

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
 Data File : BG028418.D
 Acq On : 22 Aug 2017 14:40
 Operator : SJ/JU
 Sample : I4827-19
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B0AG1

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	3.653	8	11	15	rVB2	2036	2927	0.26%	0.022%
2	3.823	37	40	48	rVB4	7741	13471	1.21%	0.099%
3	4.005	68	71	76	rVB3	2463	3078	0.28%	0.023%
4	4.064	76	81	85	rBV5	2365	4613	0.41%	0.034%
5	4.252	106	113	116	rVB4	2538	4663	0.42%	0.034%
6	4.334	120	127	133	rVB6	2881	6233	0.56%	0.046%
7	4.446	143	146	151	rVB3	2497	3601	0.32%	0.027%
8	4.499	151	155	158	rVV4	2089	2909	0.26%	0.021%
9	4.587	163	170	174	rBV7	2478	4601	0.41%	0.034%
10	4.716	191	192	197	rVB4	2429	2973	0.27%	0.022%
11	5.462	315	319	322	rVB3	3089	3706	0.33%	0.027%
12	6.449	483	487	491	rBV3	2405	3364	0.30%	0.025%
13	6.772	538	542	544	rBV2	2265	3147	0.28%	0.023%
14	7.137	599	604	609	rBV3	1650	3635	0.33%	0.027%
15	7.495	653	665	679	rVV	133537	255118	22.84%	1.884%
16	7.660	685	693	703	rVB	94831	162927	14.59%	1.203%
17	7.724	703	704	712	rBV4	2322	3638	0.33%	0.027%
18	7.877	720	730	740	rVB	123081	226928	20.32%	1.676%
19	8.200	782	785	791	rVV	1871	2942	0.26%	0.022%
20	8.341	798	809	817	rBV2	114238	205241	18.38%	1.516%
21	9.040	919	928	938	rBV	148741	283290	25.36%	2.092%
22	9.434	989	995	996	rBV2	4255	5609	0.50%	0.041%
23	9.510	1001	1008	1020	rVB	132471	256024	22.92%	1.891%
24	9.604	1020	1024	1030	rVV4	2165	4211	0.38%	0.031%
