%	0.552%
52	23.092	3429	3435	3440	rVV2	1146198	1883254	80.46%	6.934%
53	23.227	3451	3458	3465	rBV2	979031	1713301	73.20%	6.308%
54	23.762	3543	3549	3555	rVB	115186	219224	9.37%	0.807%
55	23.839	3557	3562	3573	rVB8	89893	179359	7.66%	0.660%
56	24.462	3662	3668	3673	rVB3	90376	190002	8.12%	0.700%
57	25.280	3802	3807	3812	rBV3	62149	121437	5.19%	0.447%

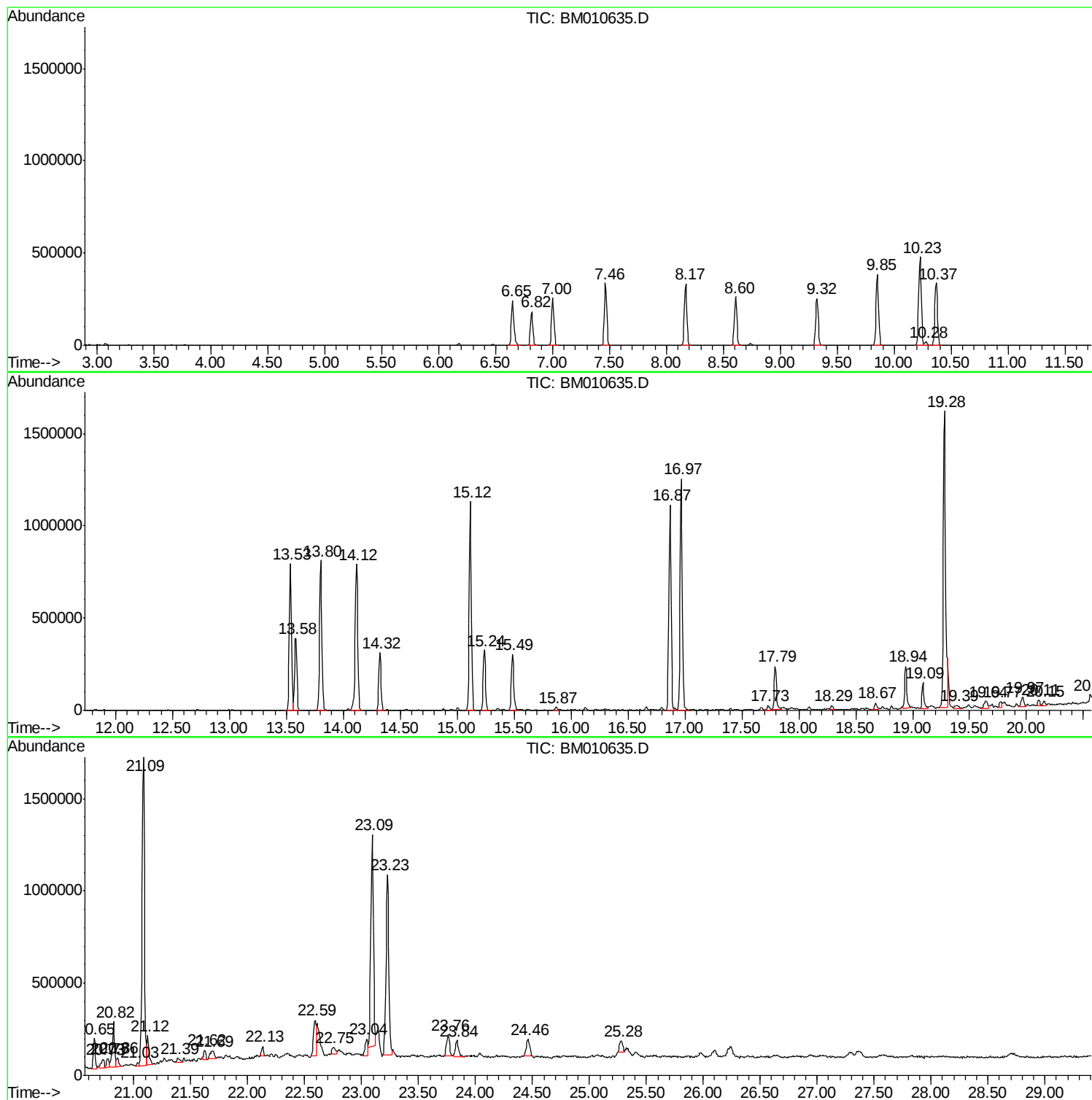
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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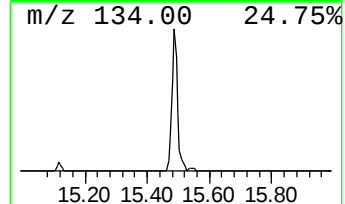
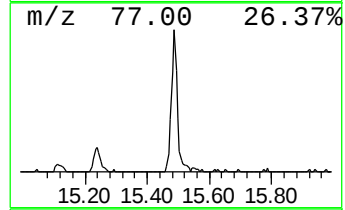
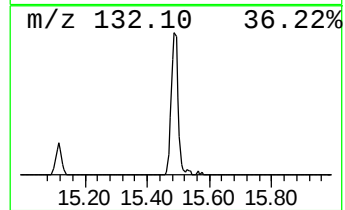
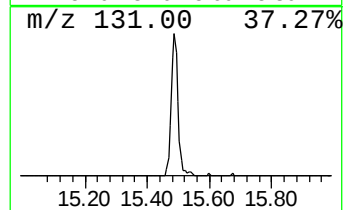
