

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
 Data File : BG024282.D
 Acq On : 12 Oct 2016 2:01
 Operator : UM/SJ
 Sample : H5113-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BDP64

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG0100716.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	3.648	135	138	148	rVB7	30422	64509	1.40%	0.106%
2	3.947	186	189	194	rBV5	8316	16240	0.35%	0.027%
3	4.247	239	240	249	rBV7	15727	33744	0.73%	0.055%
4	4.412	266	268	275	rBV5	21339	37301	0.81%	0.061%
5	4.741	322	324	328	rBV4	11254	18363	0.40%	0.030%
6	5.363	425	430	435	rVB9	12365	26606	0.58%	0.044%
7	5.898	515	521	526	rBV9	15780	34124	0.74%	0.056%
8	6.333	589	595	597	rBV5	10535	18263	0.40%	0.030%
9	6.480	612	620	623	rBV10	11393	16247	0.35%	0.027%
10	6.638	644	647	652	rBV7	10133	15245	0.33%	0.025%
11	6.897	688	691	697	rVB8	10193	15810	0.34%	0.026%
12	6.967	701	703	708	rBV4	13471	19029	0.41%	0.031%
13	7.420	771	780	792	rVB	590357	1110213	24.09%	1.825%
14	7.602	805	811	821	rBV	420872	712158	15.45%	1.171%
15	7.814	838	847	857	rBV	550953	996967	21.63%	1.639%
16	8.289	921	928	939	rBV	588688	1089821	23.65%	1.792%
17	8.460	953	957	961	rVB7	8759	14940	0.32%	0.025%
18	8.519	961	967	969	rBV7	9525	16307	0.35%	0.027%
19	8.977	1037	1045	1052	rVB2	711792	1270715	27.57%	2.089%
20	9.465	1120	1128	1135	rVV	579406	1078677	23.41%	1.773%
21	9.523	1135	1138	1144	rVV8	23884	37232	0.81%	0.061%
22	9.564	1144	1145	1153	rVV7	6934	16309	0.35%	0.027%
23	9.811	1185	1187	1192	rBV5	11877	19121	0.41%	0.031%
24	9.888	1196	1200	1204	rBV5	9346	15843	0.34%	0.026%
25	10.040	1222	1226	1229	rBV3	10575	20400	0.44%	0.034%
26	10.193	1244	1252	1261	rBV2	472002	898555	19.50%	1.477%
27	10.722	1335	1342	1357	rVB	744334	1342909	29.14%	2.208%
28	11.121	1402	1410	1419	rVB	785382	1491886	32.37%	2.453%