25	10.168	1114	1120	1122	rVB2	2483	3618	0.32%	0.027%
26	10.233	1122	1131	1144	rBV	116641	231928	20.77%	1.713%
27	10.456	1163	1169	1173	rBV5	6096	14390	1.29%	0.106%
28	10.780	1216	1224	1238	rVV	176586	332315	29.75%	2.454%
29	11.161	1281	1289	1300	rBV	181629	337273	30.20%	2.491%
30	11.297	1300	1312	1329	rBV	150546	309661	27.72%	2.287%
31	11.620	1359	1367	1379	rBV	40093	93902	8.41%	0.694%
32	12.513	1513	1519	1521	rBV2	1827	3131	0.28%	0.023%
33	12.548	1521	1525	1530	rVB3	2491	3405	0.30%	0.025%
34	12.718	1551	1554	1561	rVB3	3806	5370	0.48%	0.040%

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35	13.224	1633	1640	1643	rBV5	5711	10305	0.92%	0.076%
36	13.541	1691	1694	1699	rVB3	3776	4572	0.41%	0.034%
37	13.741	1724	1728	1731	rBV2	3288	3633	0.33%	0.027%
38	14.340	1818	1830	1834	rVV	406364	587738	52.62%	4.341%
39	14.387	1834	1838	1845	rVB	126925	186030	16.66%	1.374%
40	14.651	1873	1883	1892	rBV	393606	646899	57.92%	4.778%
41	14.804	1904	1909	1916	rBV4	5055	10532	0.94%	0.078%
42	14.951	1926	1934	1943	rBV2	331742	545720	48.86%	4.031%
43	15.151	1960	1968	1985	rBV3	111914	262714	23.52%	1.940%
44	15.327	1992	1998	2009	rBV3	48057	98181	8.79%	0.725%
45	15.709	2060	2063	2066	rBV3	3202	4663	0.42%	0.034%
46	15.750	2066	2070	2075	rVB3	12037	15376	1.38%	0.114%
47	15.938	2095	2102	2111	rBV	551720	865477	77.49%	6.392%
48	16.056	2116	2122	2131	rBV	191384	299777	26.84%	2.214%
49	16.179	2135	2143	2149	rVB7	7867	17243	1.54%	0.127%
50	16.308	2161	2165	2173	rBV5	3239	7765	0.70%	0.057%