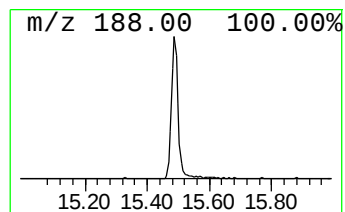
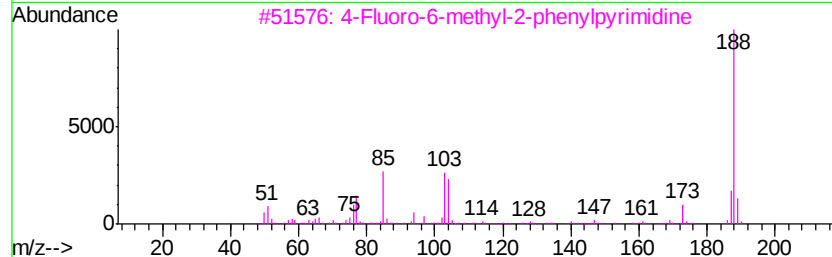
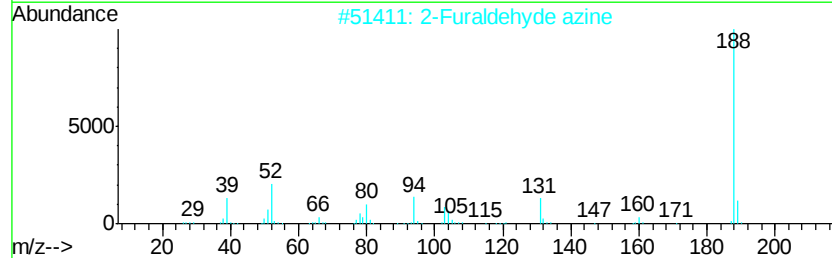
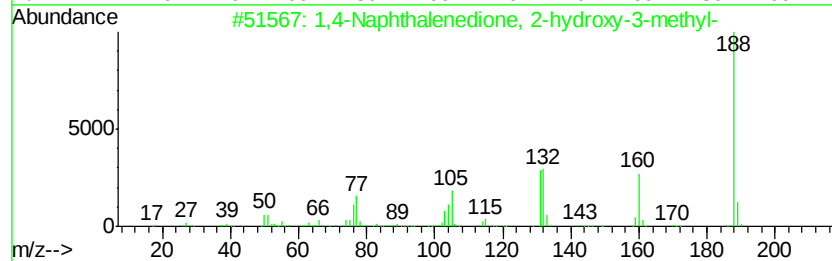
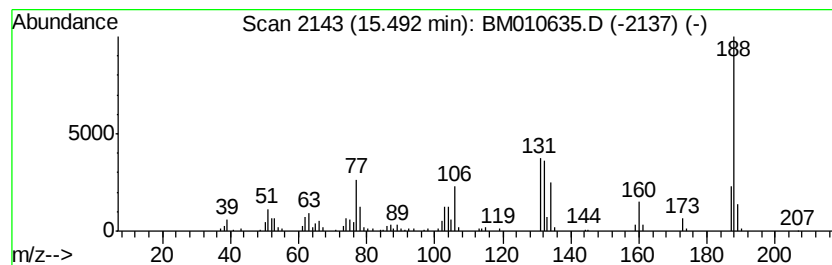
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,4-Naphthalenedione, 2-hyd... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.49	6.90 ng/ul	422633	Acenaphthene-d10	14.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Naphthalenedione, 2-hydroxy-...	188	C11H8O3	000483-55-6	58	
2	2-Furaldehyde azine	188	C10H8N2O2	005428-37-5	50	
3	4-Fluoro-6-methyl-2-phenylpyrimi...	188	C11H9FN2	051421-92-2	49	
4	5H-Pyrazolo[3,4-b]quinolin-3-ami...	188	C10H12N4	1000362-40-8	49	
