

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
 Data File : BG028120.D
 Acq On : 2 Aug 2017 22:37
 Operator : SJ/JU
 Sample : I4405-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JJ2X6

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\SOM-EPA-BG080217.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	3.770	26	31	40	rVV4	11456	16889	1.54%	0.117%
2	3.852	40	45	55	rVB6	6896	16319	1.49%	0.113%
3	4.358	128	131	138	rBV4	2979	4701	0.43%	0.032%
4	4.581	165	169	181	rVB2	11484	19614	1.79%	0.135%
5	4.781	198	203	206	rVB6	5100	6999	0.64%	0.048%
6	4.933	225	229	234	rVB3	2300	4206	0.38%	0.029%
7	5.180	267	271	279	rBV5	2958	5854	0.53%	0.040%
8	5.480	316	322	326	rBV6	3063	4987	0.45%	0.034%
9	6.261	449	455	459	rBV2	1632	2956	0.27%	0.020%
10	7.507	658	667	683	rBV2	120359	255641	23.32%	1.765%
11	7.677	690	696	708	rBV	88242	148246	13.52%	1.024%
12	7.895	726	733	745	rBV	104566	195691	17.85%	1.351%
13	8.171	775	780	787	rVB2	1727	3144	0.29%	0.022%
14	8.365	804	813	826	rBV	130022	232304	21.19%	1.604%
15	8.623	852	857	862	rVB2	2175	4554	0.42%	0.031%
16	9.052	922	930	948	rBV2	144700	273634	24.96%	1.889%
17	9.199	949	955	961	rBV3	2167	5536	0.50%	0.038%
18	9.534	1004	1012	1024	rBV	120777	235329	21.47%	1.625%
19	9.898	1070	1074	1081	rVB3	2231	3810	0.35%	0.026%
20	10.257	1128	1135	1151	rVB	103964	195695	17.85%	1.351%
21	10.797	1218	1227	1242	rBV	146572	292652	26.69%	2.021%
22	11.109	1274	1280	1284	rVV3	2338	4517	0.41%	0.031%
23	11.185	1284	1293	1304	rVV	206304	393009	35.85%	2.714%
24	11.314	1308	1315	1333	rBV	76891	179751	16.40%	1.241%
25	11.614	1363	1366	1370	rBV2	1648	2830	0.26%	0.020%
26	11.720	1379	1384	1386	rBV2	1830	2752	0.25%	0.019%
27	12.178	1459	1462	1472	rVB2	1307	2858	0.26%	0.020%
28	12.748	1552	1559	1566	rVB3	2265	5654	0.52%	0.039%
29	12.942	1586	1592	1598	rBV2	1899	3223	0.29%	0.022%
30	13.564	1691	1698	1705	rVB6	2515	7019	0.64%	0.048%
31	13.776	1725	1734	1740	rBV6	3965	10395	0.95%	0.072%
