

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
 Data File : BG027508.D
 Acq On : 17 Jun 2017 15:51
 Operator : SJ/MA
 Sample : I3599-19
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 F5C96

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-BG061617.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	4.081	27	33	39	rBV	7929	12866	0.94%	0.073%
2	5.086	200	204	209	rVV4	3536	3620	0.26%	0.021%
3	6.602	459	462	472	rBV3	2013	4023	0.29%	0.023%
4	7.454	603	607	616	rBV2	3030	5748	0.42%	0.033%
5	7.654	633	641	653	rVB	175746	334810	24.40%	1.903%
6	7.830	663	671	682	rBV	144534	249544	18.19%	1.418%
7	8.053	701	709	719	rBV	163071	300476	21.90%	1.708%
8	8.517	779	788	802	rBV	167097	311958	22.74%	1.773%
9	8.846	837	844	849	rVV3	1781	3413	0.25%	0.019%
10	9.193	895	903	913	rBV	216900	399409	29.11%	2.270%
11	9.681	977	986	993	rVV	162964	310327	22.62%	1.764%
12	9.740	993	996	1006	rVV2	7319	12667	0.92%	0.072%
13	10.403	1100	1109	1120	rVB	137607	258326	18.83%	1.468%
14	10.580	1135	1139	1147	rBV4	1836	3519	0.26%	0.020%
15	10.944	1192	1201	1216	rBV	216044	403943	29.44%	2.296%
16	11.338	1260	1268	1274	rBV	275364	516384	37.64%	2.935%
17	11.391	1274	1277	1282	rVV	27282	43551	3.17%	0.248%
18	11.461	1282	1289	1303	rVB	204260	410808	29.94%	2.335%
19	11.772	1333	1342	1354	rBV	59653	108086	7.88%	0.614%
20	12.889	1524	1532	1537	rBV4	2639	5511	0.40%	0.031%
21	12.953	1537	1543	1551	rVB3	1827	3586	0.26%	0.020%
22	13.171	1570	1580	1586	rVB2	5142	10274	0.75%	0.058%
23	13.459	1624	1629	1637	rVB4	2615	3730	0.27%	0.021%
24	13.706	1662	1671	1674	rBV4	2813	4896	0.36%	0.028%
25	14.299	1763	1772	1782	rBV3	10007	23699	1.73%	0.135%