5	Fumaric acid, monoamide, N-methy...	383	C17H12Cl3N03	1000357-46-5	47	



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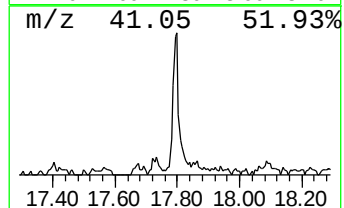
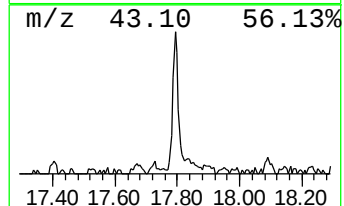
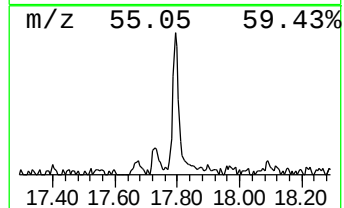
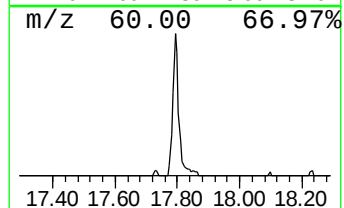
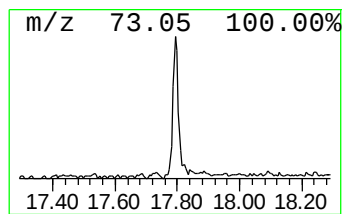
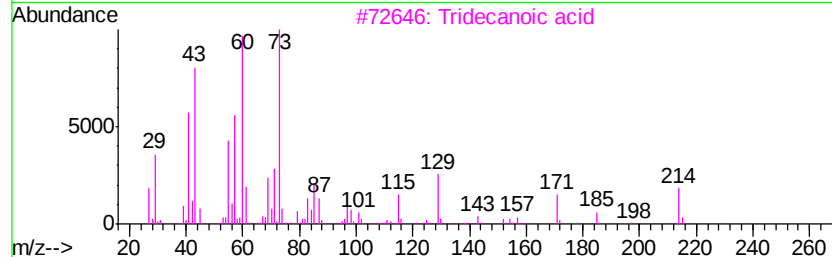
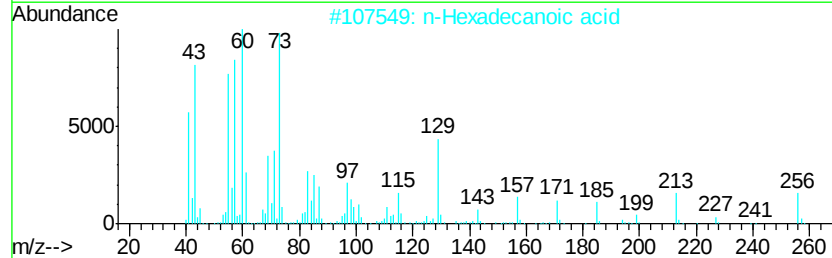
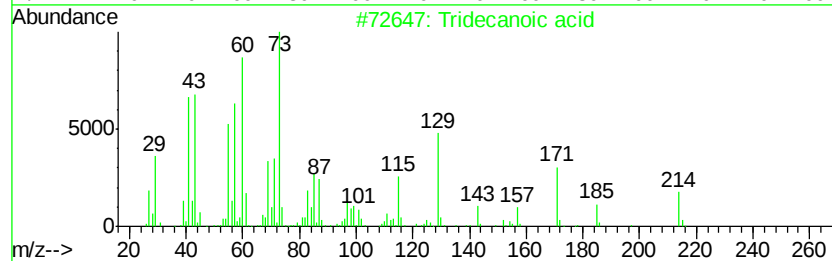
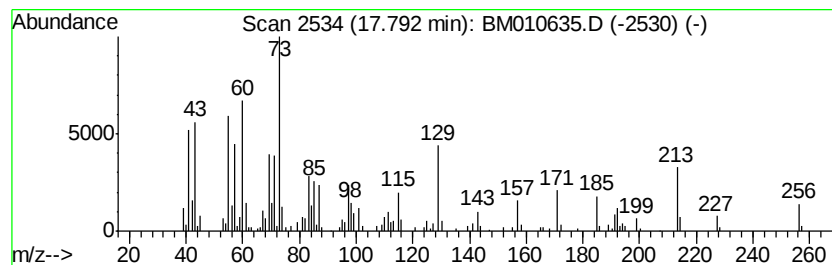
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	3.94 ng/ul	309107	Phenanthrene-d10	16.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5		Tridecanoic acid	214	C13H26O2	000638-53-9	90