32	13.852	1741	1747	1749	rVV4	2307	3580	0.33%	0.025%
33	14.358	1824	1833	1838	rBV	374452	558266	50.92%	3.855%
34	14.405	1838	1841	1850	rVB	98862	141793	12.93%	0.979%

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35	14.604	1868	1875	1878	rBV2	3367	4656	0.42%	0.032%
36	14.663	1878	1885	1893	rBV	364481	604448	55.13%	4.173%
37	14.828	1908	1913	1917	rBV4	5731	8466	0.77%	0.058%
38	14.892	1921	1924	1928	rBV2	2398	3446	0.31%	0.024%
39	14.969	1930	1937	1946	rBV2	372385	623387	56.86%	4.304%
40	15.157	1962	1969	1986	rVV2	67992	159699	14.57%	1.103%
41	15.262	1986	1987	1990	rVV2	4516	5736	0.52%	0.040%
42	15.321	1990	1997	2002	rVV7	8296	21765	1.99%	0.150%
43	15.368	2002	2005	2012	rVV8	5833	10281	0.94%	0.071%
44	15.439	2012	2017	2023	rVB6	4285	9548	0.87%	0.066%
45	15.515	2027	2030	2033	rBV3	2232	3353	0.31%	0.023%
46	15.615	2042	2047	2048	rBV2	1845	2895	0.26%	0.020%
47	15.691	2055	2060	2065	rVB3	9262	14158	1.29%	0.098%
48	15.774	2068	2074	2080	rVB3	17655	28324	2.58%	0.196%
49	15.832	2080	2084	2089	rBV3	2795	5181	0.47%	0.036%
50	15.897	2089	2095	2096	rBV3	2354	3381	0.31%	0.023%
51	15.956	2098	2105	2114	rVB	524008	834918	76.16%	5.765%
52	16.067	2118	2124	2134	rBV2	154879	241068	21.99%	1.664%
53	16.197	2136	2146	2155	rVB9	9280	29575	2.70%	0.204%
54	16.273	2155	2159	2162	rBV4	2452	3970	0.36%	0.027%
55	16.326	2165	2168	2171	rBV3	3118	5183	0.47%	0.036%
56	16.391	2176	2179	2184	rVB5	5396	7567	0.69%	0.052%
57	16.461	2185	2191	2195	rBV4	1956	4746	0.43%	0.033%
58	16.526	2200	2202	2207	rVB5	2359	2839	0.26%	0.020%
59	16.631	2215	2220	2233	rVB2	26367	57559	5.25%	0.397%
60	16.908	2262	2267	2271	rBV6	3690	5190	0.47%	0.036%
61	16.978	2275	2279	2284	rBV4	2977	5778	0.53%	0.040%
62	17.037	2288	2289	2294	rVB4	3875	3874	0.35%	0.027%
63	17.096	2294	2299	2303	rVB8	3663	6784	0.62%	0.047%
64	17.143	2303	2307	2315	rVB4	3934	8082	0.74%	0.056%
65	17.213	2315	2319	2322	rBV4	3878	5223	0.48%	0.036%
66	17.431	2351	2356	2361	rBV2	16095	21836	1.99%	0.151%