26	14.487	1796	1804	1809	rVV	444023	697489	50.84%	3.964%
27	14.534	1809	1812	1820	rVV	192494	277557	20.23%	1.577%
28	14.798	1849	1857	1871	rBV	458828	774751	56.47%	4.403%
29	14.957	1876	1884	1892	rBV3	7917	12253	0.89%	0.070%
30	15.104	1898	1909	1916	rBV2	458624	758341	55.28%	4.310%
31	15.168	1916	1920	1925	rVB3	12073	19756	1.44%	0.112%
32	15.268	1925	1937	1953	rBV	202333	361214	26.33%	2.053%
33	15.392	1953	1958	1965	rVB7	1897	5216	0.38%	0.030%
34	15.468	1965	1971	1983	rBV4	24919	68192	4.97%	0.388%

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Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
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35	15.568	1983	1988	1992	rVB4	4000	6134	0.45%	0.035%
36	15.633	1996	1999	2004	rVB6	2472	3662	0.27%	0.021%
37	15.903	2040	2045	2050	rVB	18401	24685	1.80%	0.140%
38	16.091	2068	2077	2084	rBV	663480	1060147	77.27%	6.025%
39	16.144	2084	2086	2089	rVV3	11616	15887	1.16%	0.090%
40	16.191	2089	2094	2104	rVB	223272	350401	25.54%	1.991%
41	16.326	2104	2117	2124	rBV8	8209	25579	1.86%	0.145%
42	16.402	2126	2130	2133	rVB4	2573	3809	0.28%	0.022%
43	16.461	2135	2140	2144	rBV4	2711	3842	0.28%	0.022%
44	16.520	2147	2150	2156	rVB5	3196	4654	0.34%	0.026%
45	16.602	2156	2164	2168	rVB9	2095	5391	0.39%	0.031%
46	16.708	2178	2182	2185	rBV5	2341	3496	0.25%	0.020%
47	16.761	2187	2191	2201	rBV	21815	39171	2.86%	0.223%
48	17.043	2233	2239	2243	rBV4	2238	3744	0.27%	0.021%
49	17.107	2244	2250	2256	rVB6	3308	7317	0.53%	0.042%
50	17.207	2263	2267	2274	rVB7	3739	7375	0.54%	0.042%
51	17.266	2274	2277	2286	rVB7	3356	7679	0.56%	0.044%
52	17.342	2286	2290	2292	rBV4	3346	4549	0.33%	0.026%