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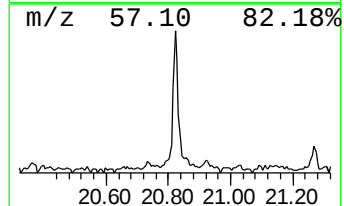
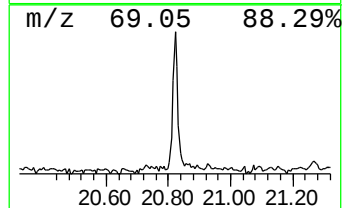
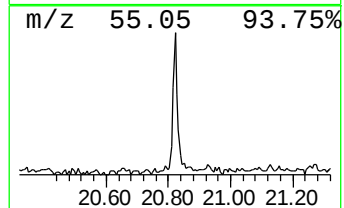
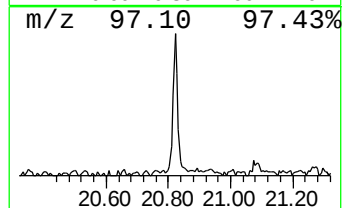
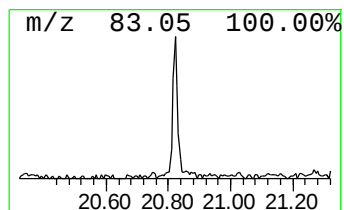
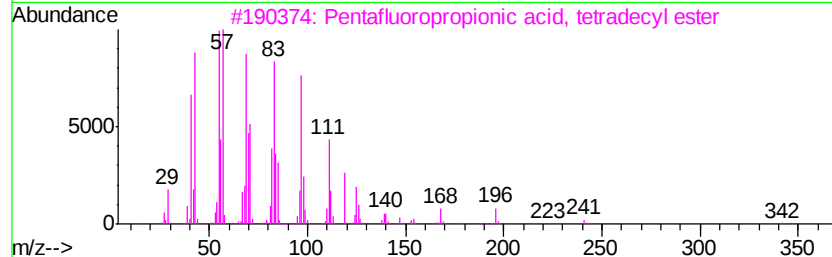
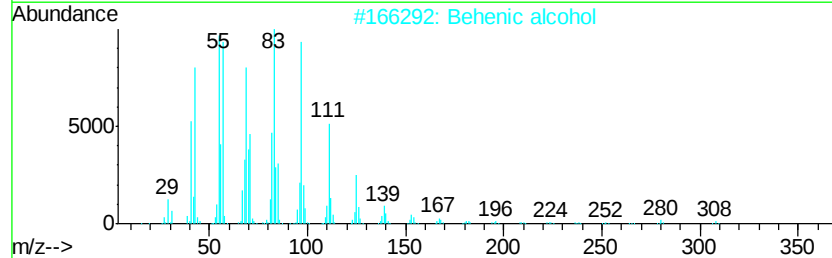
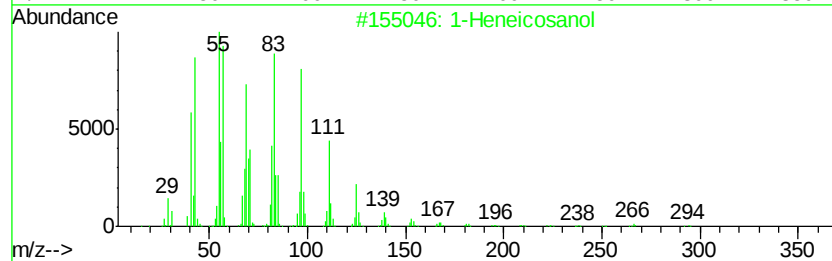
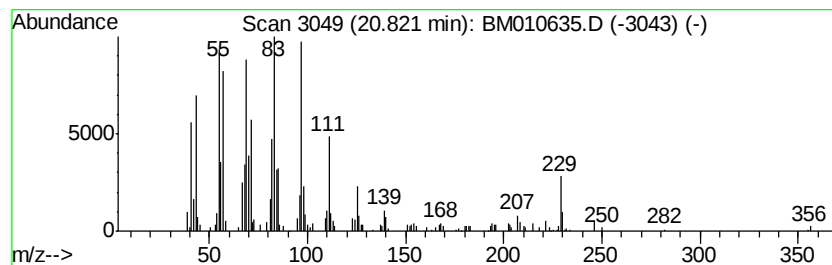
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Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.82	2.89 ng/ul	338168	Chrysene-d12	21.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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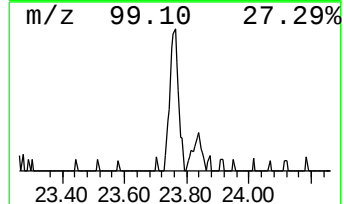