29	11.245	1422	1431	1440	rBV2	395215	761031	16.51%	1.251%
30	11.844	1528	1533	1541	rVB9	9252	22243	0.48%	0.037%
31	11.962	1550	1553	1555	rBV3	13230	15672	0.34%	0.026%
32	12.273	1600	1606	1608	rVV4	11104	17059	0.37%	0.028%
33	12.326	1608	1615	1619	rVB10	13707	29073	0.63%	0.048%
34	12.673	1670	1674	1682	rBV10	19073	43255	0.94%	0.071%

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35	13.013	1731	1732	1739	rVB5	10431	15883	0.34%	0.026%
36	13.266	1773	1775	1783	rVB9	8914	17047	0.37%	0.028%
37	13.501	1808	1815	1820	rBV7	17095	29573	0.64%	0.049%
38	13.624	1833	1836	1840	rVB5	9617	16886	0.37%	0.028%
39	13.771	1857	1861	1867	rVV3	33559	53068	1.15%	0.087%
40	13.971	1886	1895	1900	rVV7	9698	21546	0.47%	0.035%
41	14.300	1939	1951	1955	rVV	1479080	2311520	50.16%	3.800%
42	14.347	1955	1959	1969	rVB	1302811	1890048	41.01%	3.107%
43	14.606	1994	2003	2010	rBV	1483951	2456865	53.31%	4.039%
44	14.764	2025	2030	2036	rBV5	38044	62129	1.35%	0.102%
45	14.905	2047	2054	2063	rVB	1419793	2282526	49.53%	3.753%
46	15.064	2072	2081	2096	rBV	871859	1424143	30.90%	2.341%
47	15.217	2102	2107	2109	rBV5	13262	18487	0.40%	0.030%
48	15.270	2112	2116	2121	rVB6	30747	45577	0.99%	0.075%
49	15.369	2130	2133	2139	rBV5	23011	38304	0.83%	0.063%
50	15.616	2172	2175	2178	rBV5	12008	16067	0.35%	0.026%
51	15.663	2180	2183	2186	rVB5	15084	16513	0.36%	0.027%
52	15.710	2186	2191	2196	rBV	103191	142504	3.09%	0.234%
53	15.763	2197	2200	2205	rVB7	11570	21850	0.47%	0.036%
54	15.892	2214	2222	2230	rBV	2195495	3384698	73.44%	5.565%
55	15.992	2231	2239	2246	rBV2	790171	1227038	26.62%	2.017%
56	16.110	2252	2259	2271	rVB10	46017	154903	3.36%	0.255%
57	16.210	2271	2276	2280	rVB8	21848	35436	0.77%	0.058%
58	16.262	2281	2285	2293	rVB10	22937	33506	0.73%	0.055%
59	16.327	2293	2296	2304	rBV9	17548	26894	0.58%	0.044%