53	17.560	2320	2327	2331	rVV	16784	23101	1.68%	0.131%
54	17.619	2332	2337	2339	rBV4	3412	5933	0.43%	0.034%
55	17.854	2369	2377	2388	rBV	590860	1000183	72.90%	5.684%
56	17.953	2388	2394	2404	rVB	750640	1186734	86.50%	6.744%
57	18.089	2414	2417	2421	rBV4	2528	4868	0.35%	0.028%
58	18.130	2421	2424	2430	rVB5	3648	5206	0.38%	0.030%
59	18.253	2439	2445	2449	rBV2	7818	11488	0.84%	0.065%
60	18.300	2449	2453	2457	rBV2	6110	7284	0.53%	0.041%
61	18.482	2479	2484	2488	rVB6	2865	5347	0.39%	0.030%
62	18.694	2513	2520	2530	rBV2	80170	144288	10.52%	0.820%
63	18.982	2564	2569	2573	rBV8	2786	6005	0.44%	0.034%
64	19.105	2589	2590	2595	rVB5	2469	3640	0.27%	0.021%
65	19.381	2633	2637	2641	rBV5	5897	7401	0.54%	0.042%
66	19.422	2641	2644	2650	rVV2	10021	11812	0.86%	0.067%
67	19.857	2713	2718	2721	rBV3	8565	14488	1.06%	0.082%
68	19.951	2729	2734	2749	rBV7	29838	65195	4.75%	0.371%
69	20.116	2756	2762	2768	rBV3	7177	13238	0.96%	0.075%
70	20.221	2774	2780	2793	rVB	884978	1371925	100.00%	7.797%
71	20.492	2821	2826	2829	rBV	103964	118624	8.65%	0.674%

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72	20.527	2829	2832	2838	rVB	204309	229151	16.70%	1.302%
73	20.909	2892	2897	2902	rBV6	3685	9888	0.72%	0.056%
74	21.156	2936	2939	2940	rBV3	3470	3384	0.25%	0.019%
75	21.538	2999	3004	3007	rBV	50565	69213	5.04%	0.393%
76	21.579	3007	3011	3021	rVB	106251	138569	10.10%	0.788%
77	21.784	3040	3046	3054	rBV10	19715	52633	3.84%	0.299%
78	22.055	3089	3092	3098	rVB8	4427	6057	0.44%	0.034%
79	22.231	3114	3122	3131	rBV	575587	1121669	81.76%	6.375%
80	22.760	3206	3212	3216	rBV3	24077	48444	3.53%	0.275%