67	17.483	2361	2365	2377	rVB8	8188	19489	1.78%	0.135%
68	17.589	2379	2383	2385	rBV3	2904	3892	0.36%	0.027%
69	17.718	2398	2405	2416	rBV	516077	841480	76.75%	5.810%
70	17.818	2416	2422	2432	rVB2	605713	936092	85.38%	6.463%
71	17.977	2446	2449	2456	rBV7	3236	6462	0.59%	0.045%

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72	18.089	2464	2468	2469	rBV4	4599	3391	0.31%	0.023%
73	18.177	2478	2483	2485	rVB3	9931	13698	1.25%	0.095%
74	18.570	2546	2550	2561	rBV3	44767	97965	8.94%	0.676%
75	18.852	2594	2598	2604	rBV6	8455	12341	1.13%	0.085%
76	18.929	2608	2611	2613	rBV4	4422	6138	0.56%	0.042%
77	19.129	2641	2645	2647	rBV5	4606	8405	0.77%	0.058%
78	19.393	2689	2690	2693	rBV3	3374	3846	0.35%	0.027%
79	19.469	2701	2703	2708	rBV2	14742	17781	1.62%	0.123%
80	19.828	2759	2764	2771	rBV5	45326	85810	7.83%	0.592%
81	20.022	2794	2797	2803	rBV3	25553	43402	3.96%	0.300%
82	20.092	2803	2809	2820	rVB	753539	1096326	100.00%	7.570%
83	20.580	2887	2892	2898	rVB4	51230	93325	8.51%	0.644%
84	20.862	2936	2940	2946	rVB8	33065	45397	4.14%	0.313%
85	21.085	2975	2978	2982	rVB3	35257	40223	3.67%	0.278%
86	21.626	3065	3070	3080	rBV4	98720	196685	17.94%	1.358%
87	21.890	3111	3115	3120	rVB2	40522	61930	5.65%	0.428%
88	22.055	3135	3143	3153	rVB	507475	960478	87.61%	6.632%
89	22.207	3165	3169	3175	rVB3	32264	51960	4.74%	0.359%
90	22.865	3276	3281	3287	rBV	87668	157877	14.40%	1.090%
91	23.617	3405	3409	3416	rVB3	44554	80016	7.30%	0.552%
92	24.487	3550	3557	3564	rBV	132392	293995	26.82%	2.030%
93	24.569	3565	3571	3588	rVB4	62774	208569	19.02%	1.440%
94	25.321	3688	3699	3713	rVB2	331320	953848	87.00%	6.586%
95	25.562	3727	3740	3755	rVB2	280008	993700	90.64%	6.861%
96	26.755	3937	3943	3957	rVB2	116701	384153	35.04%	2.652%
97	26.914	3963	3970	3975	rBV10	24469	60623	5.53%	0.419%
98	28.241	4187	4196	4210	rVB5	38681	140978	12.86%	0.973%
99	30.033	4490	4501	4515	rBV6	41222	168907	15.41%	1.166%