60	16.568	2331	2337	2346	rBV	136619	249939	5.42%	0.411%
61	16.844	2379	2384	2389	rBV8	19379	43717	0.95%	0.072%
62	16.915	2392	2396	2402	rBV6	17372	35825	0.78%	0.059%
63	16.997	2407	2410	2414	rBV5	28195	37221	0.81%	0.061%
64	17.073	2419	2423	2430	rBV9	23916	56327	1.22%	0.093%
65	17.138	2431	2434	2438	rVB6	14208	18911	0.41%	0.031%
66	17.355	2467	2471	2476	rBV	96295	141699	3.07%	0.233%
67	17.408	2476	2480	2489	rVB10	41061	100112	2.17%	0.165%
68	17.643	2512	2520	2527	rBV	1890425	2948603	63.98%	4.848%
69	17.743	2530	2537	2546	rBV	2397986	3838064	83.28%	6.310%
70	17.884	2555	2561	2566	rBV2	80156	104738	2.27%	0.172%
71	17.931	2566	2569	2574	rVV	146430	180632	3.92%	0.297%

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72	17.978	2574	2577	2582	rVV5	24132	34199	0.74%	0.056%
73	18.101	2592	2598	2602	rVB7	34148	53641	1.16%	0.088%
74	18.143	2602	2605	2608	rBV5	12537	17937	0.39%	0.029%
75	18.366	2635	2643	2649	rBV5	30139	74057	1.61%	0.122%
76	18.489	2658	2664	2676	rBV	655880	952812	20.67%	1.567%
77	18.577	2676	2679	2684	rVB5	25890	35331	0.77%	0.058%
78	18.818	2717	2720	2728	rVB10	19314	37690	0.82%	0.062%
79	18.912	2734	2736	2742	rVB6	20401	20479	0.44%	0.034%
80	19.141	2772	2775	2778	rBV5	16182	21206	0.46%	0.035%
81	19.183	2778	2782	2786	rVV2	115906	149824	3.25%	0.246%
82	19.230	2786	2790	2795	rVB	228479	277165	6.01%	0.456%
83	19.641	2851	2860	2868	rBV6	64638	174627	3.79%	0.287%
84	19.747	2873	2878	2894	rBV2	430957	608759	13.21%	1.001%
85	19.899	2901	2904	2910	rVB6	54944	80473	1.75%	0.132%
86	20.011	2917	2923	2936	rVB	3032790	4608653	100.00%	7.577%
87	20.293	2966	2971	2974	rBV	1061813	1228738	26.66%	2.020%
88	20.334	2974	2978	2984	rVB	2034272	2436622	52.87%	4.006%
89	21.304	3138	3143	3146	rBV	391492	516862	11.22%	0.850%
90	21.345	3146	3150	3155	rVB	755243	962918	20.89%	1.583%