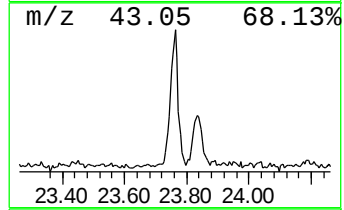
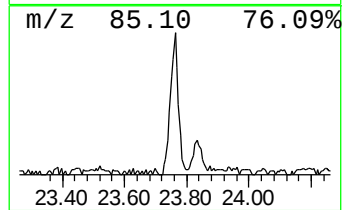
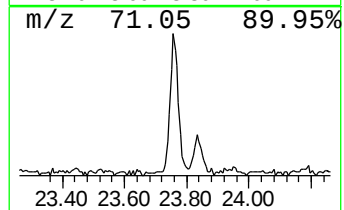
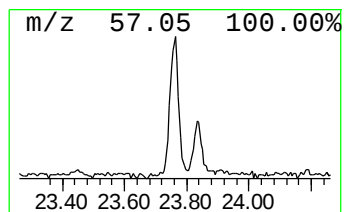
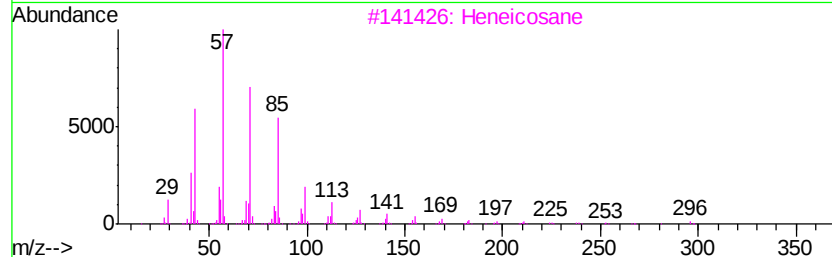
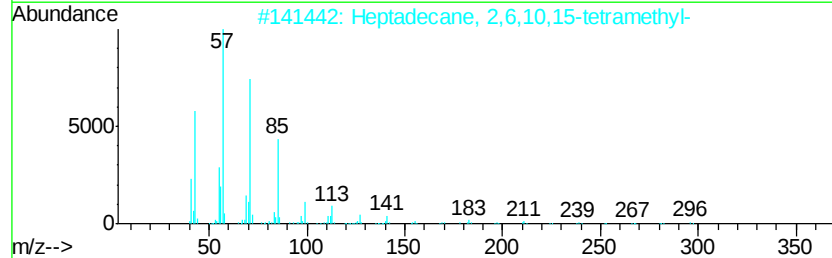
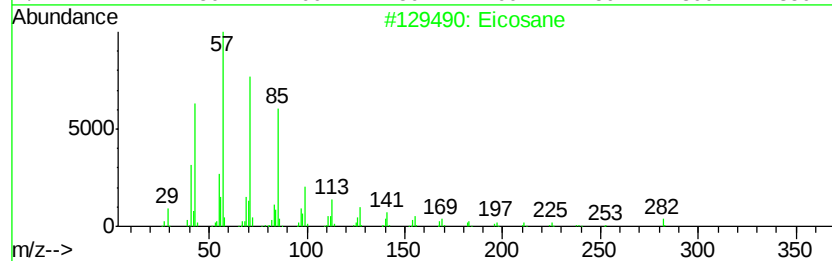
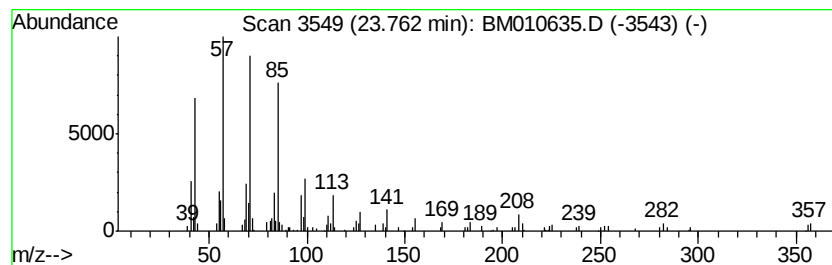
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

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23.76	2.56 ng/ul	219224	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Eicosane	282	C20H42	000112-95-8	87
5		Tetracosane	338	C24H50	000646-31-1	87



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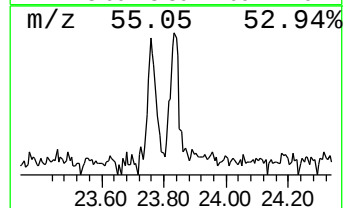