100	31.367	4714	4728	4747	rBV6	68002	396864	36.20%	2.740%

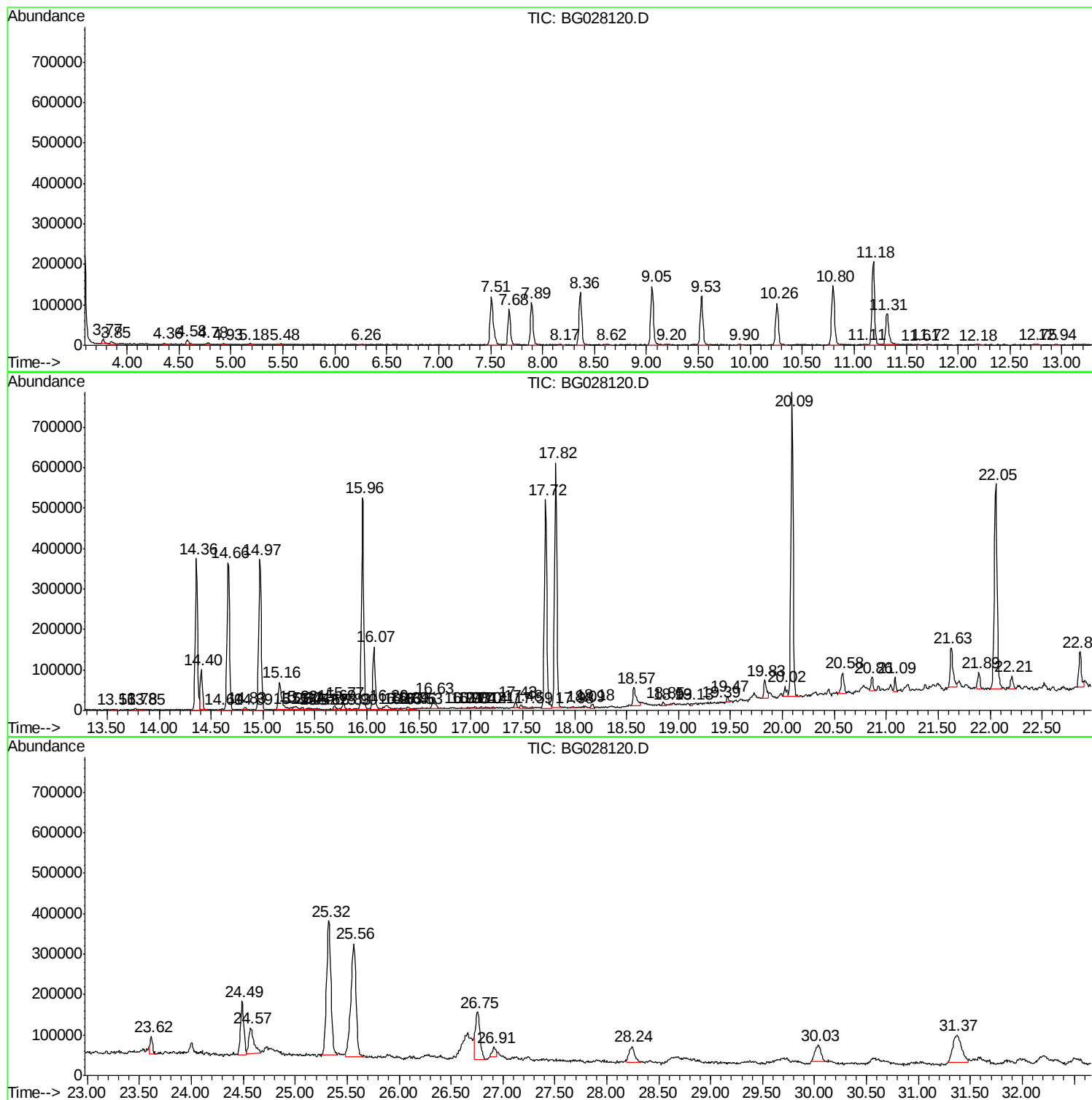
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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



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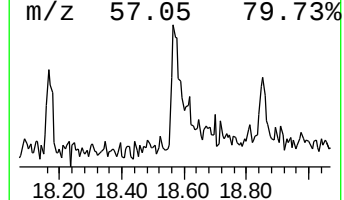
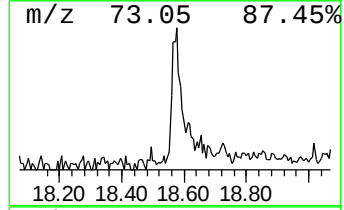
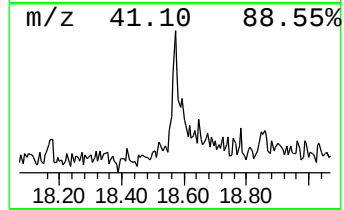
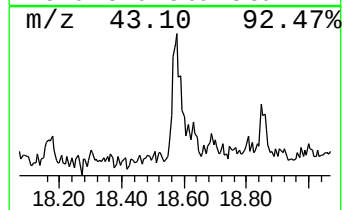
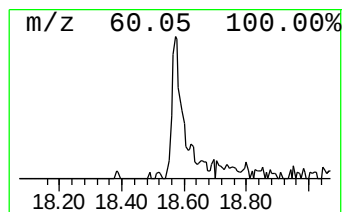
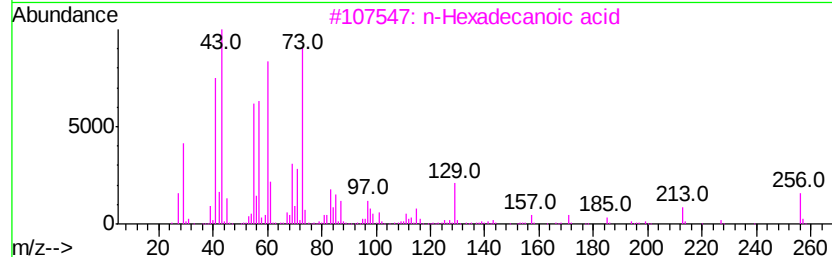
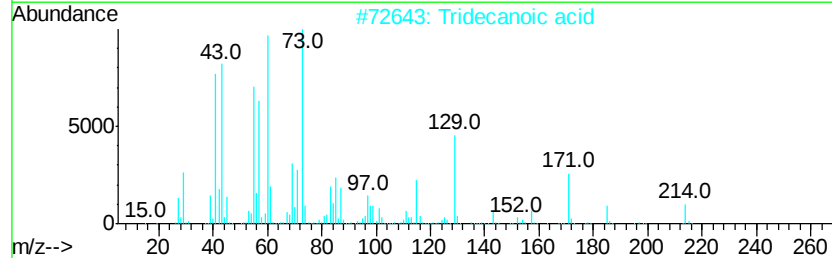
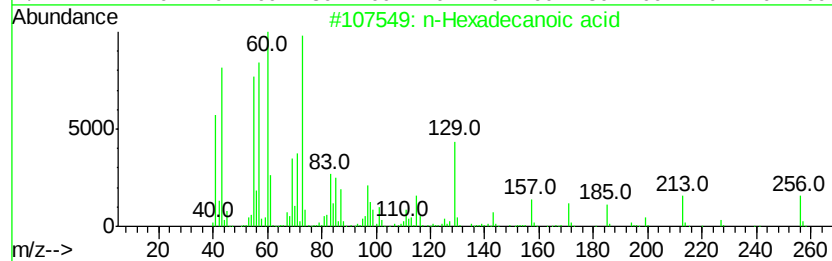
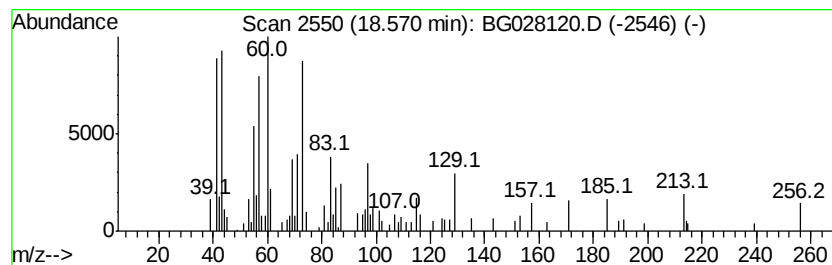
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.33 ng/ul	97965	Phenanthrene-d10	17.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96	
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70	
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58	
4	Undecanoic acid	186	C11H22O2	000112-37-8	58	
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52	



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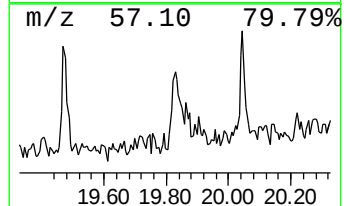
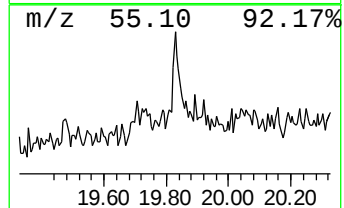
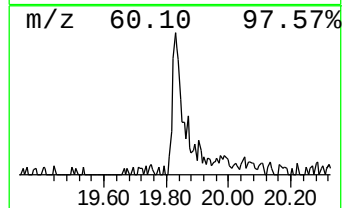
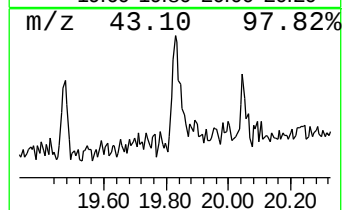
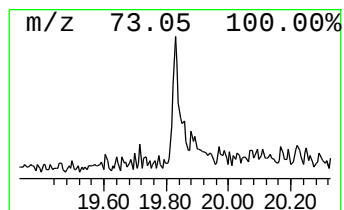
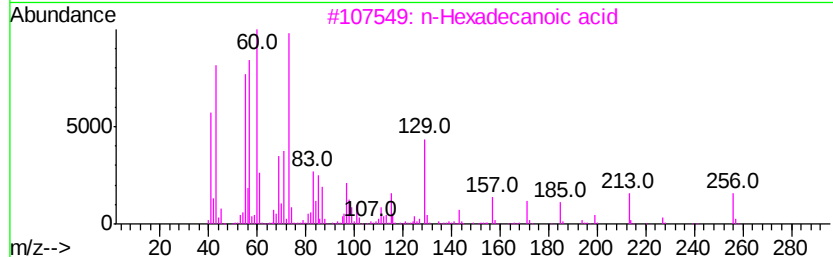
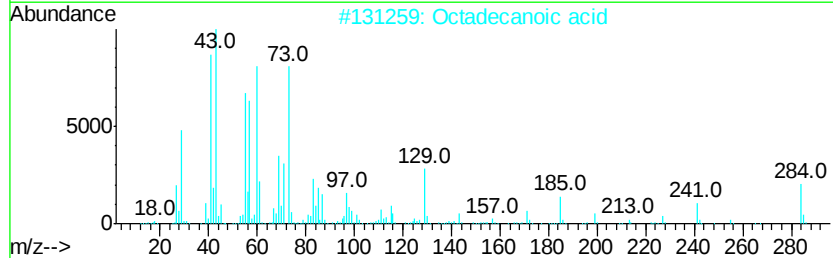
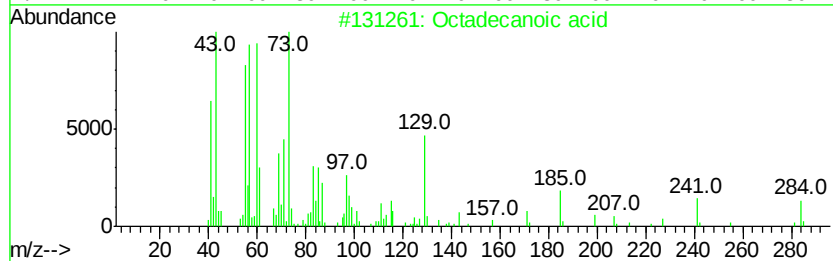
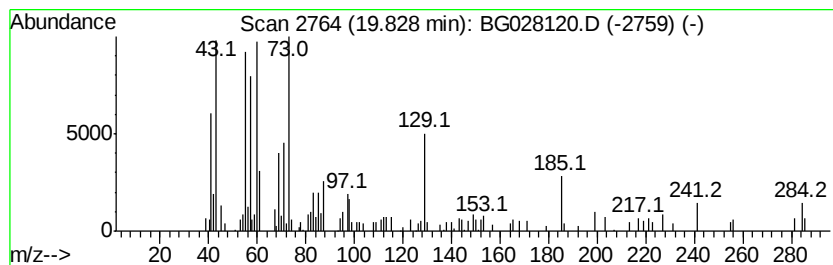
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.83	2.04 ng/ul	85810	Phenanthrene-d10	17.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Octadecanoic acid	284	C18H36O2	000057-11-4	74



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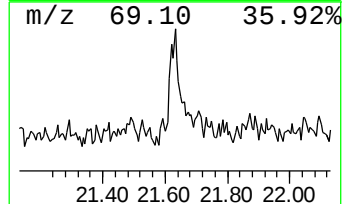
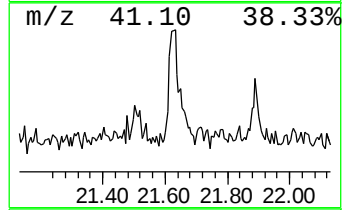
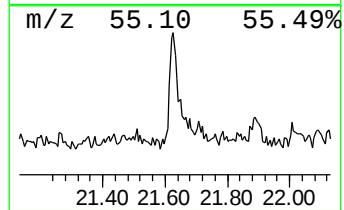
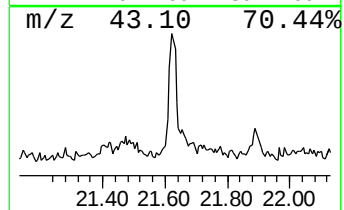
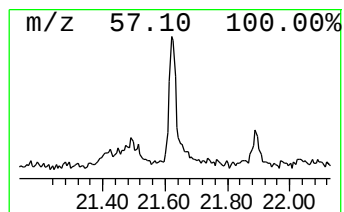
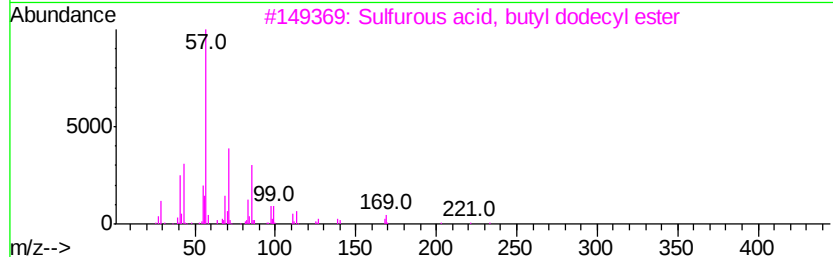
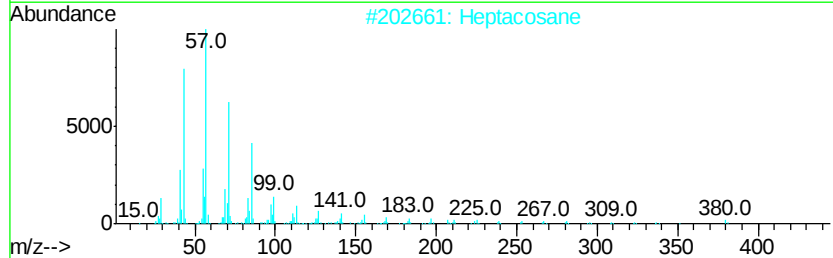