51	16.379	2173	2177	2180	rVB4	2864	3561	0.32%	0.026%
52	16.496	2195	2197	2204	rVB4	2237	3361	0.30%	0.025%
53	16.561	2204	2208	2211	rBV3	2049	3163	0.28%	0.023%
54	16.614	2211	2217	2228	rVV3	14697	24330	2.18%	0.180%
55	16.802	2244	2249	2252	rVB4	3496	3775	0.34%	0.028%
56	16.890	2261	2264	2271	rBV6	2158	3596	0.32%	0.027%
57	16.961	2271	2276	2281	rVV6	2084	3957	0.35%	0.029%
58	17.060	2288	2293	2308	rVB8	17160	40285	3.61%	0.298%
59	17.213	2314	2319	2325	rBV2	12098	17164	1.54%	0.127%
60	17.401	2348	2351	2358	rBV3	8486	13718	1.23%	0.101%
61	17.572	2376	2380	2386	rVB3	3946	7028	0.63%	0.052%
62	17.701	2391	2402	2412	rBV	465331	725336	64.94%	5.357%
63	17.801	2412	2419	2429	rVV	615057	963284	86.25%	7.115%
64	18.106	2470	2471	2475	rVB3	2245	2868	0.26%	0.021%
65	18.147	2475	2478	2481	rBV4	4964	6077	0.54%	0.045%
66	18.324	2506	2508	2511	rVB3	3455	3264	0.29%	0.024%
67	18.435	2524	2527	2532	rVB3	2418	3315	0.30%	0.024%
68	18.506	2535	2539	2541	rVB3	2567	3312	0.30%	0.024%
69	18.547	2541	2546	2556	rBV3	66388	117283	10.50%	0.866%
70	18.899	2604	2606	2609	rBV2	2681	3398	0.30%	0.025%
71	19.199	2654	2657	2658	rBV2	3691	2895	0.26%	0.021%

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72	19.275	2666	2670	2675	rBV4	6579	10258	0.92%	0.076%
73	19.463	2696	2702	2703	rBV5	3508	5584	0.50%	0.041%
74	19.516	2708	2711	2713	rBV3	3398	2930	0.26%	0.022%
75	19.704	2740	2743	2751	rVB6	8658	12681	1.14%	0.094%
76	19.804	2756	2760	2766	rBV3	29607	48640	4.35%	0.359%