91	21.533	3177	3182	3191	rBV2	422160	662933	14.38%	1.090%
92	21.944	3244	3252	3259	rVB	1958613	3404393	73.87%	5.597%
93	22.461	3335	3340	3344	rBV4	164389	266500	5.78%	0.438%
94	22.508	3344	3348	3355	rVB2	310556	470222	10.20%	0.773%
95	23.431	3501	3505	3511	rVB8	94630	167472	3.63%	0.275%
96	23.713	3547	3553	3559	rVB3	108430	247040	5.36%	0.406%
97	23.959	3590	3595	3600	rBV5	120796	213637	4.64%	0.351%
98	24.024	3601	3606	3613	rVB3	264167	543426	11.79%	0.893%
99	25.152	3787	3798	3810	rBV2	1394407	4292601	93.14%	7.058%
100	25.393	3828	3839	3851	rVB2	1118393	3427796	74.38%	5.636%

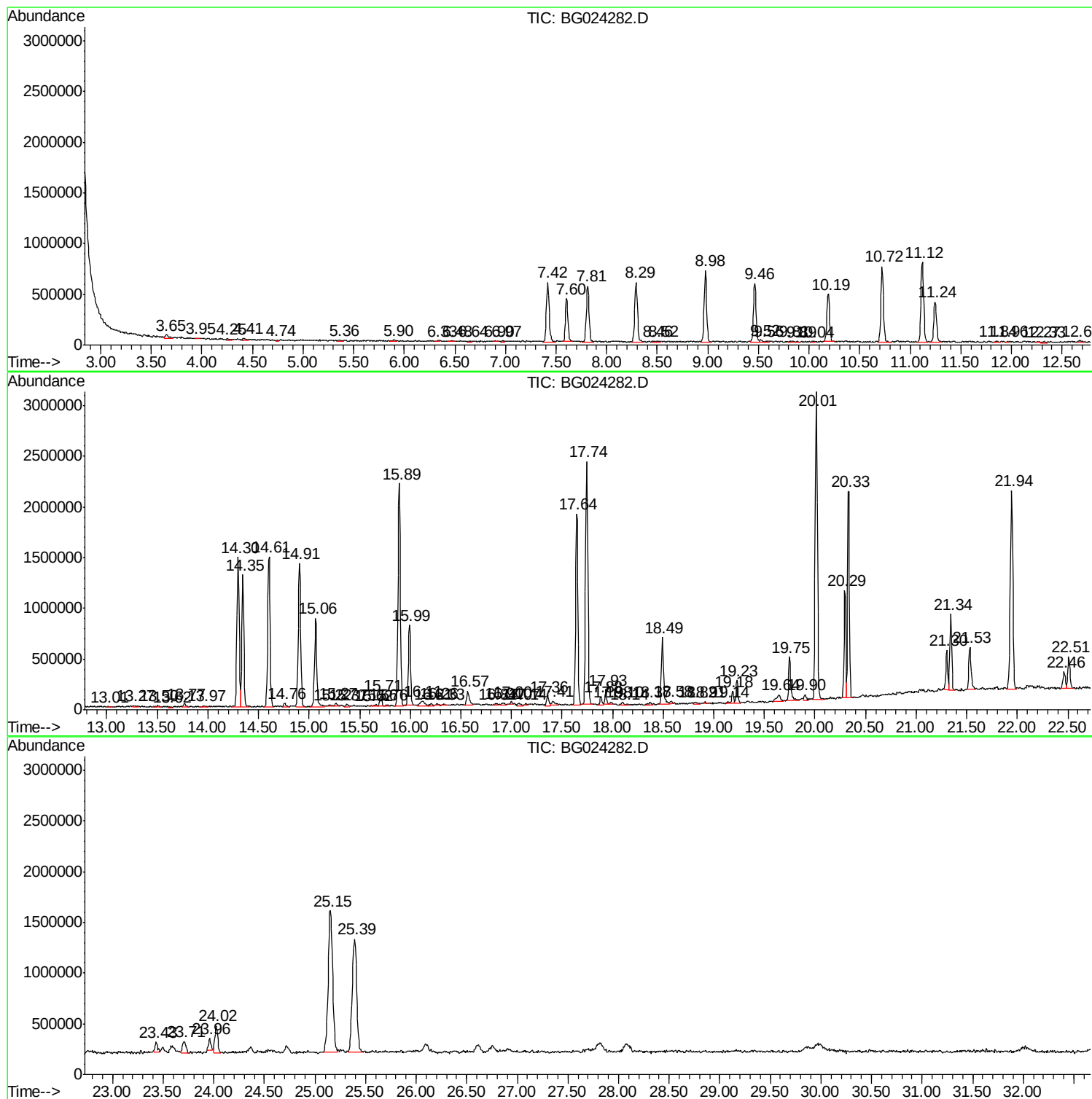
Sum of corrected areas: 60822679

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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



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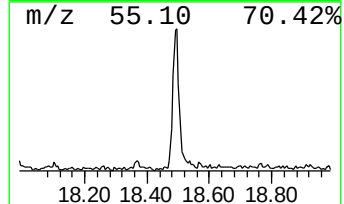
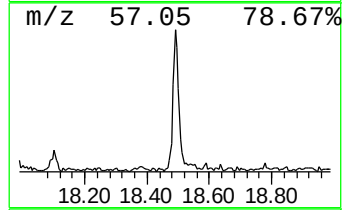
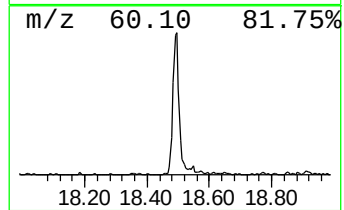
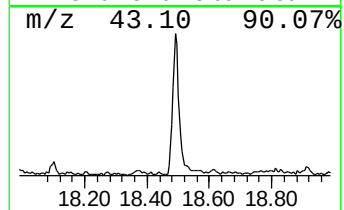
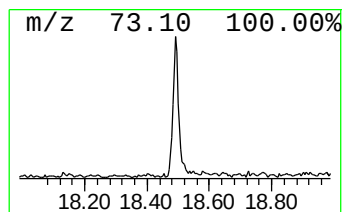
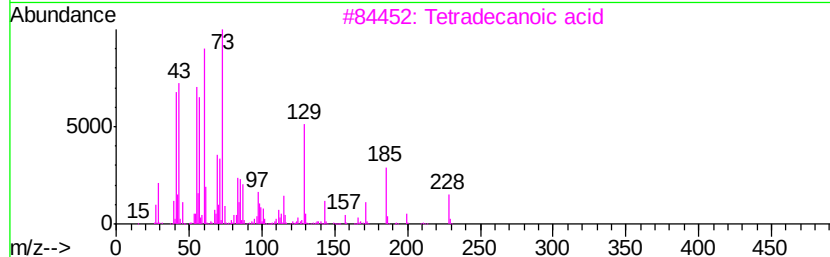
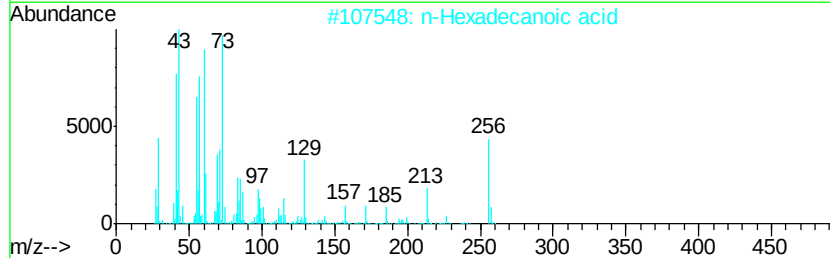
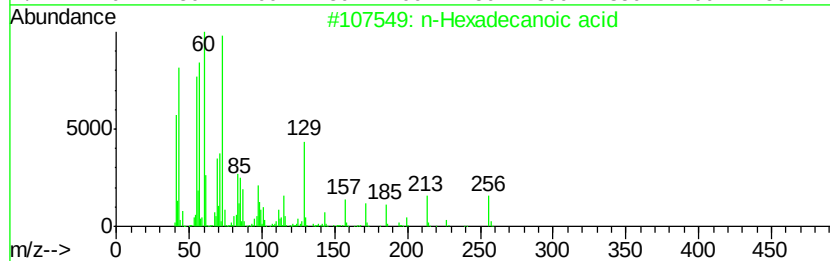
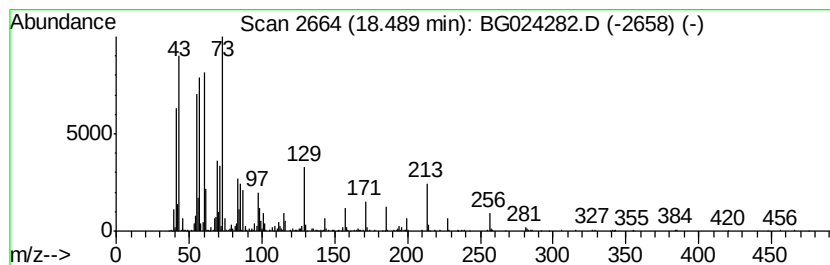
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	6.46 ng/ul	952812	Phenanthrene-d10	17.64

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	90	
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87	
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83	



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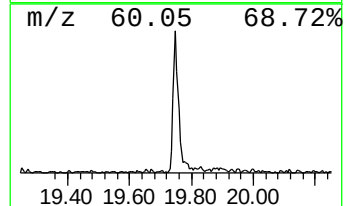
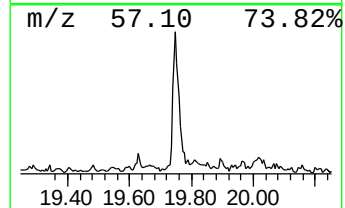
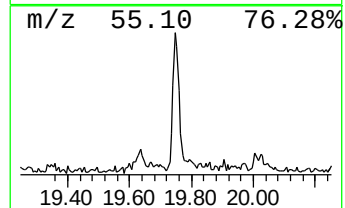
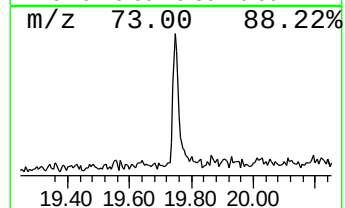
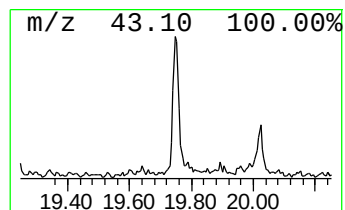
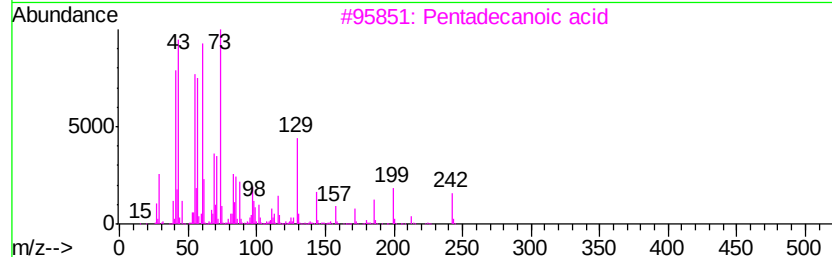
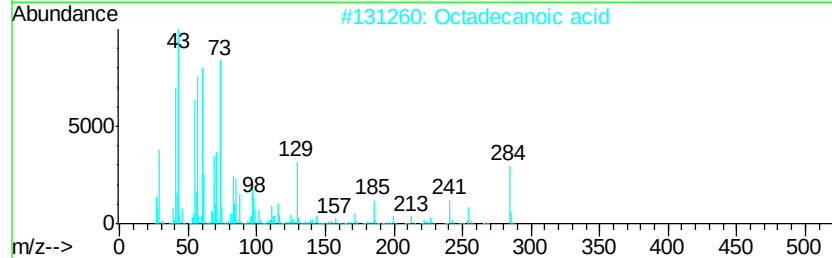