81	22.807	3216	3220	3228	rVB	47436	80242	5.85%	0.456%
82	23.065	3259	3264	3271	rBV4	9750	19495	1.42%	0.111%
83	23.788	3382	3387	3391	rVB6	5051	8219	0.60%	0.047%
84	23.852	3391	3398	3408	rVB4	26015	59501	4.34%	0.338%
85	24.087	3432	3438	3445	rVB7	6909	15019	1.09%	0.085%
86	24.340	3476	3481	3486	rBV5	16586	33965	2.48%	0.193%
87	24.411	3487	3493	3501	rVB4	36667	78861	5.75%	0.448%
88	24.599	3521	3525	3528	rBV5	4845	7898	0.58%	0.045%
89	24.769	3547	3554	3564	rVB2	40239	93365	6.81%	0.531%
90	25.633	3688	3701	3718	rBV2	412912	1329832	96.93%	7.558%
91	25.879	3729	3743	3759	rVB3	338201	1243567	90.64%	7.067%
92	27.154	3949	3960	3972	rBV3	59068	199361	14.53%	1.133%
93	28.706	4211	4224	4238	rBV3	55425	221432	16.14%	1.258%
94	29.646	4381	4384	4388	rVB4	4491	6541	0.48%	0.037%
95	29.687	4388	4391	4394	rBV4	3767	5066	0.37%	0.029%
96	29.804	4407	4411	4414	rBV6	4234	7745	0.56%	0.044%
97	30.233	4483	4484	4490	rBV5	4594	6981	0.51%	0.040%
98	30.274	4490	4491	4494	rBV3	3801	3670	0.27%	0.021%
99	30.586	4529	4544	4560	rBV3	38199	188147	13.71%	1.069%
100	32.201	4818	4819	4822	rBV3	4086	3887	0.28%	0.022%

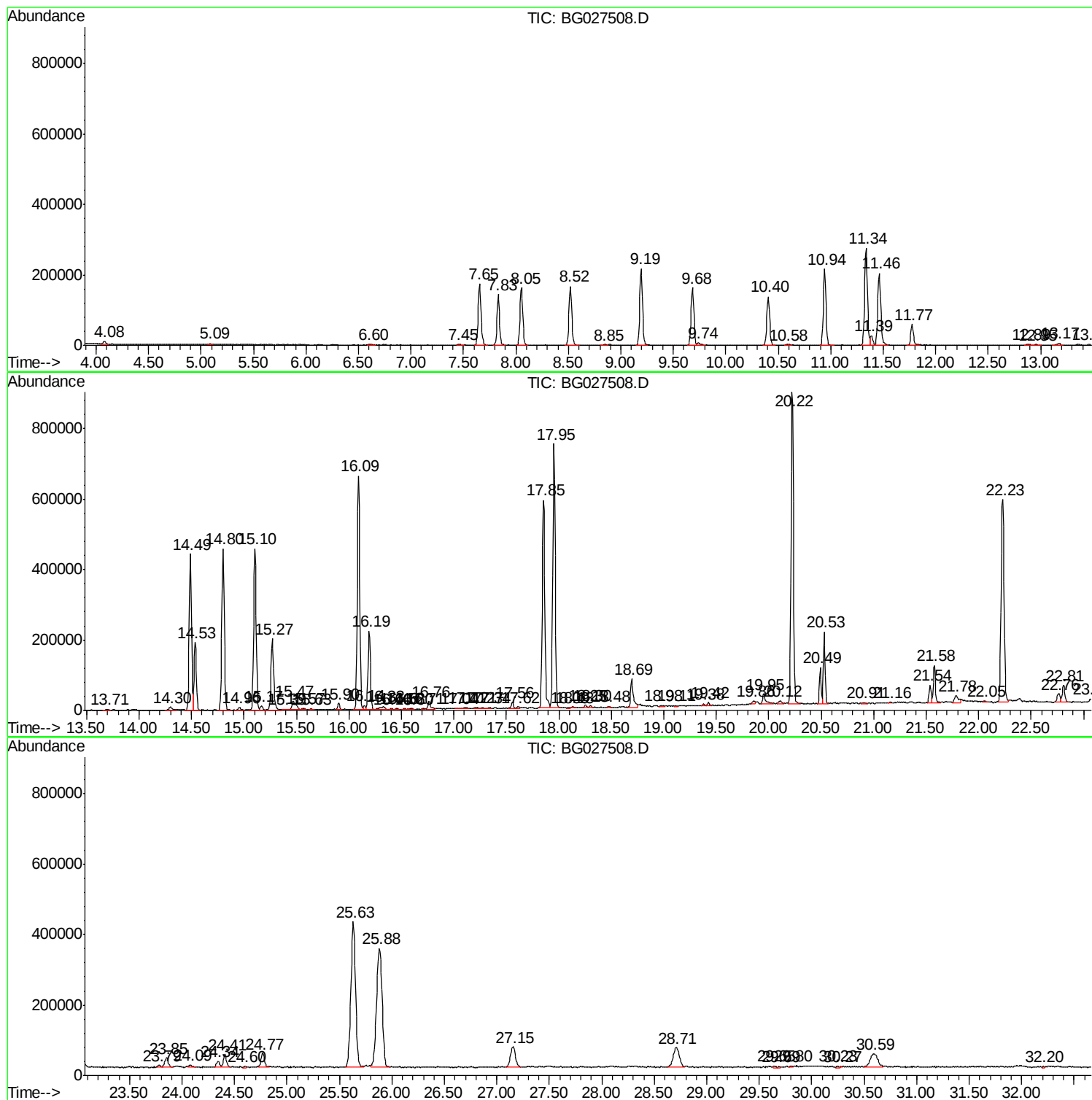
Sum of corrected areas: 17596027

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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



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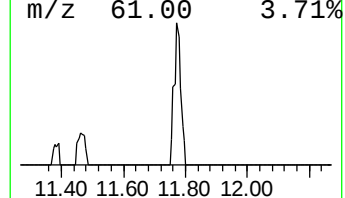
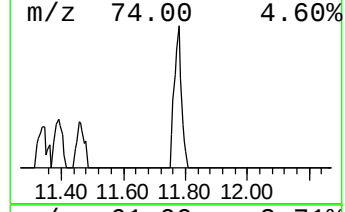
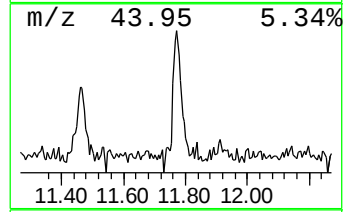
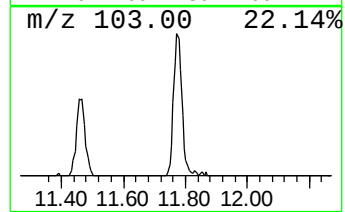
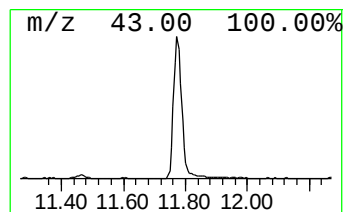
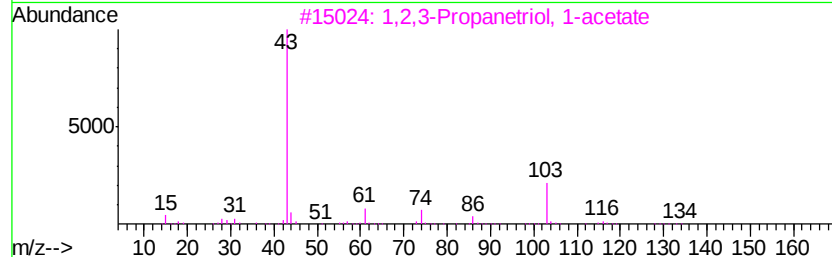
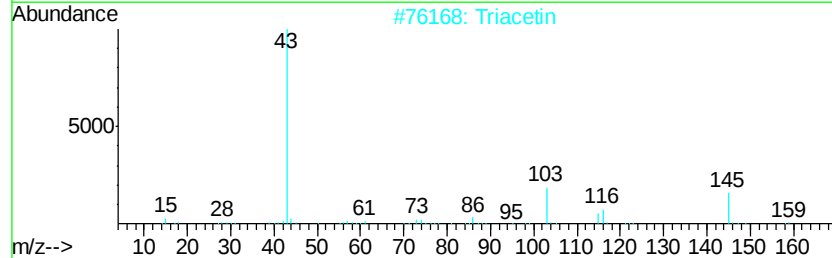
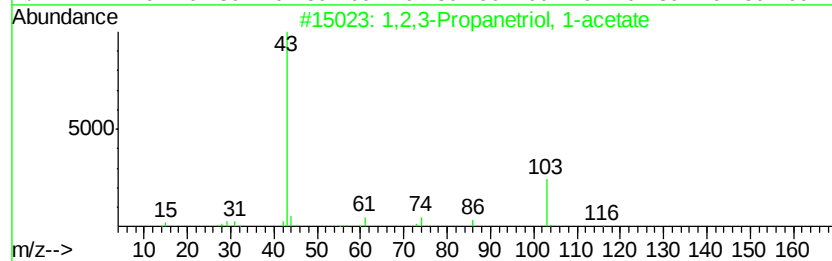