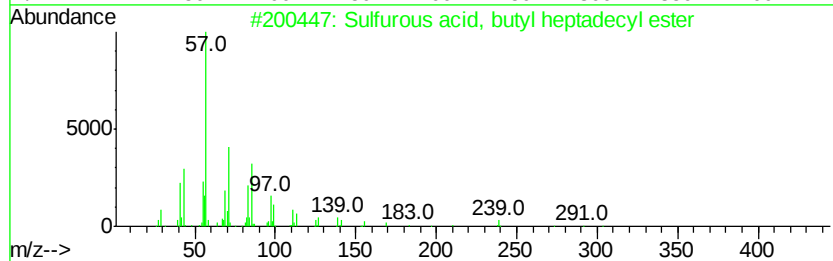
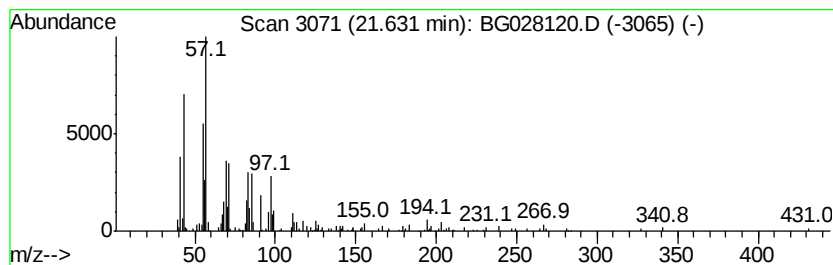
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Peak Number 3 Sulfurous acid, butyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.63	4.10 ng/ul	196685	Chrysene-d12	22.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	78
2		Heptacosane	380	C27H56	000593-49-7	53
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
4		Tridecane	184	C13H28	000629-50-5	52
5		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	47



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
Acq On : 2 Aug 2017 22:37
Operator : SJ/JU
Sample : I4405-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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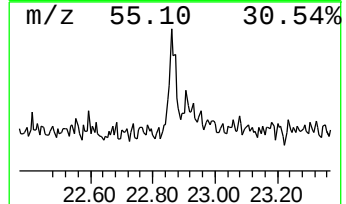
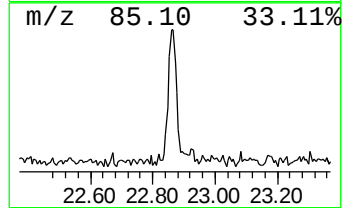
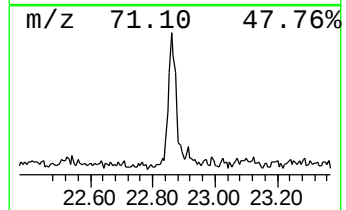
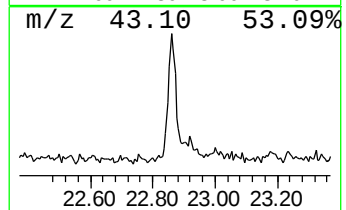
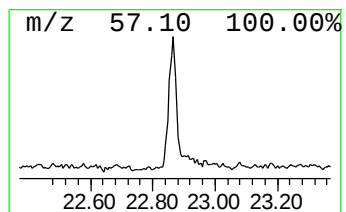
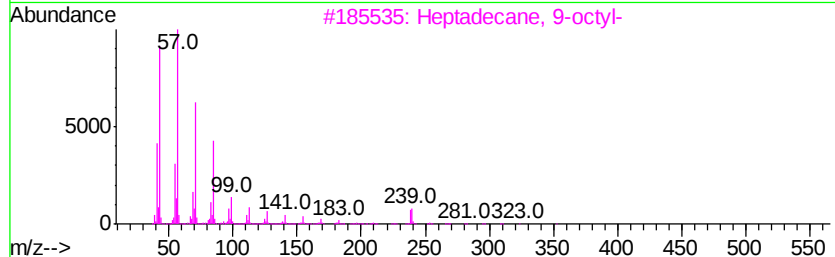
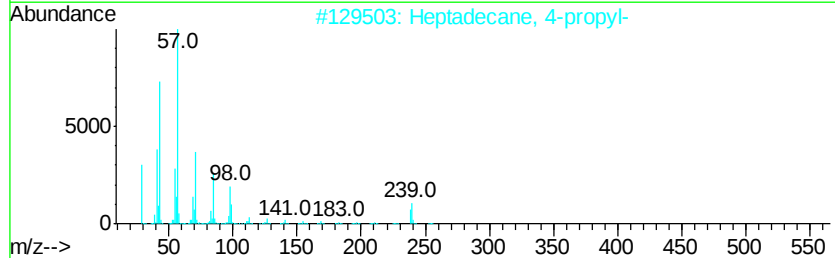
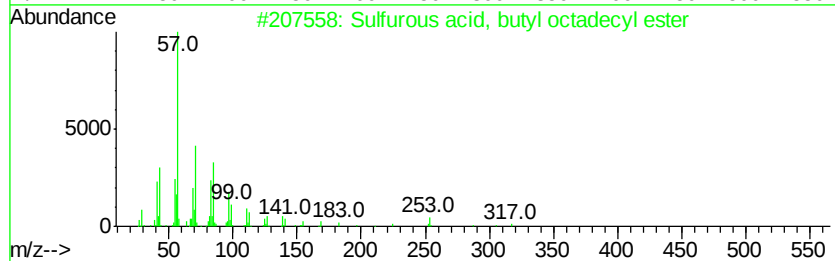
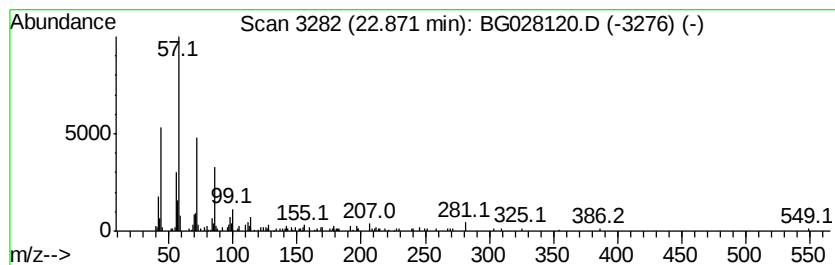
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Sulfurous acid, butyl octadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.87	3.29 ng/ul	157877	Chrysene-d12	22.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	80
2		Heptadecane, 4-propyl-	282	C20H42	055044-10-5	80
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	68
4		Pentadecane	212	C15H32	000629-62-9	64
5		Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
Acq On : 2 Aug 2017 22:37
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Sample : I4405-09
Misc :
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Instrument :
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ClientSampleId :
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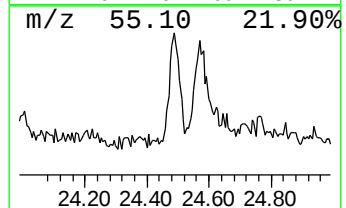
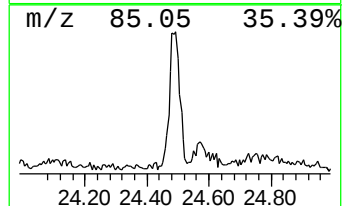