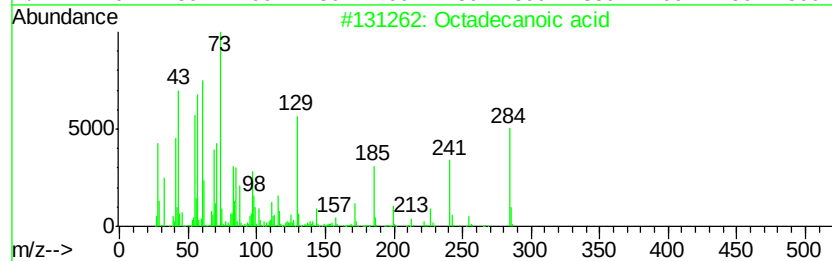
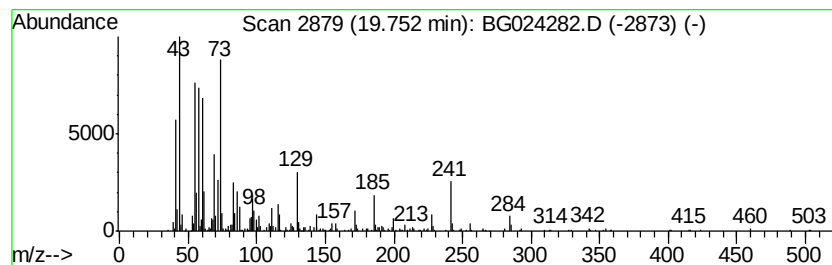
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	4.13 ng/ul	608759	Phenanthrene-d10	17.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Octadecanoic acid	284	C18H36O2	000057-11-4	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Tridecanoic acid	214	C13H26O2	000638-53-9	89
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	86



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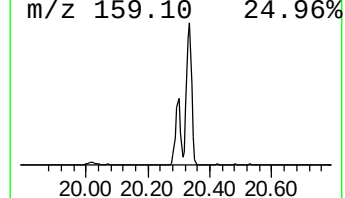
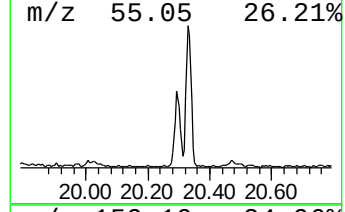
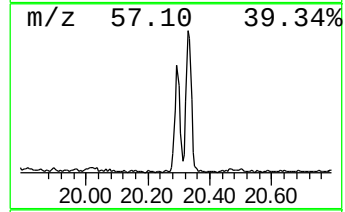
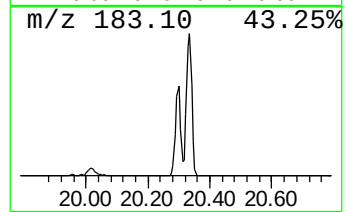
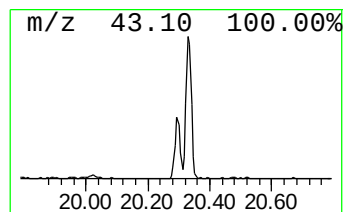
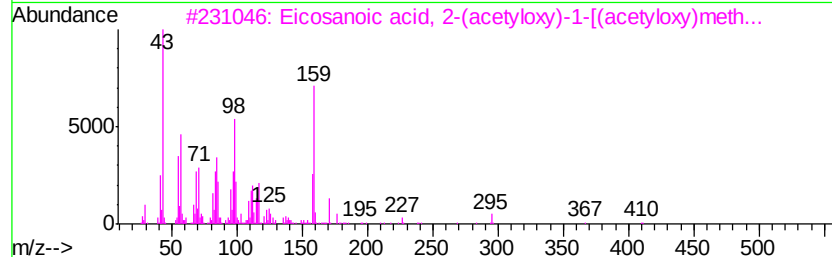
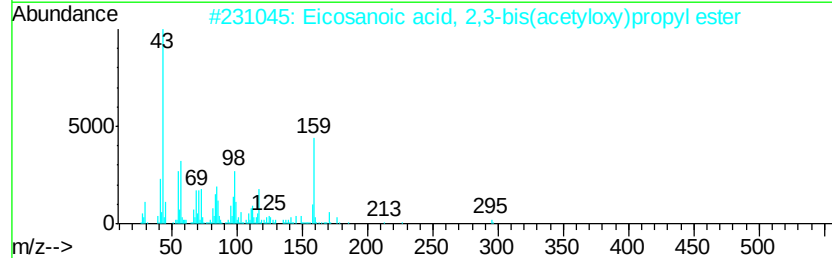
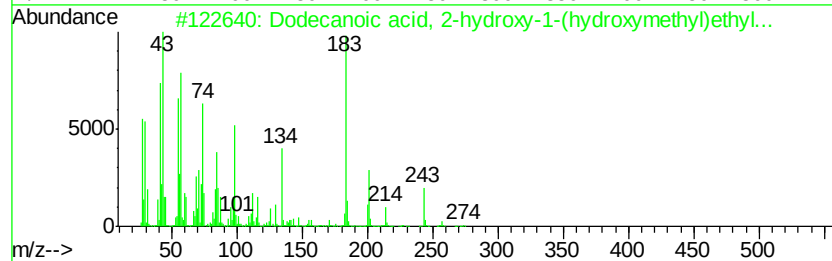
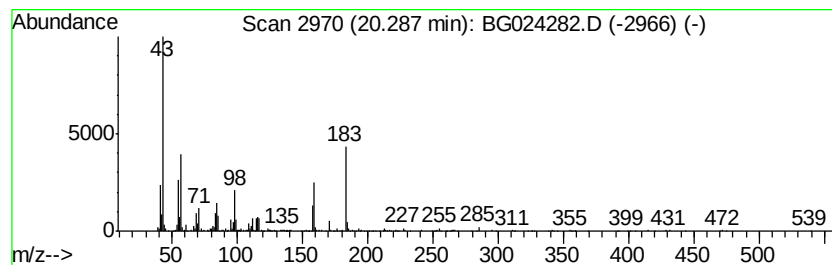
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecanoic acid, 2-hydroxy-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	7.22 ng/ul	1228740	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	50
2		Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	38
3		Eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]...	470	C27H50O6	055429-68-0	27
4		1,2-Dicarbadodecaborane(12), 1-hydroxy-2,3-bis(hydroxymethyl)ethyl...	230	C8H24B10	020740-05-0	14
5		9-Octadecenoic acid (Z)-, 2,3-bis(hydroxymethyl)ethyl...	440	C25H44O6	055401-64-4	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024282.D
Acq On : 12 Oct 2016 2:01
Operator : UM/SJ
Sample : H5113-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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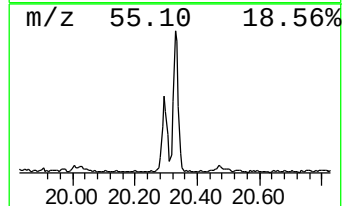
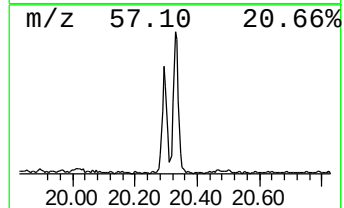
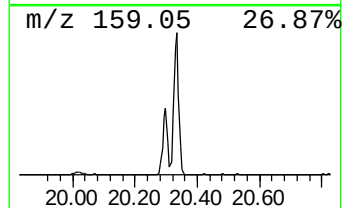
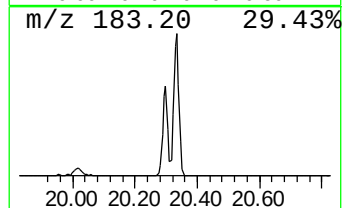