77	19.939	2781	2783	2785	rBV3	4878	4620	0.41%	0.034%
78	19.957	2785	2786	2793	rVB4	8844	12964	1.16%	0.096%
79	20.075	2800	2806	2818	rVB	776196	1116903	100.00%	8.249%
80	20.345	2846	2852	2855	rBV	127413	142076	12.72%	1.049%
81	20.380	2855	2858	2865	rVB	197139	216691	19.40%	1.600%
82	21.244	3000	3005	3006	rVB5	4249	6081	0.54%	0.045%
83	21.361	3020	3025	3028	rBV2	58721	80839	7.24%	0.597%
84	21.402	3028	3032	3042	rVB	74547	113541	10.17%	0.839%
85	21.608	3063	3067	3074	rVB7	11577	22535	2.02%	0.166%
86	22.031	3131	3139	3150	rBV	447001	823377	73.72%	6.081%
87	22.530	3221	3224	3228	rBV4	18659	29219	2.62%	0.216%
88	22.577	3229	3232	3239	rVB6	27899	44239	3.96%	0.327%
89	22.824	3271	3274	3280	rVB7	11382	19704	1.76%	0.146%
90	23.512	3386	3391	3395	rBV8	8125	15115	1.35%	0.112%
91	23.570	3397	3401	3409	rVB7	20128	41252	3.69%	0.305%
92	23.788	3433	3438	3444	rVB4	23082	40706	3.64%	0.301%
93	24.046	3476	3482	3487	rBV9	15759	33014	2.96%	0.244%
94	24.105	3488	3492	3501	rVB7	25293	53902	4.83%	0.398%
95	24.446	3545	3550	3559	rVB5	24380	53711	4.81%	0.397%
96	25.292	3683	3694	3708	rBV	344657	1059197	94.83%	7.823%
97	25.533	3717	3735	3746	rBV4	251535	872978	78.16%	6.448%
98	26.696	3926	3933	3948	rVB7	33410	108554	9.72%	0.802%
99	28.183	4174	4186	4195	rBV5	32433	123640	11.07%	0.913%
100	29.951	4479	4487	4501	rVB10	23963	99053	8.87%	0.732%

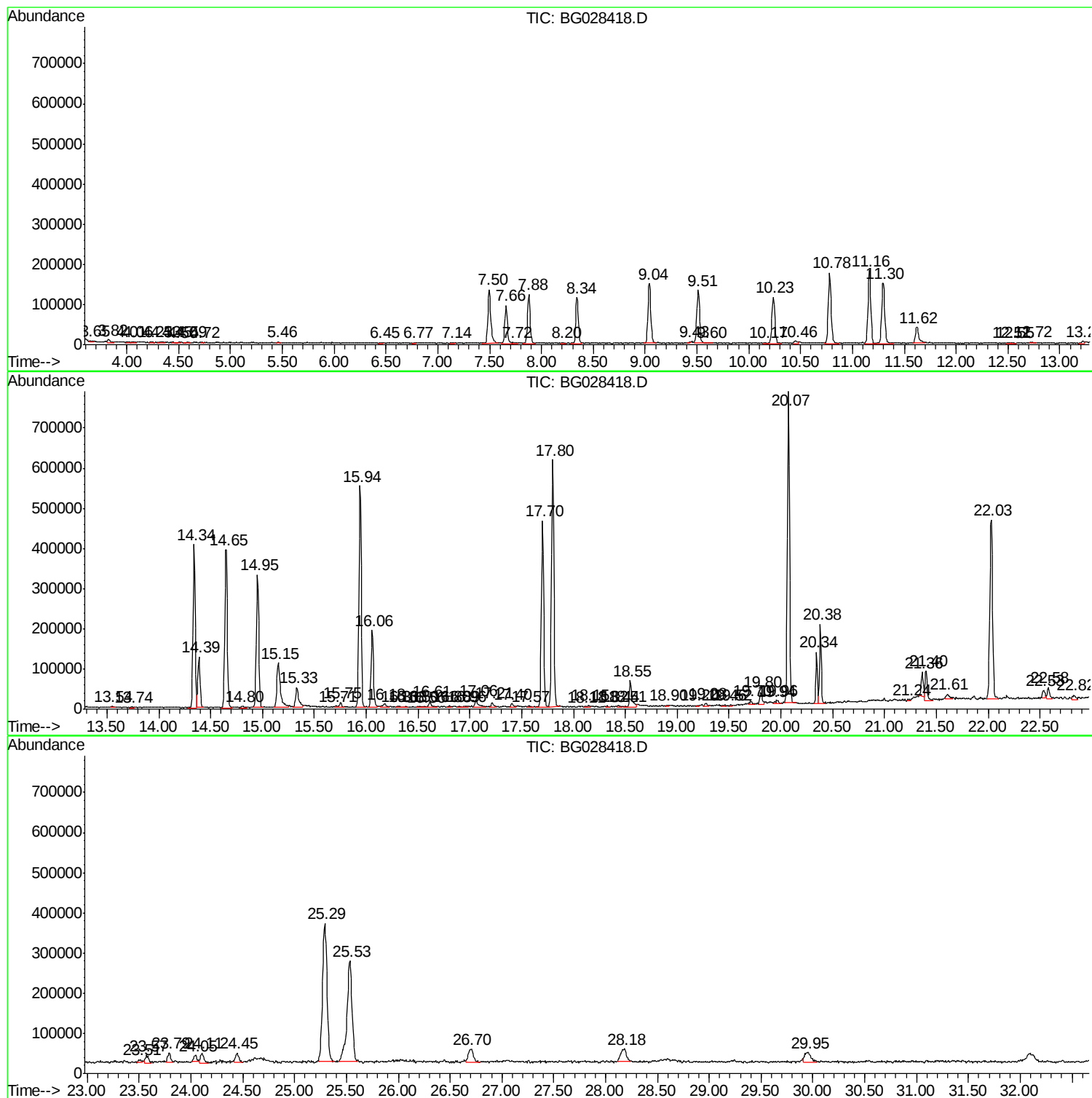
Sum of corrected areas: 13539441

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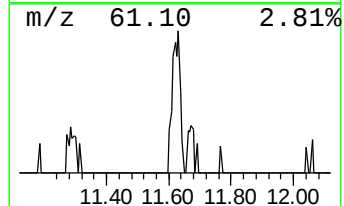