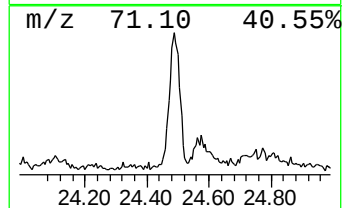
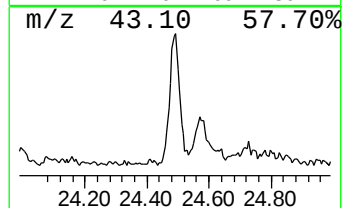
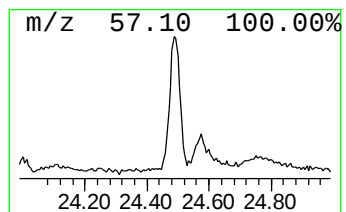
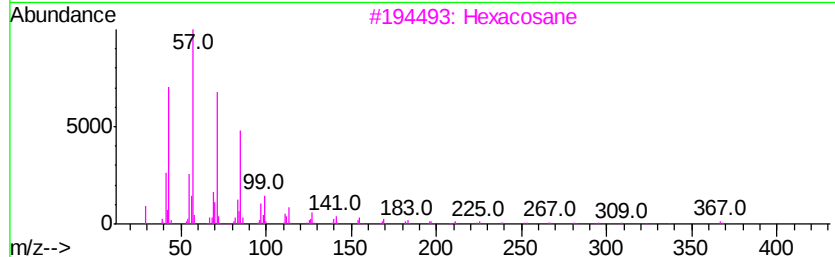
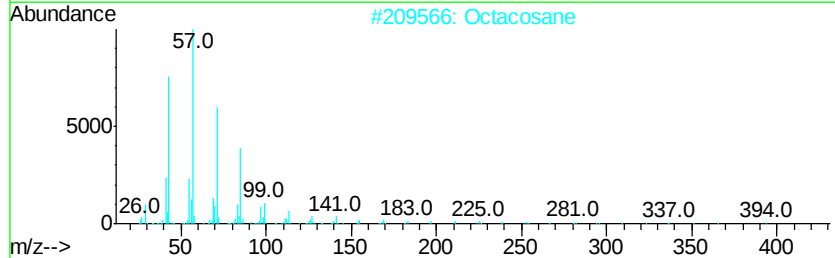
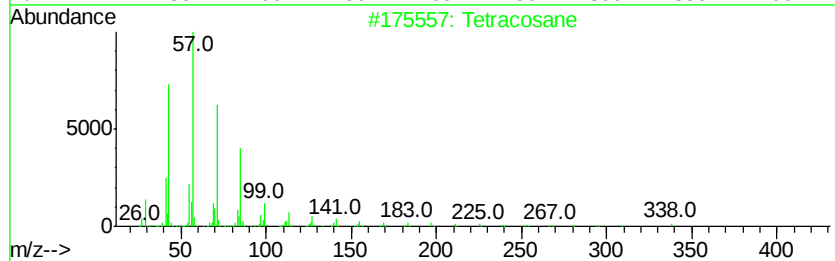
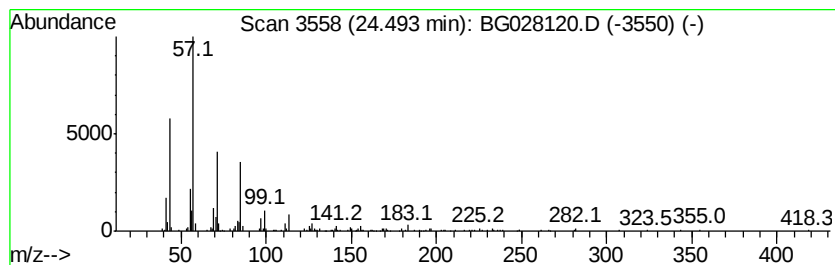
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.49	5.92 ng/ul	293995	Perylene-d12	25.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Eicosane	282	C20H42	000112-95-8	83



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
Acq On : 2 Aug 2017 22:37
Operator : SJ/JU
Sample : I4405-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
JJ2X6

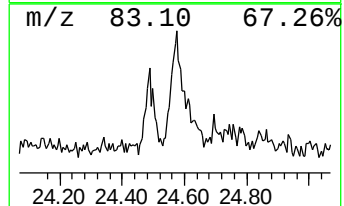
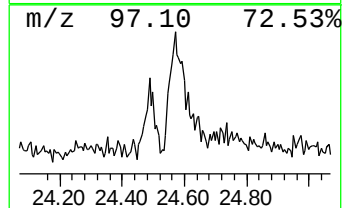
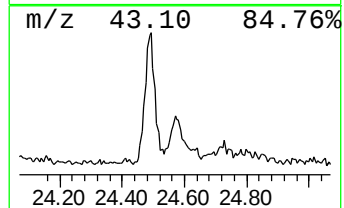
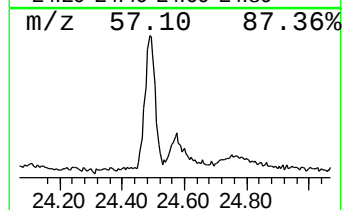
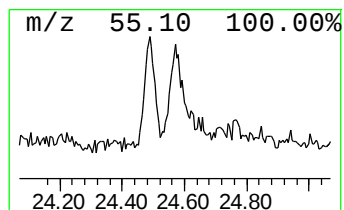
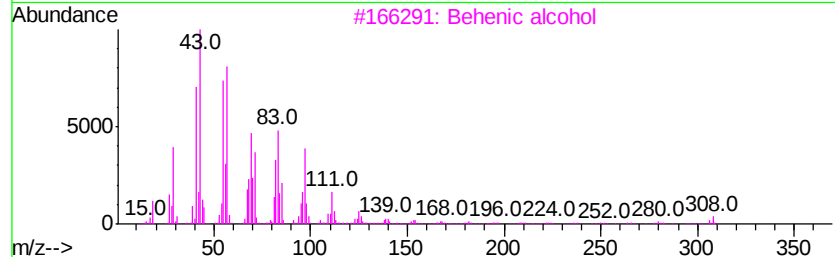
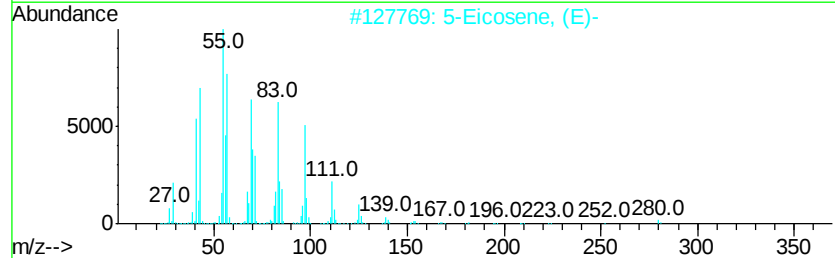
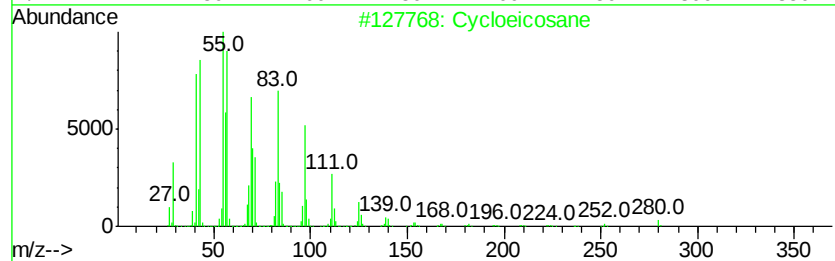
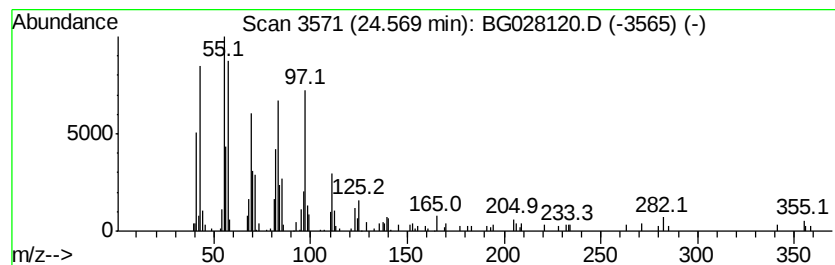
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Cyclic24.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.57	4.20 ng/ul	208569	Perylene-d12	25.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloeicosane	280	C20H40	000296-56-0	96
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	92
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	90
5		1-Eicosanol	298	C20H42O	000629-96-9	87



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
Acq On : 2 Aug 2017 22:37
Operator : SJ/JU
Sample : I4405-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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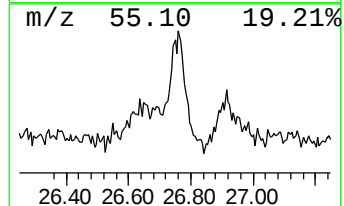
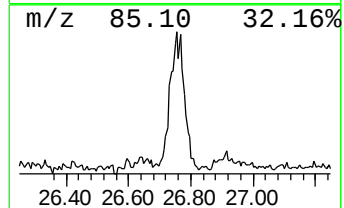
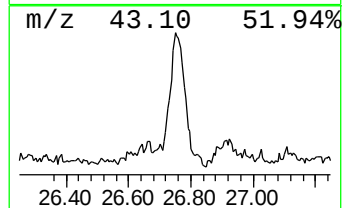
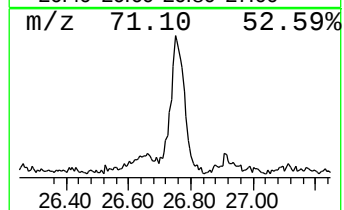
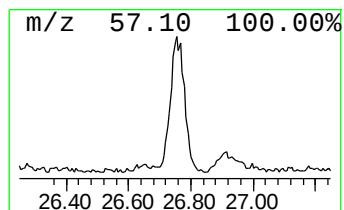
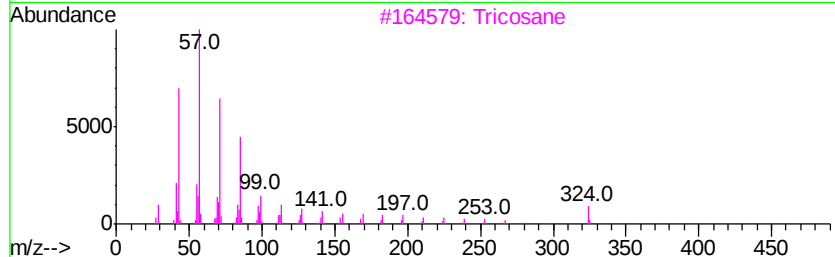
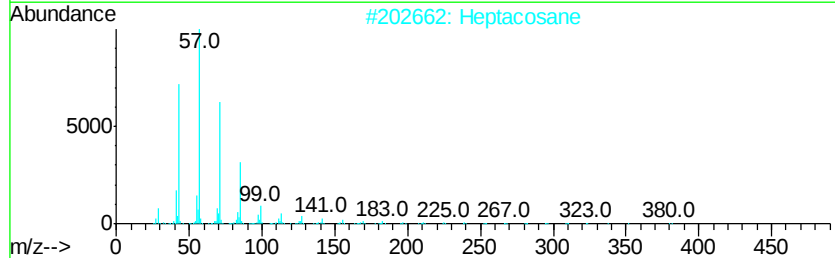
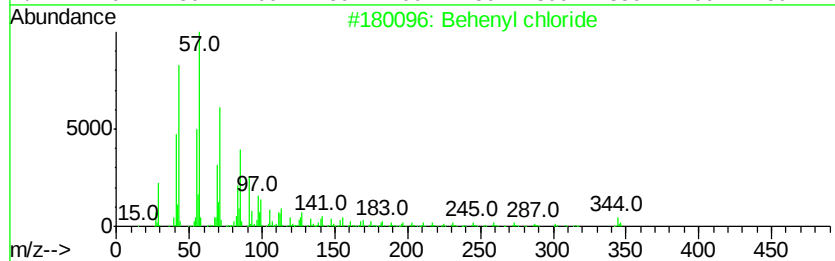