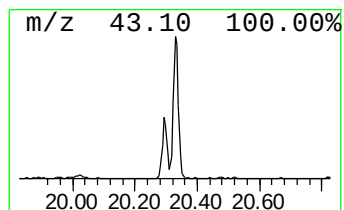
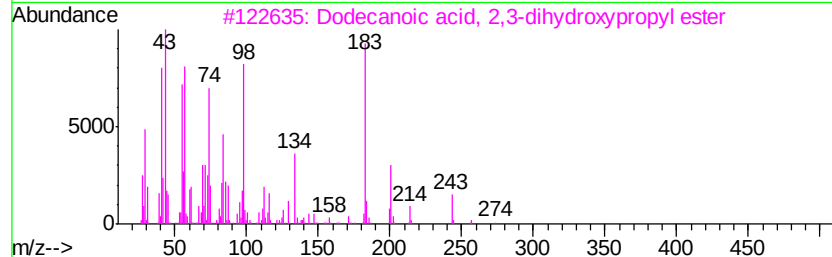
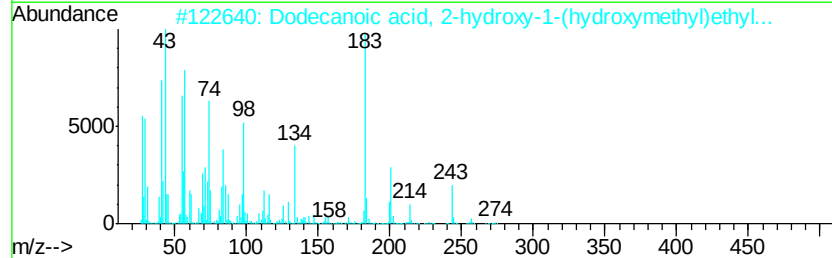
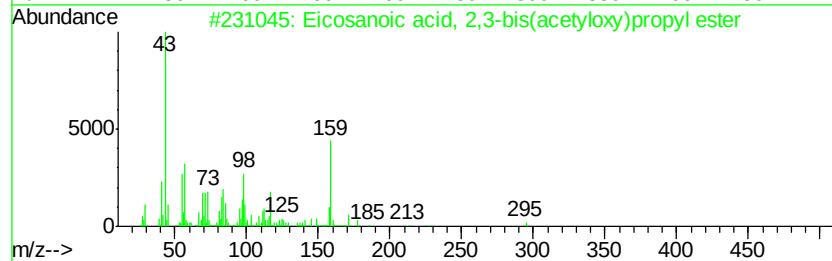
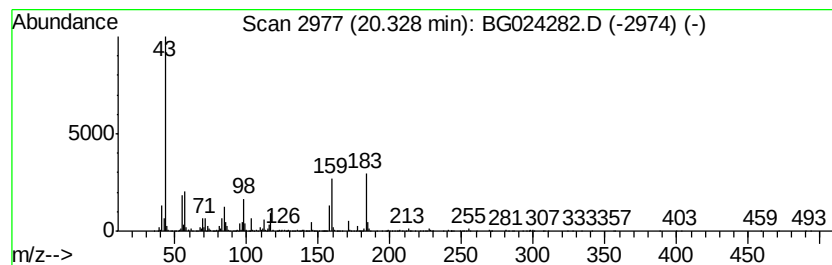
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.33	14.31 ng/ul	2436620	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	38
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	32
3		Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	32
4		9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	17
5		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024282.D
Acq On : 12 Oct 2016 2:01
Operator : UM/SJ
Sample : H5113-07
Misc :
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Instrument :
BNA_G
ClientSampleId :
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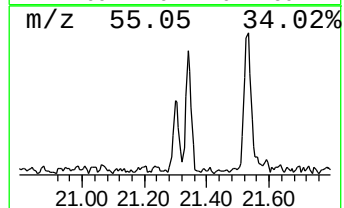
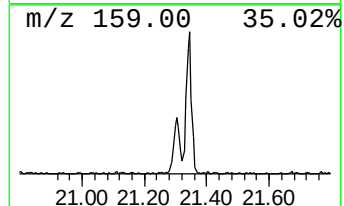
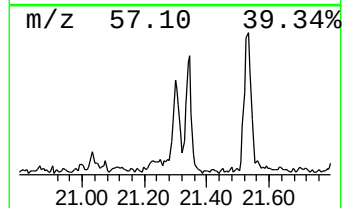
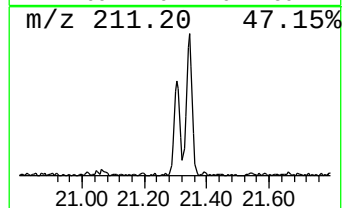
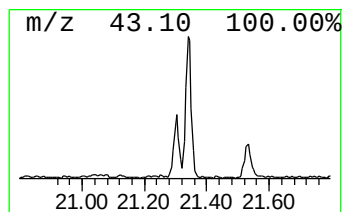
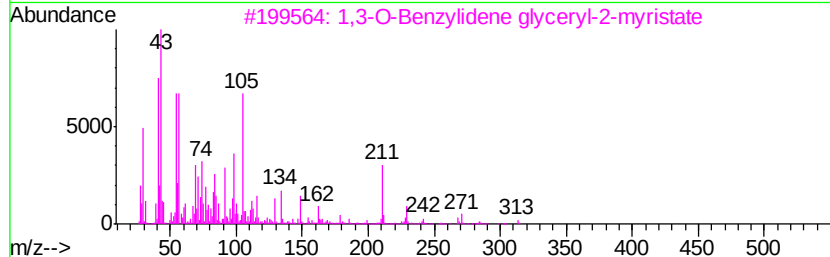
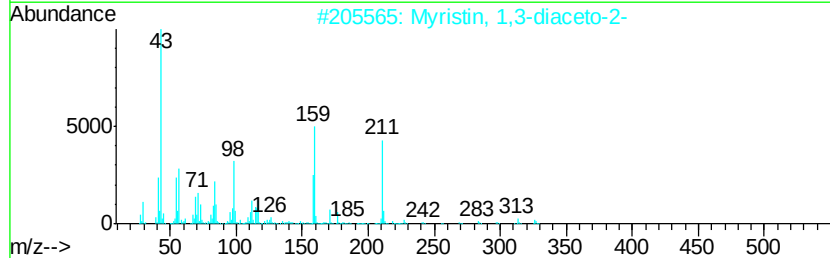
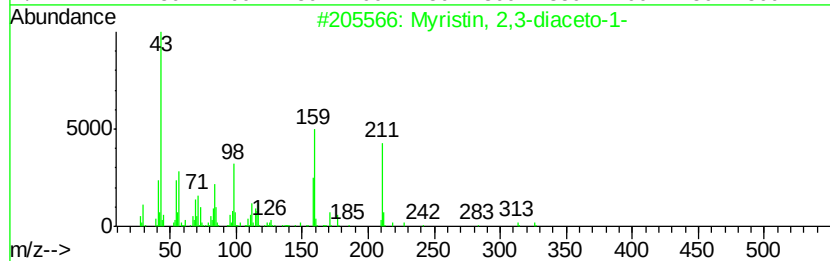
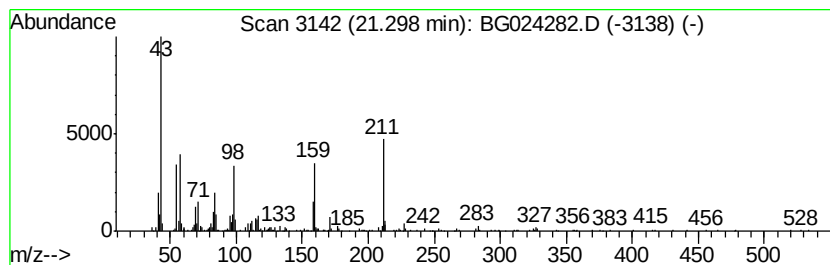
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Myristin, 2,3-diaceto-1- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	3.04 ng/ul	516862	Chrysene-d12	21.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	72	
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	32	
3	1,3-O-Benzylidene glyceryl-2-myristate	374	C24H38O3	1000036-49-3	23	
4	Tetradecanoic acid, 2-hydroxy-1-	302	C17H34O4	003443-83-2	23	
5	3-Acetoxy-3-(2-bromocyclobut-1-ethyl)-2-methylbutanoic acid	290	C11H15BrO4	1000193-56-1	12	



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
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Acq On : 12 Oct 2016 2:01