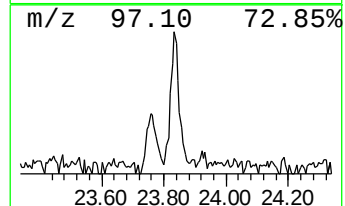
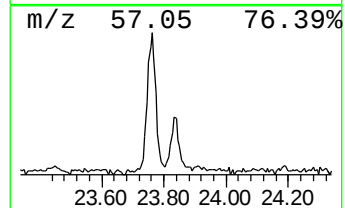
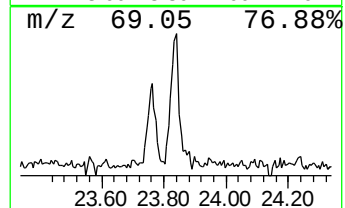
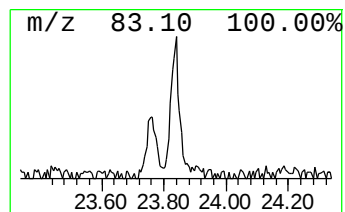
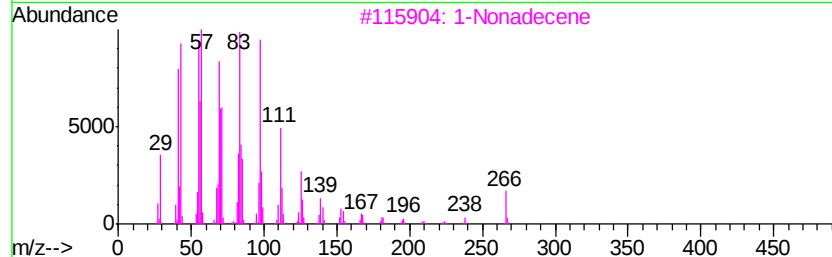
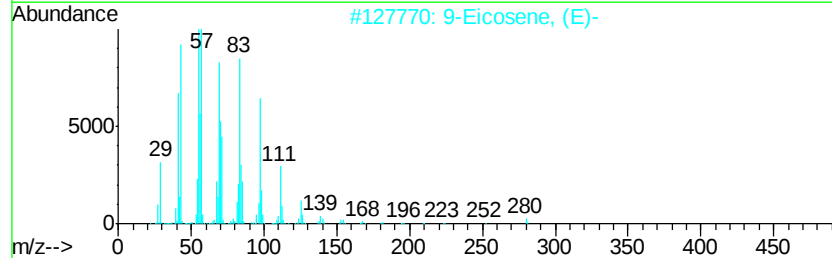
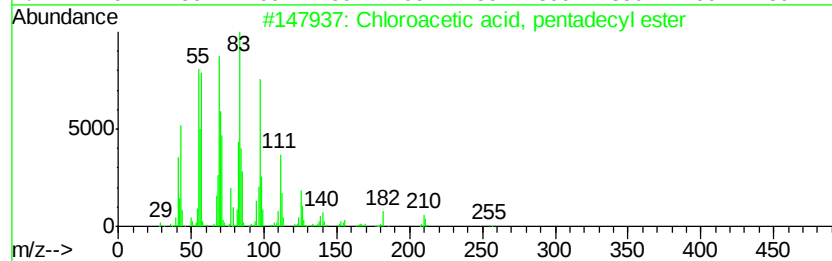
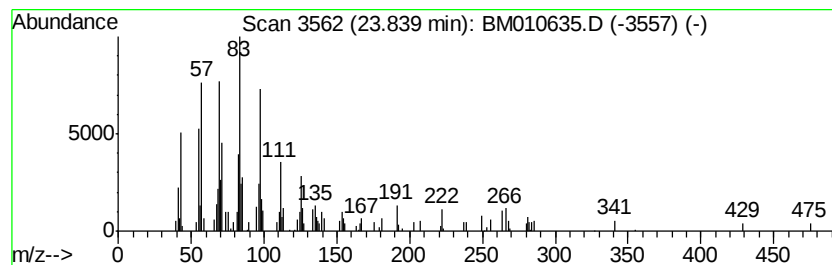
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Chloroacetic acid, pentadec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.84	2.09 ng/ul	179359	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	74
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	72
3		1-Nonadecene	266	C19H38	018435-45-5	59