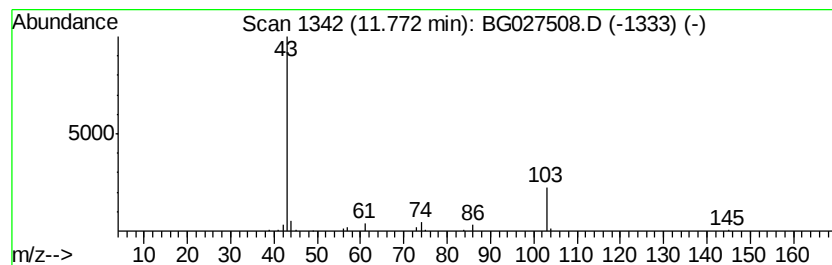
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,2,3-Propanetriol, 1-acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.19 ng/ul	108086	Naphthalene-d8	11.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	78
2			Triacetin	218	C9H14O6	000102-76-1	56
3			1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	45
4			Triacetin	218	C9H14O6	000102-76-1	25
5			Ethyl N-hydroxyacetimidate	103	C4H9NO2	010576-12-2	9



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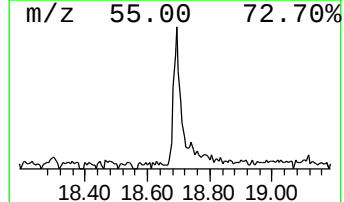
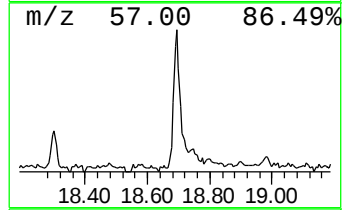
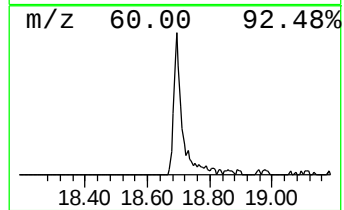
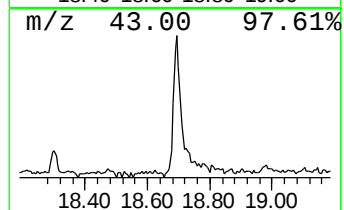
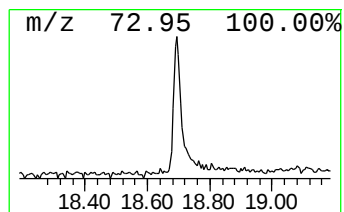
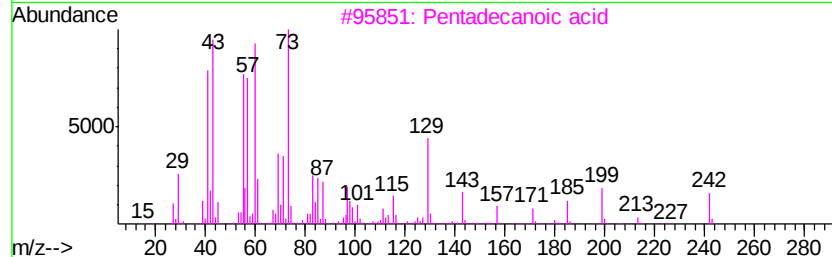
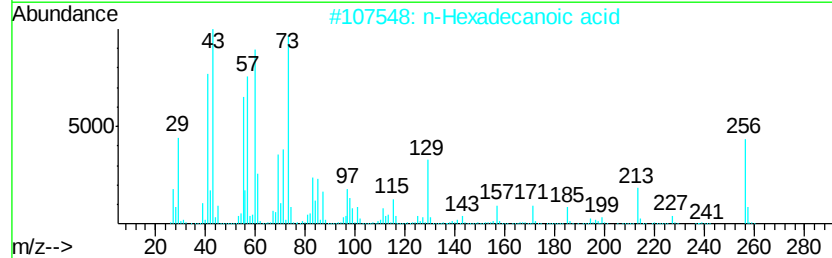
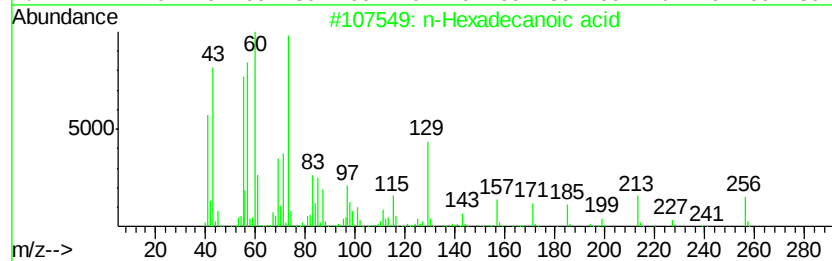
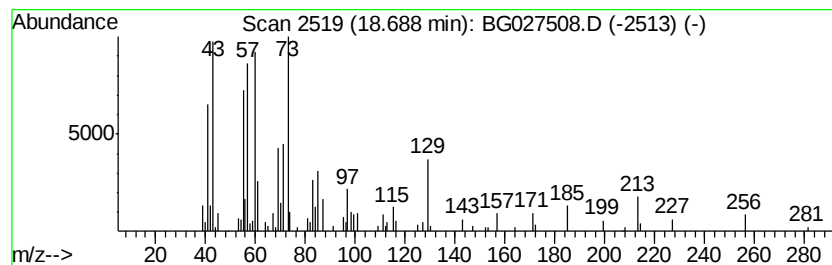
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.69	2.89 ng/ul	144288	Phenanthrene-d10	17.85	
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	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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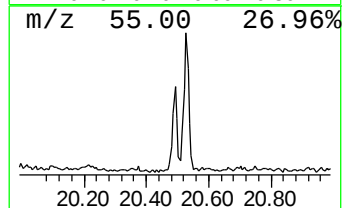
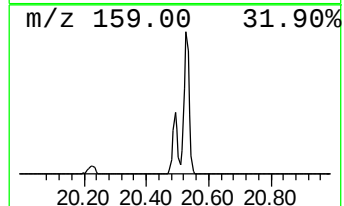
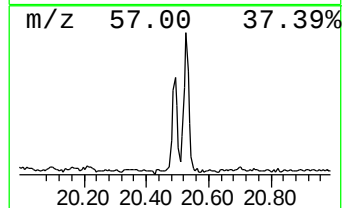
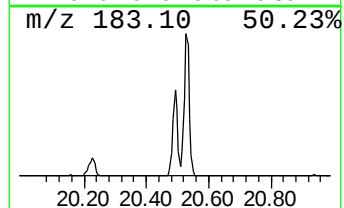
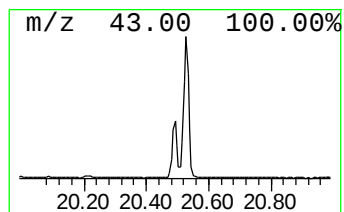
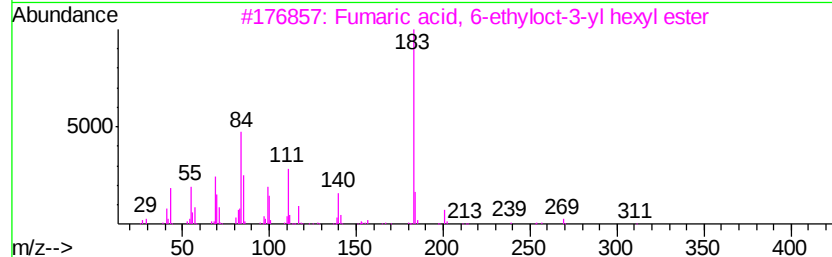
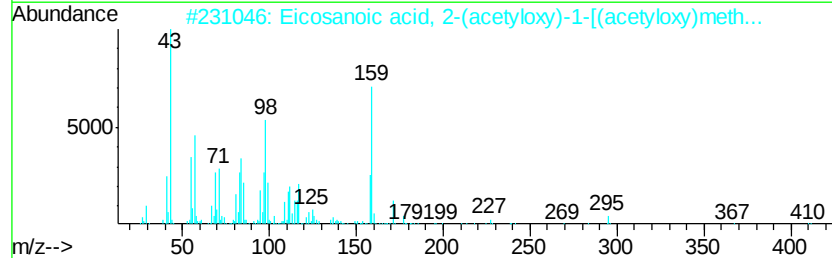
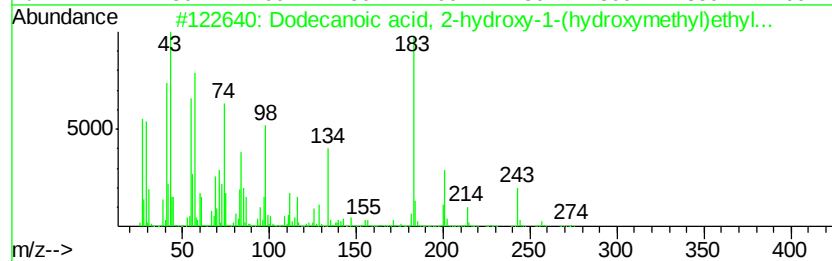
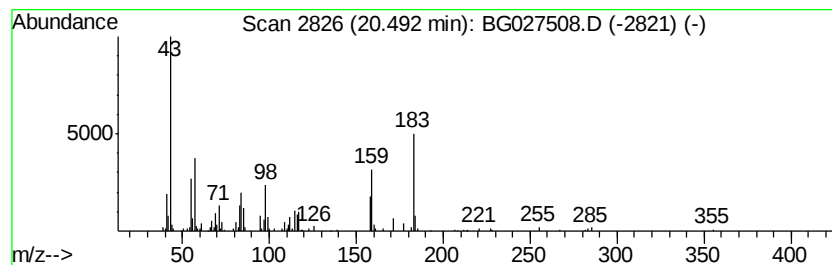