Operator : UM/SJ
Sample : H5113-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

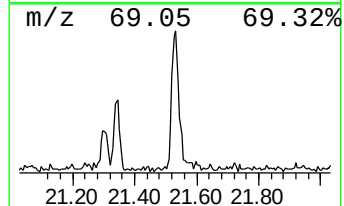
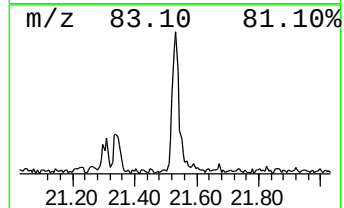
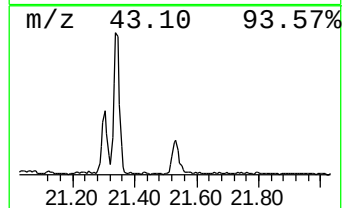
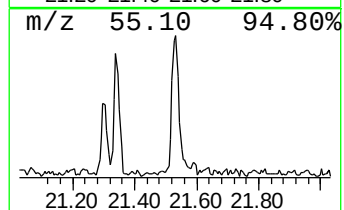
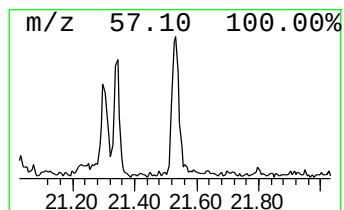
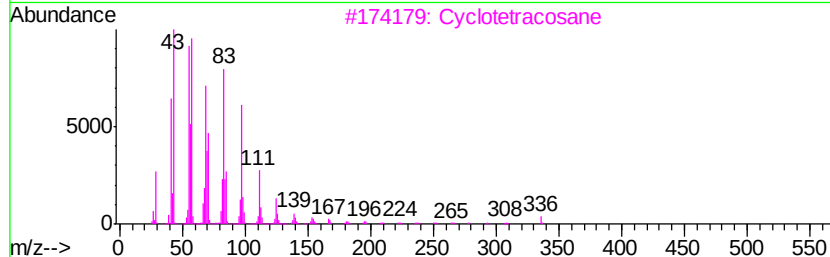
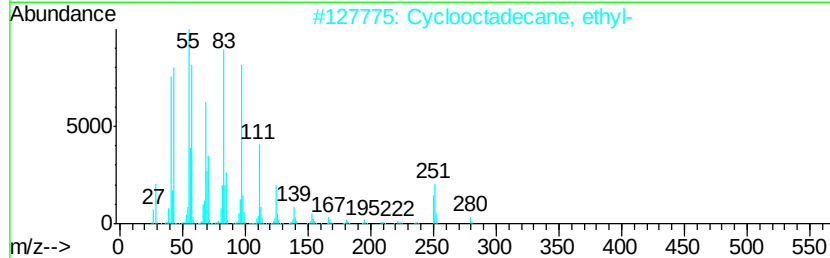
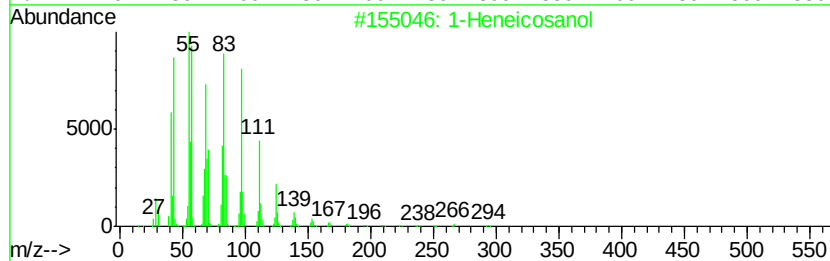
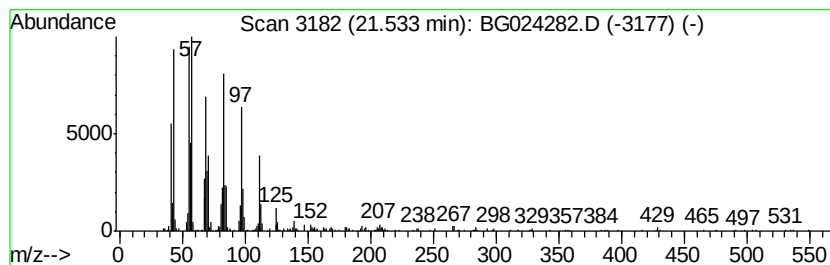
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.53	3.89 ng/ul	662933	Chrysene-d12	21.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol		312 C21H44O	015594-90-8 91
2	Cyclooctadecane, ethyl-		280 C20H40	1000151-22-5 91
3	Cyclotetracosane		336 C24H48	000297-03-0 87
4	1-Tricosanol		340 C23H48O	003133-01-5 87
5	5-Eicosene, (E)-		280 C20H40	074685-30-6 83



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024282.D
Acq On : 12 Oct 2016 2:01
Operator : UM/SJ
Sample : H5113-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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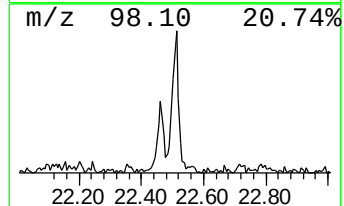
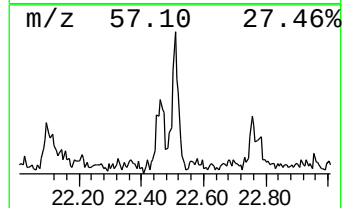
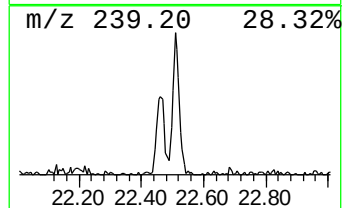
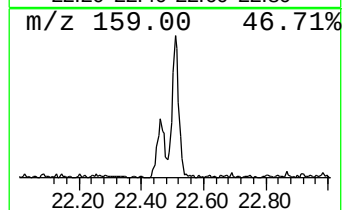
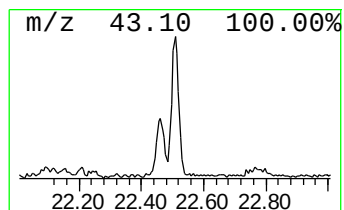
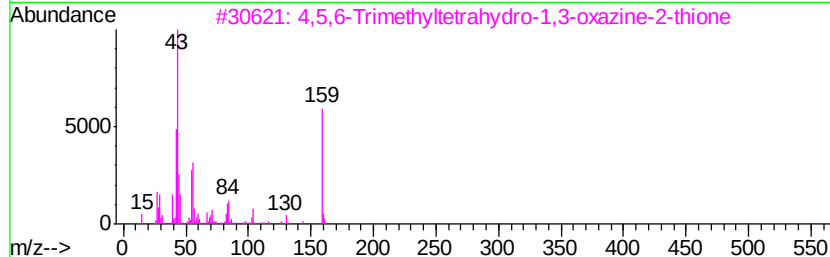
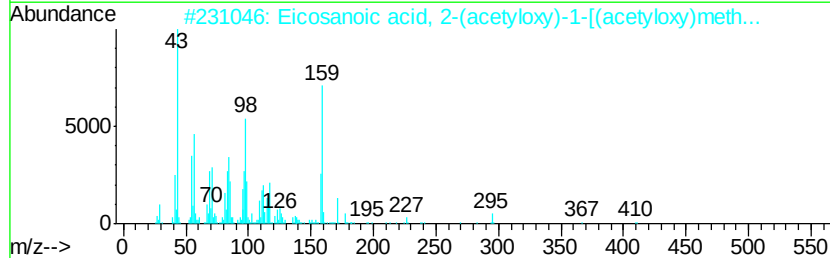
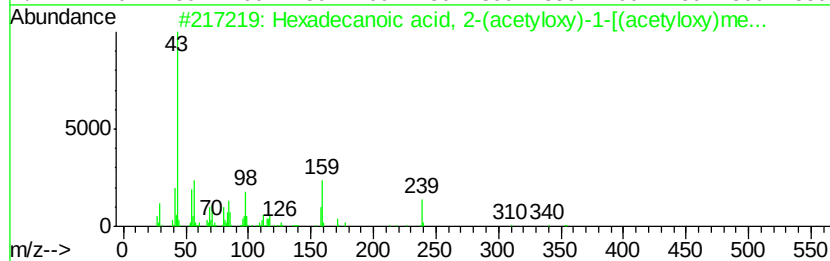
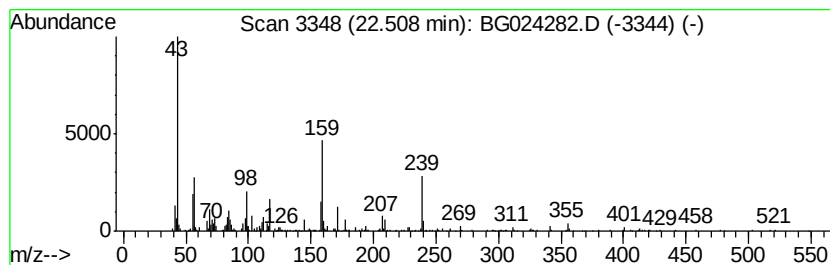
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	2.76 ng/ul	470222	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	38
2		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	38
3		4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	12
4		N-[3-(Cyano-dimethyl-methyl)-1-m...	208	C12H20N2O	1000301-04-6	10