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	58
5		Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010635.D
Acq On : 21 Jun 2017 22:28
Operator : SJ/JU
Sample : I3627-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F5E25

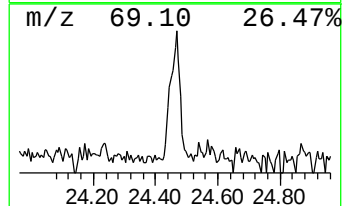
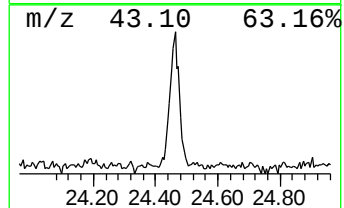
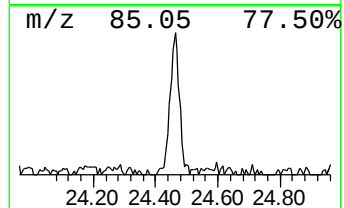
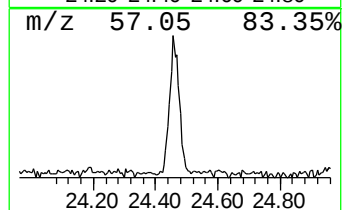
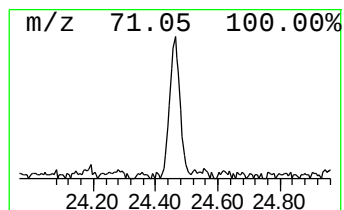
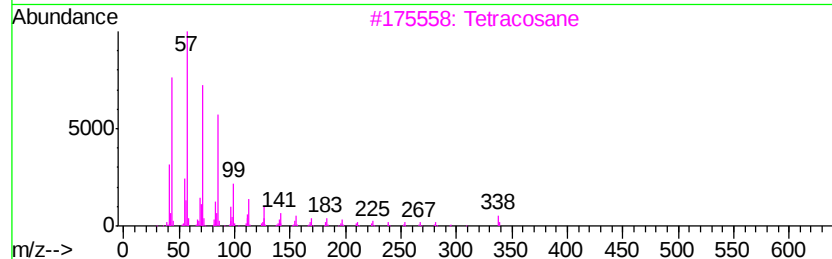
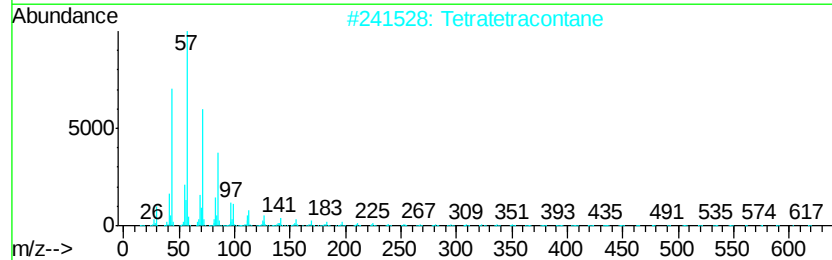
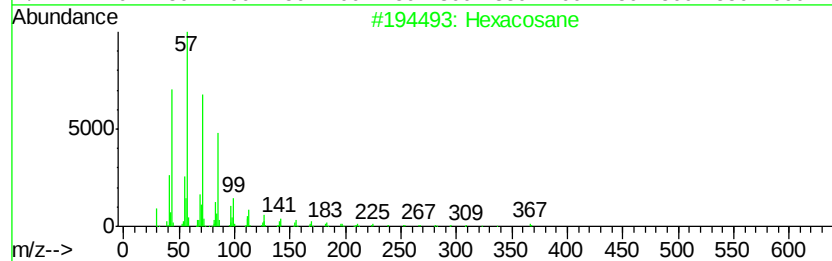
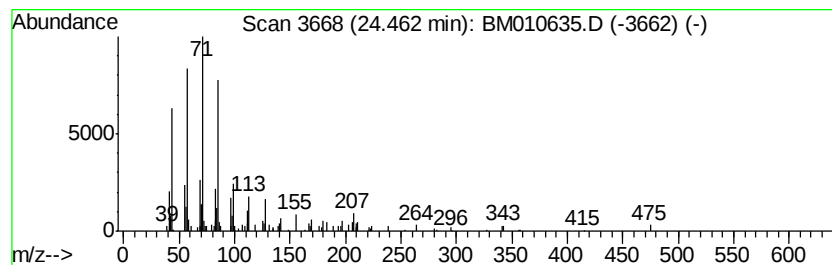
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	2.22 ng/ul	190002	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Hentriacontane	437	C31H64	000630-04-6	87
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010635.D
Acq On : 21 Jun 2017 22:28
Operator : SJ/JU
Sample : I3627-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F5E25

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Naphthalenedi...	15.49	6.9	ng/ul	422633	3	14.12	1225320	20.0
Tridecanoic acid	17.79	3.9	ng/ul	309107	4	16.87	1568470	20.0
1-Heneicosanol	20.82	2.9	ng/ul	338168	5	21.09	2337350	20.0
(DEL) Alkane: Str...	23.76	2.6	ng/ul	219224	6	23.23	1713300	20.0
Chloroacetic acid...	23.84	2.1	ng/ul	179359	6	23.23	1713300	20.0
(DEL) Alkane: Str...	24.46	2.2	ng/ul	190002	6	23.23	1713300	20.0