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Peak Number 3 Dodecanoic acid, 2-hydroxy-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	2.12 ng/ul	118624	Chrysene-d12	22.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid, 2-hydroxy-1-(hy...	274 C15H30O4	001678-45-1	50
2	Eicosanoic acid, 2-(acetyloxy)-1...	470 C27H50O6	055429-68-0	49
3	Fumaric acid, 6-ethyloct-3-yl he...	340 C20H36O4	1000339-15-3	38
4	Lauric anhydride	382 C24H46O3	000645-66-9	38
5	Fumaric acid, 2-hexyl isohexyl e...	284 C16H28O4	1000348-74-4	32



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5C96

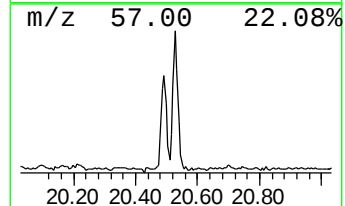
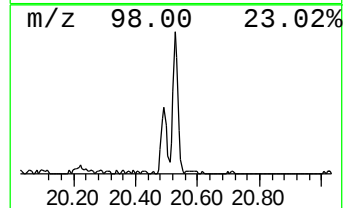
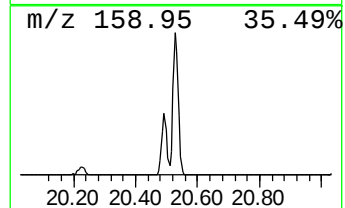
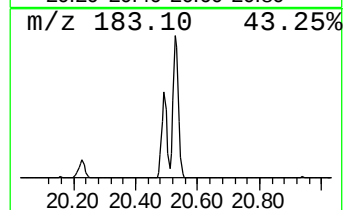
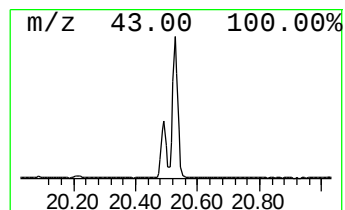
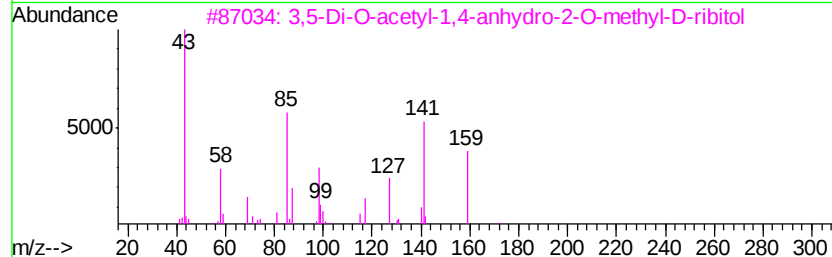
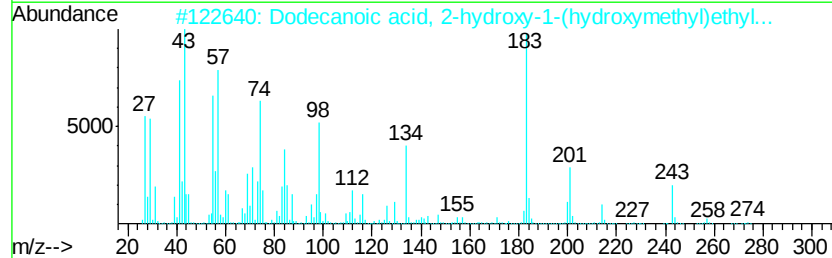
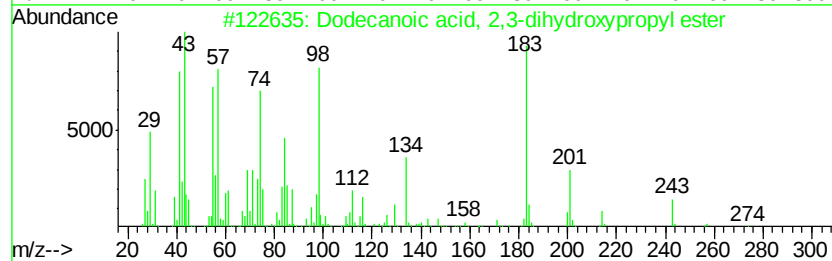
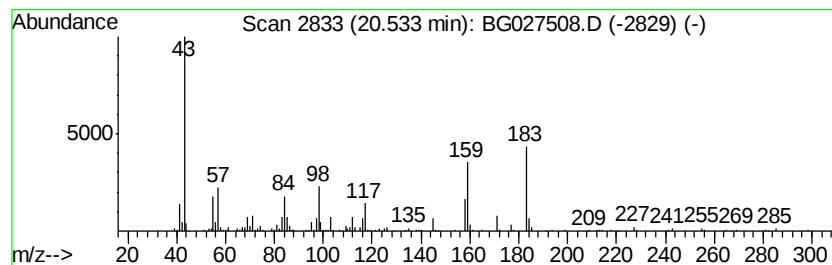
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	4.09 ng/ul	229151	Chrysene-d12	22.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	43
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	43
3		3,5-Di-O-acetyl-1,4-anhydro-2-O-...	232	C10H16O6	1000357-23-2	17
4		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	16
5		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5C96

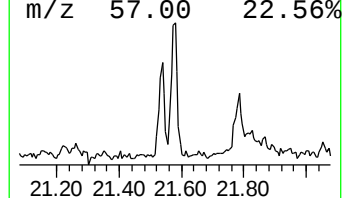
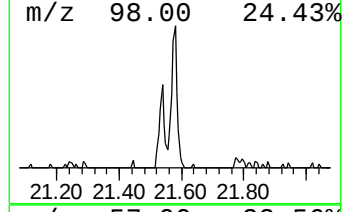
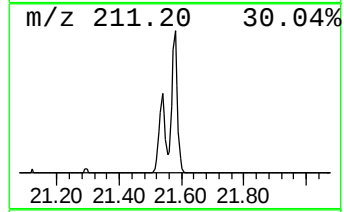
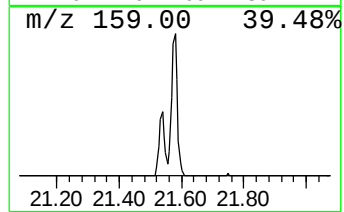
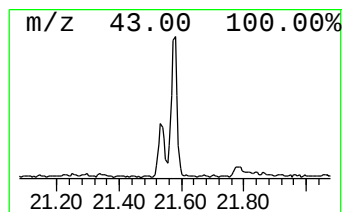
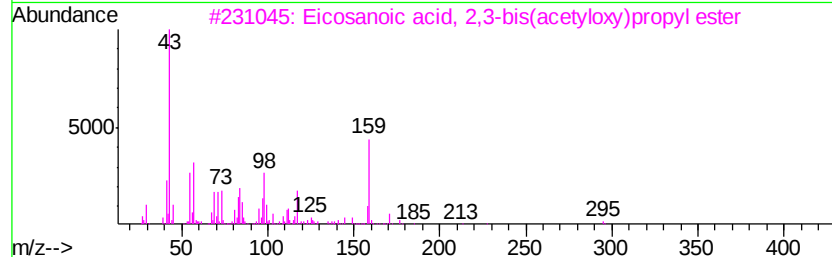
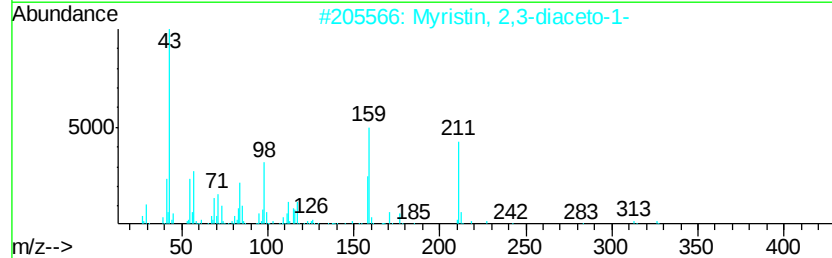
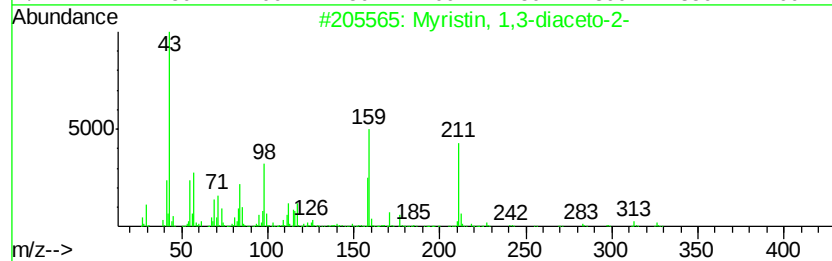
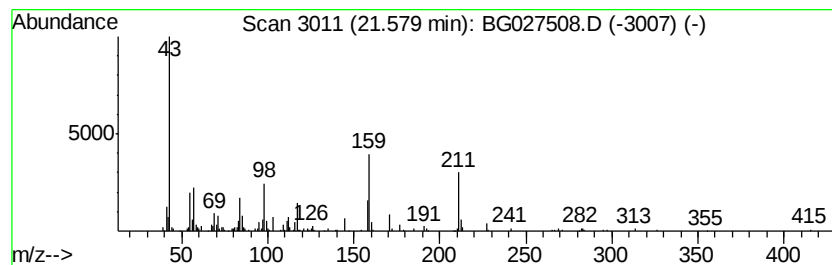