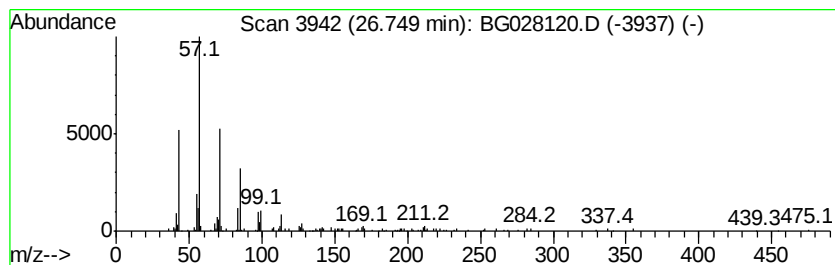
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Behenyl chloride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.75	7.73 ng/ul	384153	Perylene-d12	25.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenyl chloride	344	C22H45Cl	042217-03-8	83
2		Heptacosane	380	C27H56	000593-49-7	80
3		Tricosane	324	C23H48	000638-67-5	72
4		triacontane, 1-bromo-	500	C30H61Br	004209-22-7	72
5		Heneicosane, 10-methyl-	310	C22H46	013287-25-7	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
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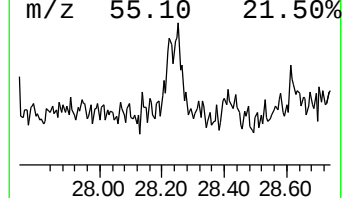
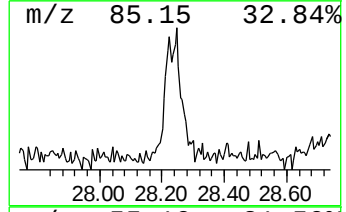
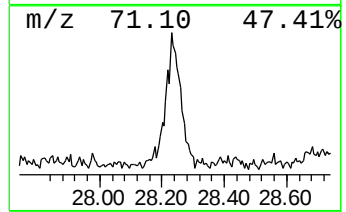
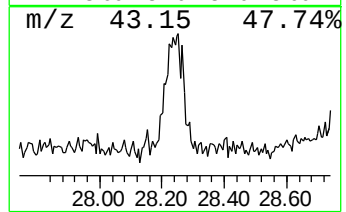
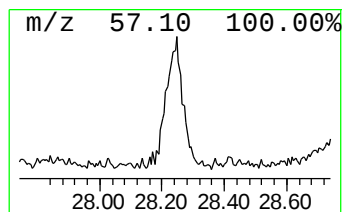
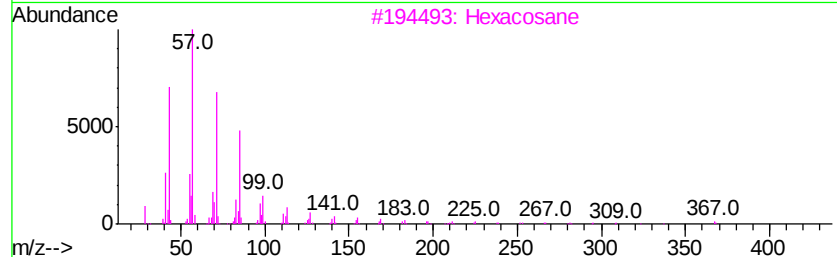
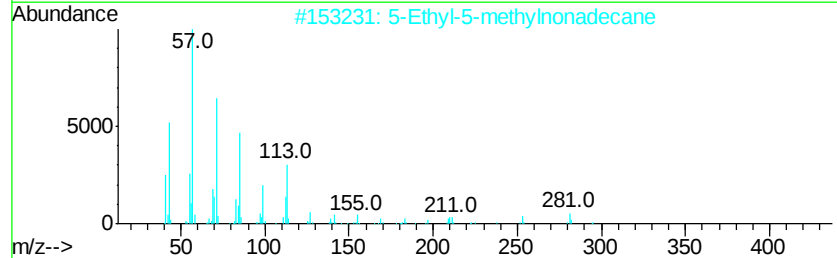
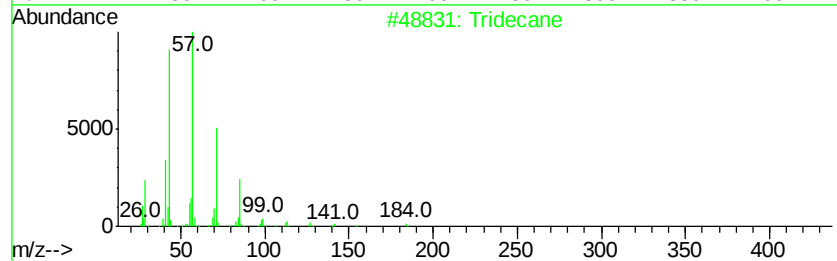
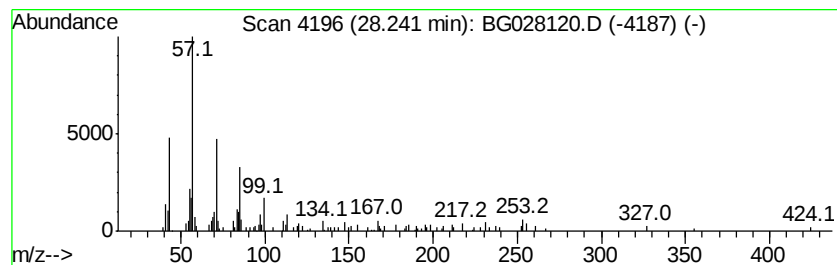
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.24	2.84 ng/ul	140978	Perylene-d12	25.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	81
2		5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
3		Hexacosane	366	C26H54	000630-01-3	80
4		Tetradecane, 2-methyl-	212	C15H32	001560-95-8	72
5		Tridecane	184	C13H28	000629-50-5	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
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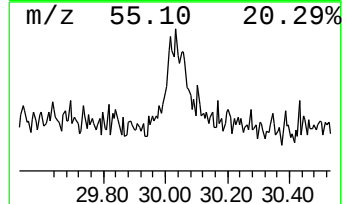
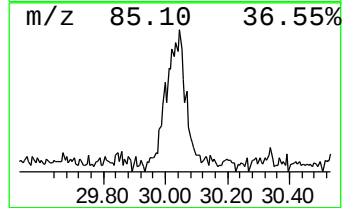
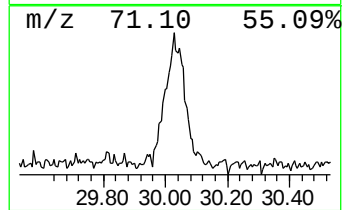
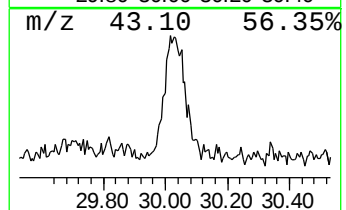
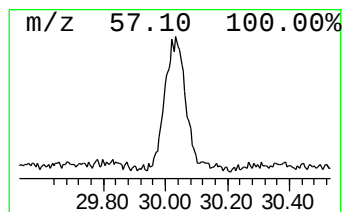
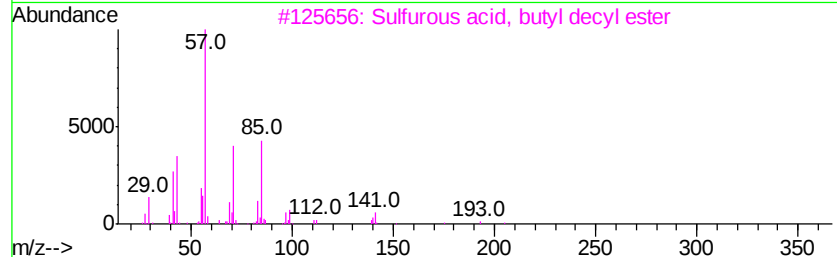
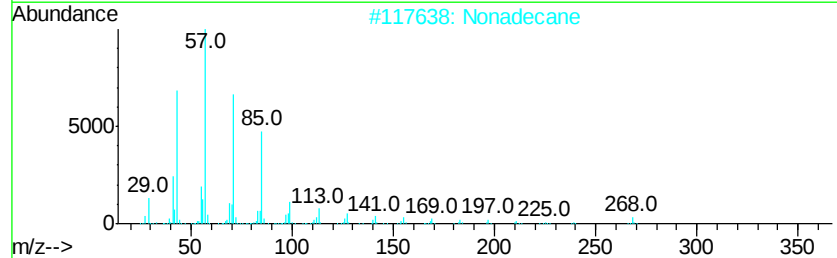
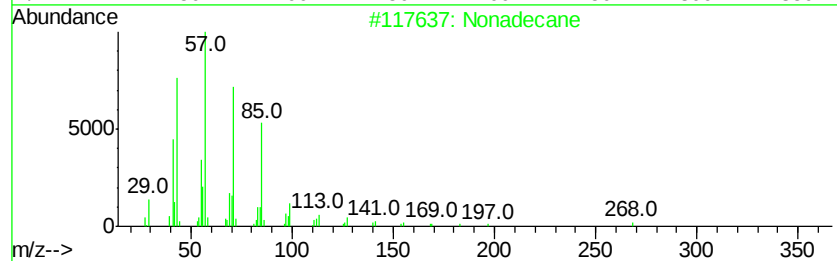
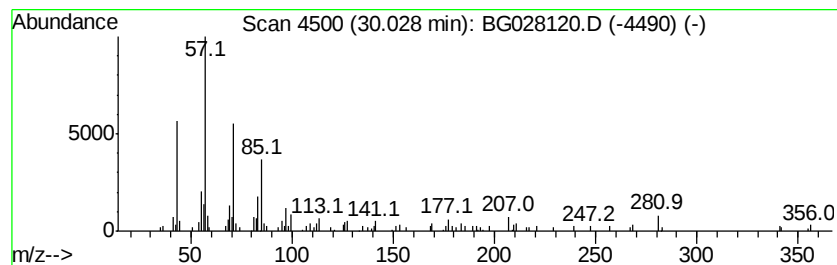
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.03	3.40 ng/ul	168907	Perylene-d12	25.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	89