5		Furan, 2,3-dihydro-2,5-dimethyl-	98	C6H10O	017108-52-0	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024282.D
Acq On : 12 Oct 2016 2:01
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Sample : H5113-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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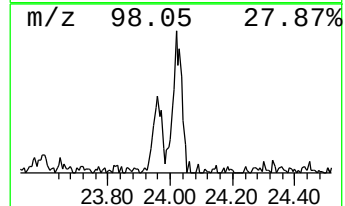
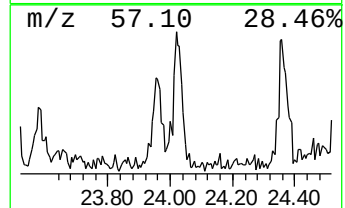
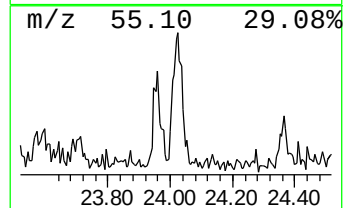
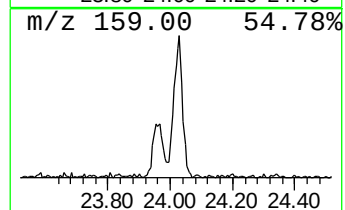
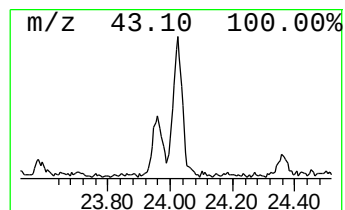
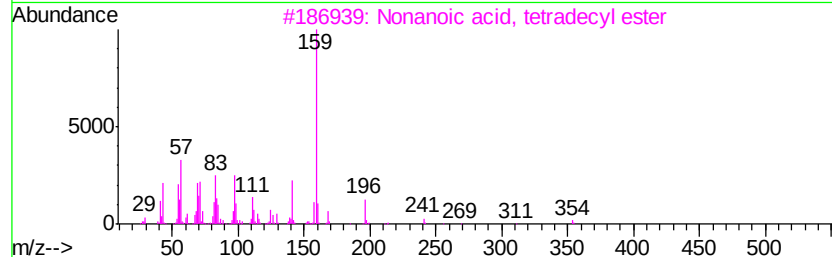
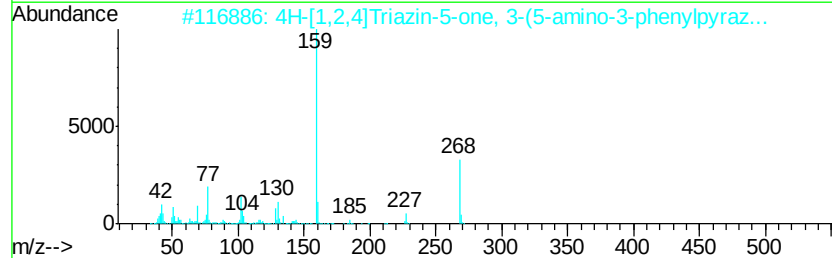
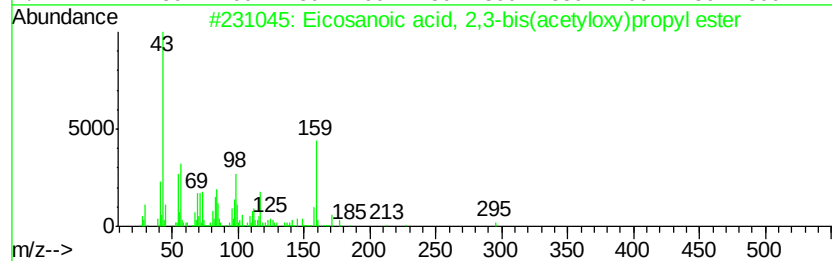
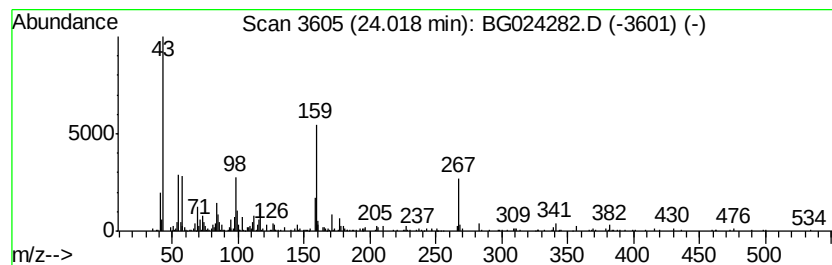
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.02	3.17 ng/ul	543426	Perylene-d12	25.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	38
2		4H-[1,2,4]Triazin-5-one, 3-(5-am...	268	C13H12N6O	1000303-97-4	38
3		Nonanoic acid, tetradecyl ester	354	C23H46O2	1000340-28-1	32
4		2,5-Difluorobenzoic acid, decyl ...	298	C17H24F2O2	1000338-80-9	32
5		Diethylmalonic acid, butyl 4-tri...	374	C19H25F3O4	1000368-40-2	32



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101116\
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ClientSampleId :
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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
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Octadecanoic acid	19.75	4.1	ng/ul	608759	4	17.64	2948600	20.0
Dodecanoic acid, ...	20.29	7.2	ng/ul	1228740	5	21.94	3404390	20.0
unknown-01	20.33	14.3	ng/ul	2436620	5	21.94	3404390	20.0
Myristin, 2,3-dia...	21.30	3.0	ng/ul	516862	5	21.94	3404390	20.0
1-Heneicosanol	21.53	3.9	ng/ul	662933	5	21.94	3404390	20.0
unknown-02	22.51	2.8	ng/ul	470222	5	21.94	3404390	20.0
unknown-03	24.02	3.2	ng/ul	543426	6	25.39	3427800	20.0