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Myristin, 1,3-diaceto-2- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.58	2.47 ng/ul	138569	Chrysene-d12	22.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin,	1,3-diaceto-2-	386	C21H38O6	014290-23-4	78
2	Myristin,	2,3-diaceto-1-	386	C21H38O6	014473-55-3	49
3	Eicosanoic acid,	2,3-bis(acetylo...	470	C27H50O6	055429-67-9	12
4	Thioacetic acid,	S-(5-acetylthio...	234	C9H14O3S2	1000185-15-4	10
5	Eicosanoic acid,	2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5C96

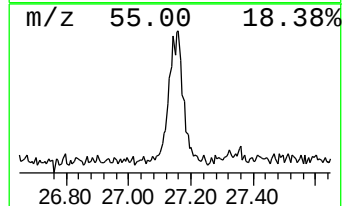
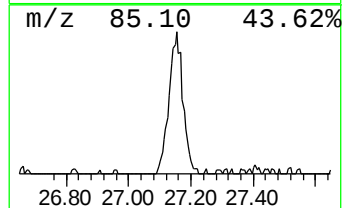
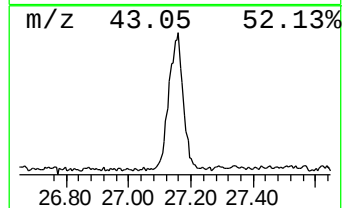
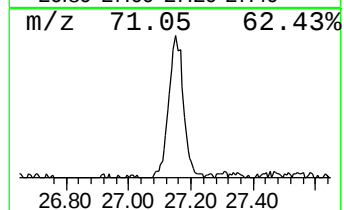
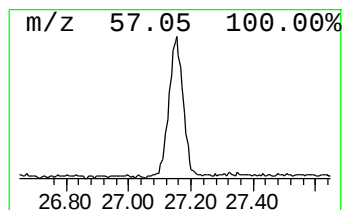
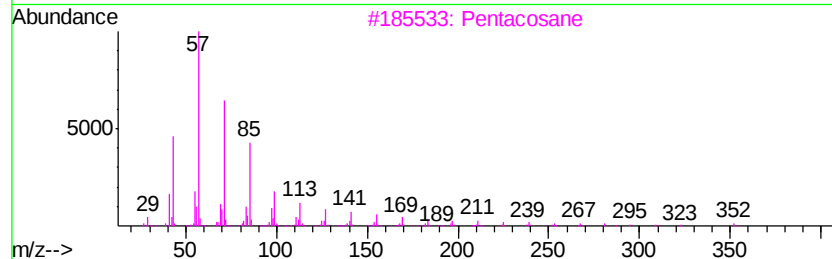
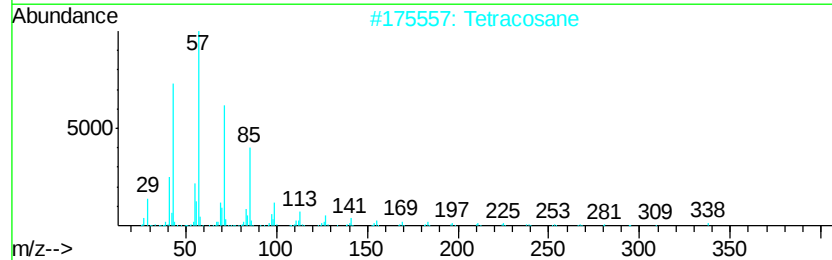
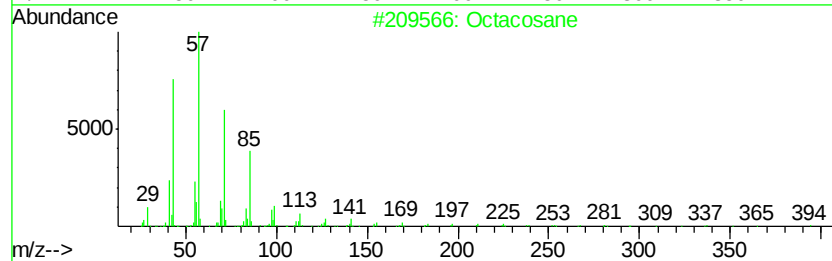
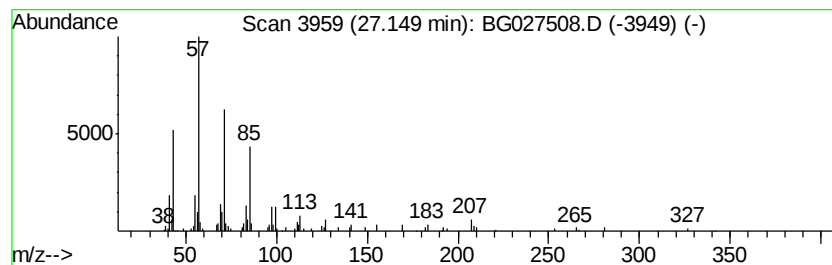
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.15	3.21 ng/ul	199361	Perylene-d12	25.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Pentacosane	352	C25H52	000629-99-2	87
4			Heptadecane	240	C17H36	000629-78-7	86
5			Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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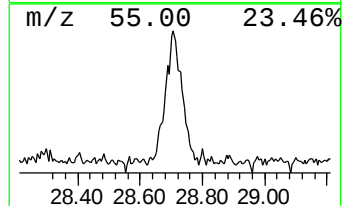
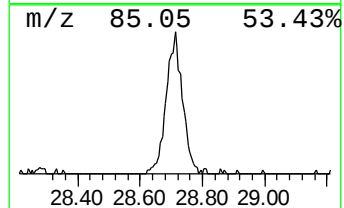
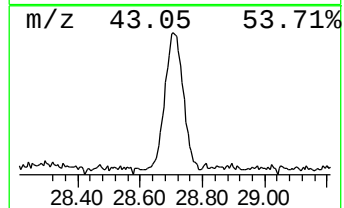
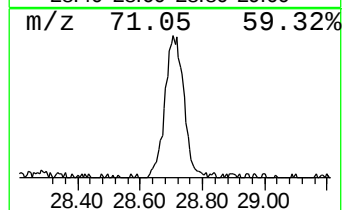
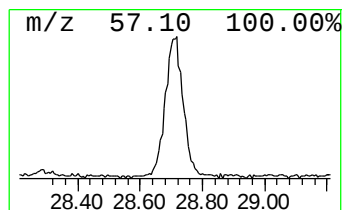
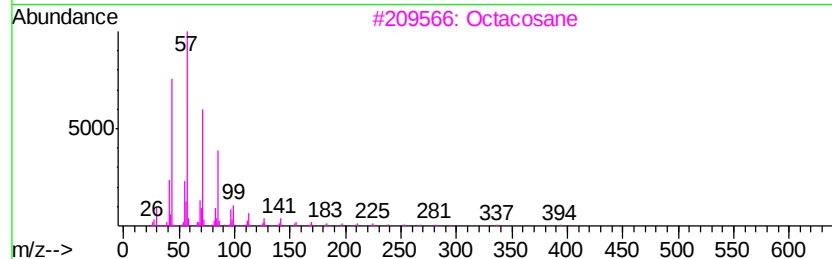
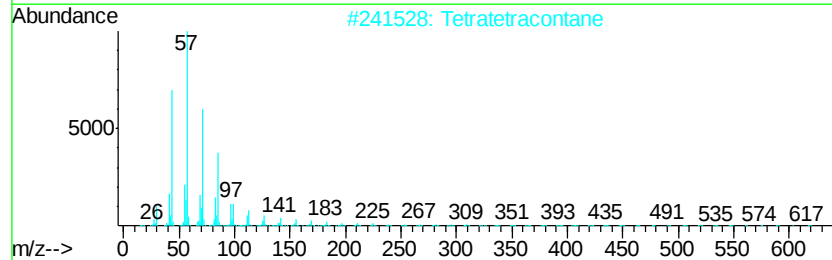
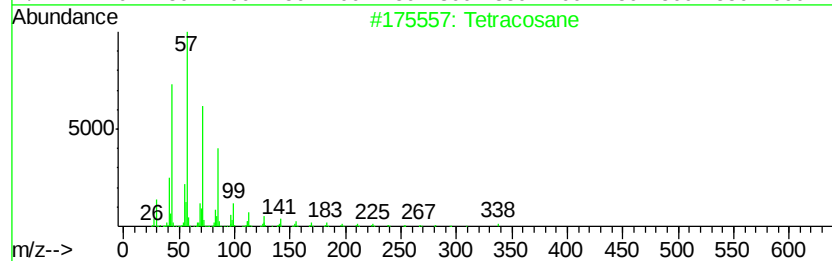
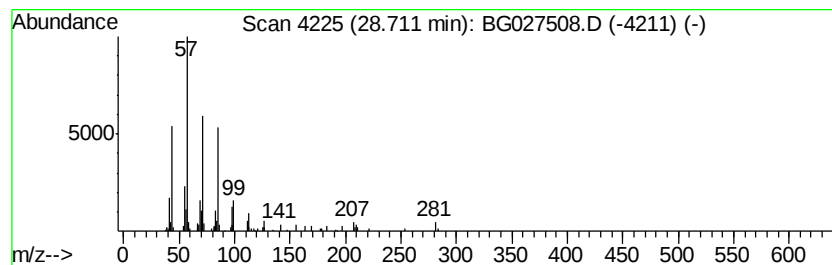