2			Nonadecane	268	C19H40	000629-92-5	76
3			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
5			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080217\
Data File : BG028120.D
Acq On : 2 Aug 2017 22:37
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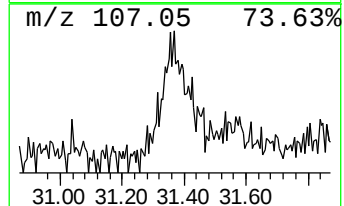
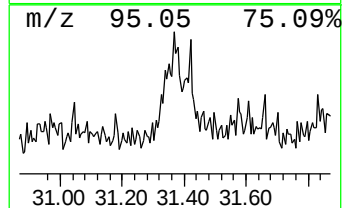
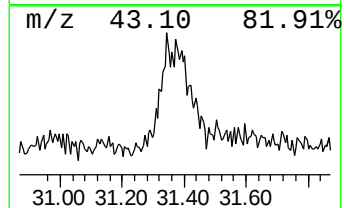
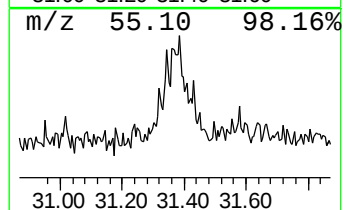
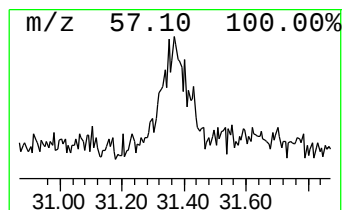
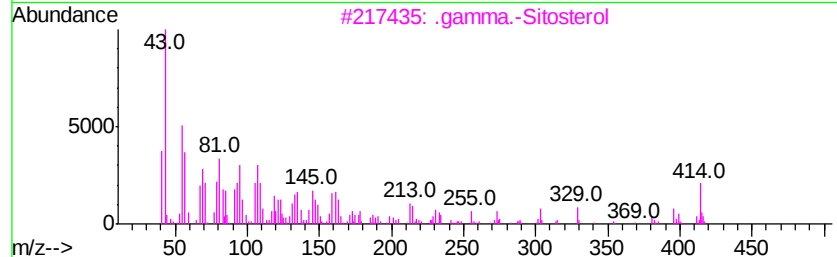
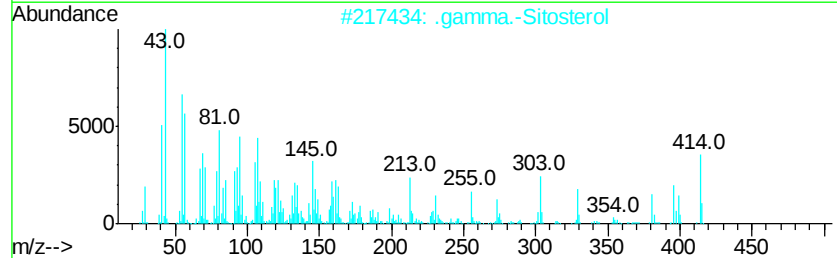
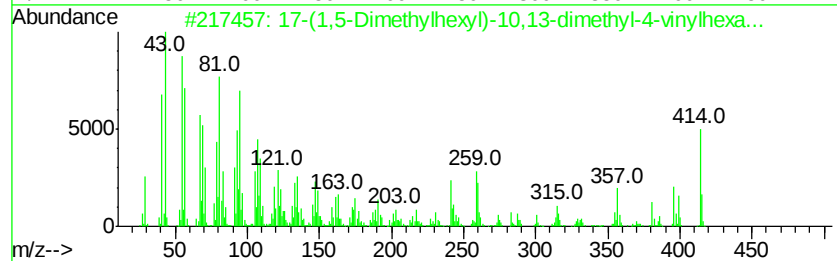
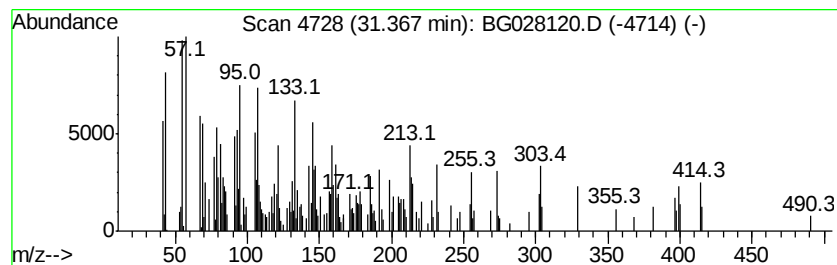
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.37	7.99 ng/ul	396864	Perylene-d12	25.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	64
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
3			.gamma.-Sitosterol	414	C29H50O	000083-47-6	53
4			.beta.-Sitosterol	414	C29H50O	000083-46-5	50
5			.beta.-Sitosterol	414	C29H50O	000083-46-5	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080217\
 Data File : BG028120.D
 Acq On : 2 Aug 2017 22:37
 Operator : SJ/JU
 Sample : I4405-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JJ2X6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.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
n-Hexadecanoic acid	18.57	2.3	ng/ul	97965	4	17.72	841480	20.0
Octadecanoic acid	19.83	2.0	ng/ul	85810	4	17.72	841480	20.0
Sulfurous acid, b...	21.63	4.1	ng/ul	196685	5	22.05	960478	20.0
Sulfurous acid, b...	22.87	3.3	ng/ul	157877	5	22.05	960478	20.0
(DEL) Alkane: Str...	24.49	5.9	ng/ul	293995	6	25.56	993700	20.0
(DEL) Alkane: Cyc...	24.57	4.2	ng/ul	208569	6	25.56	993700	20.0
Behenyl chloride	26.75	7.7	ng/ul	384153	6	25.56	993700	20.0
(DEL) Alkane: Str...	28.24	2.8	ng/ul	140978	6	25.56	993700	20.0
(DEL) Alkane: Str...	30.03	3.4	ng/ul	168907	6	25.56	993700	20.0
17-(1,5-Dimethylh...	31.37	8.0	ng/ul	396864	6	25.56	993700	20.0