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.71	3.56 ng/ul	221432	Perylene-d12	25.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Octacosane	394	C28H58	000630-02-4	90
4			2-methyloctacosane	408	C29H60	1000376-72-8	90
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
F5C96

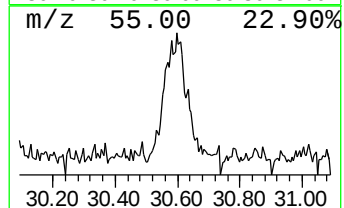
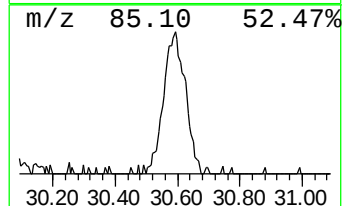
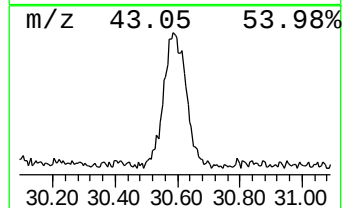
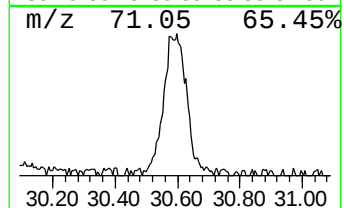
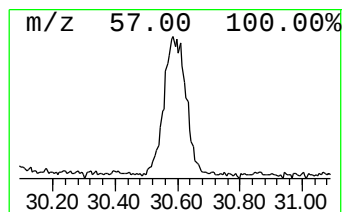
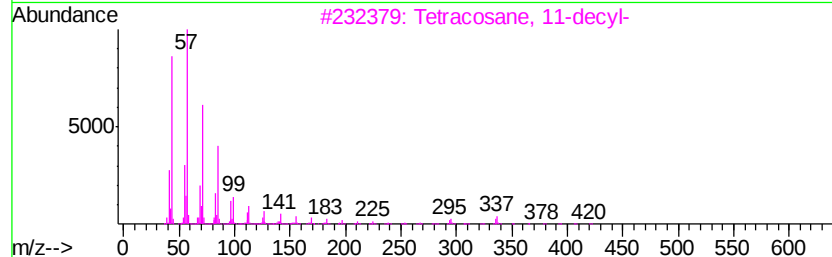
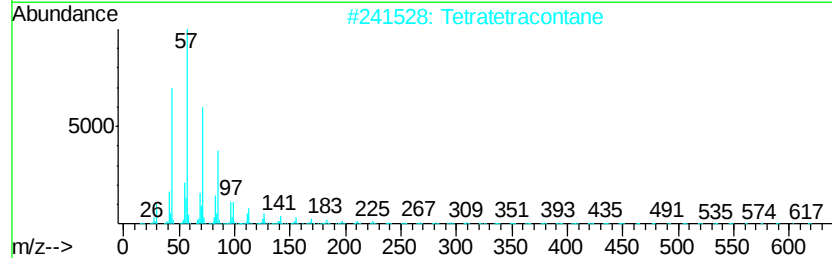
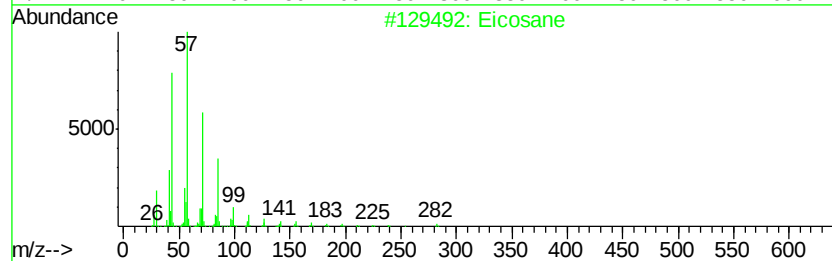
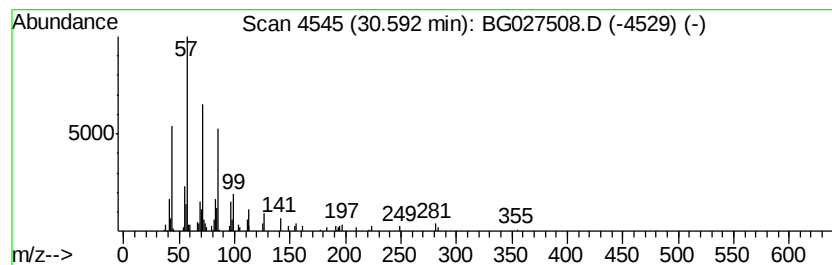
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.59	3.03 ng/ul	188147	Perylene-d12	25.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	83
4		Tritetracontane	605	C43H88	007098-21-7	83
5		2-methyloctacosane	408	C29H60	1000376-72-8	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027508.D
Acq On : 17 Jun 2017 15:51
Operator : SJ/MA
Sample : I3599-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.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
1,2,3-Propanetriol...	11.77	4.2	ng/ul	108086	2	11.34	516384	20.0
n-Hexadecanoic acid	18.69	2.9	ng/ul	144288	4	17.85	1000180	20.0
Dodecanoic acid, ...	20.49	2.1	ng/ul	118624	5	22.23	1121670	20.0
unknown-01	20.53	4.1	ng/ul	229151	5	22.23	1121670	20.0
Myristin, 1,3-dia...	21.58	2.5	ng/ul	138569	5	22.23	1121670	20.0
(DEL) Alkane: Str...	27.15	3.2	ng/ul	199361	6	25.89	1243570	20.0
(DEL) Alkane: Str...	28.71	3.6	ng/ul	221432	6	25.89	1243570	20.0
(DEL) Alkane: Str...	30.59	3.0	ng/ul	188147	6	25.89	1243570	20.0