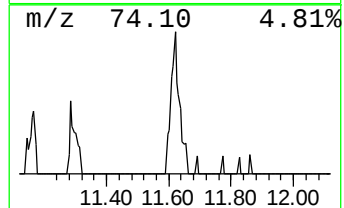
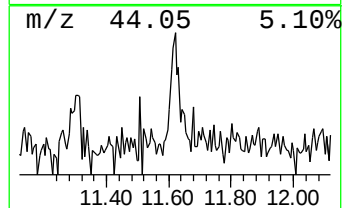
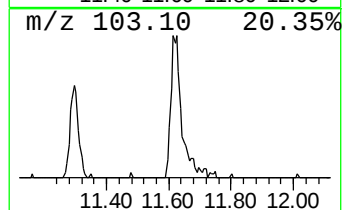
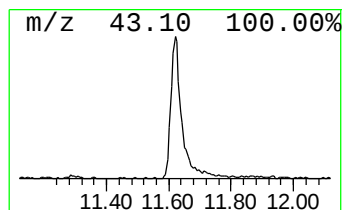
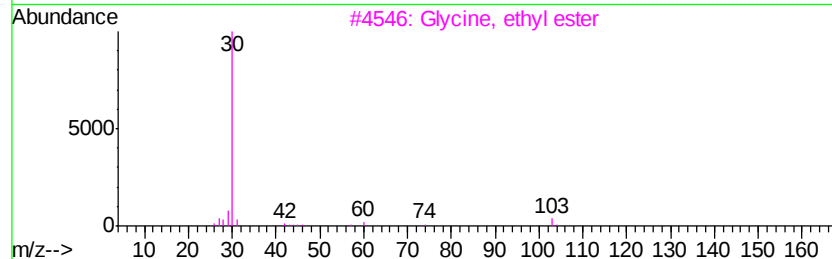
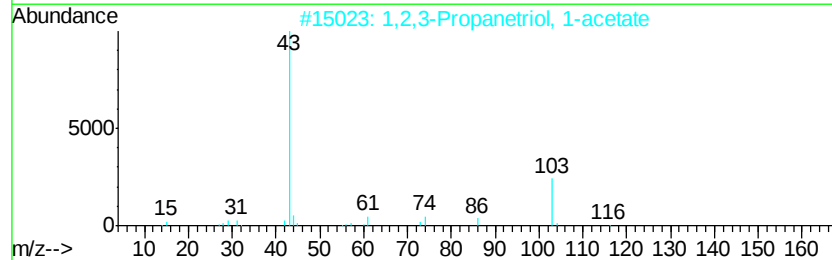
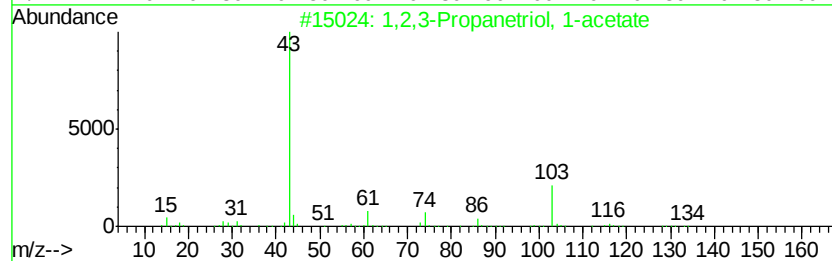
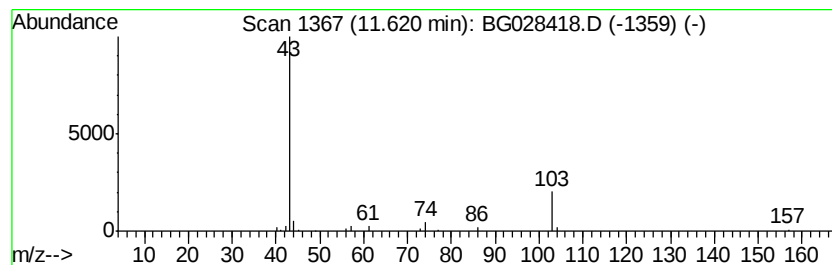
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	5.57 ng/ul	93902	Naphthalene-d8	11.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	39
2			1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	9
3			Glycine, ethyl ester	103	C4H9NO2	000459-73-4	5
4			1,2-Epoxy-3-propyl acetate	116	C5H8O3	006387-89-9	4
5			Butanedioic acid, 2-hydroxy-2-me...	148	C5H8O5	006236-09-5	4



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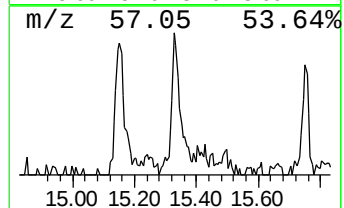
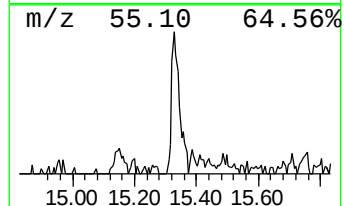
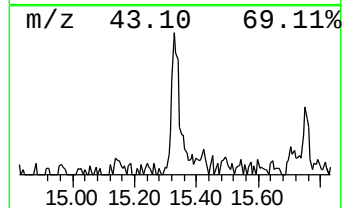
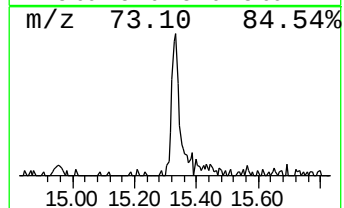
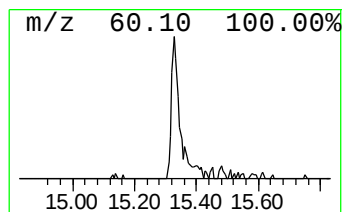
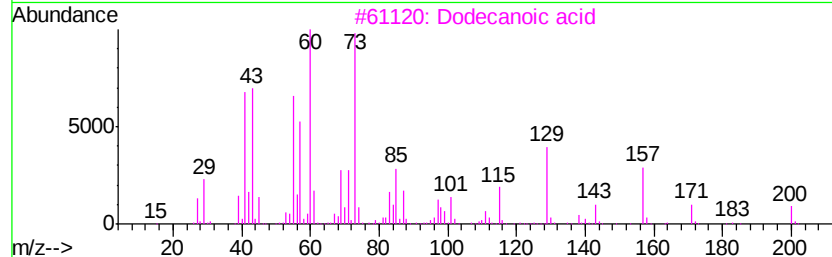
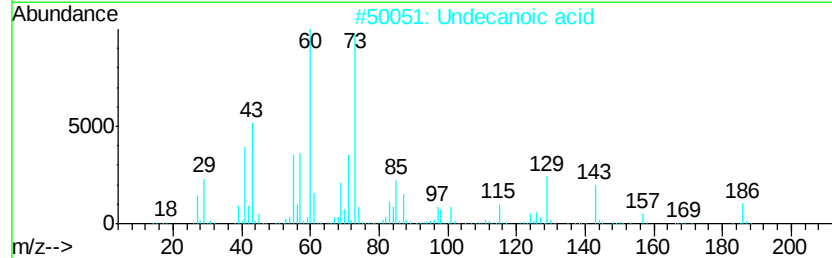
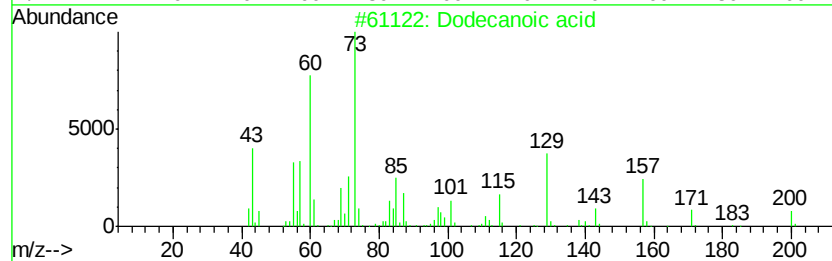
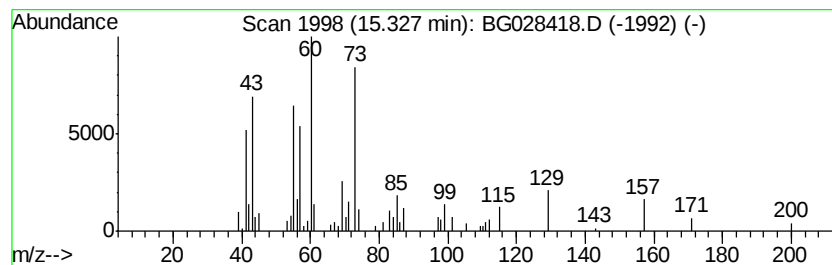
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.33	3.60 ng/ul	98181	Acenaphthene-d10		14.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	83
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			Dodecanoic acid	200	C12H24O2	000143-07-7	64
4			Nonanoic acid	158	C9H18O2	000112-05-0	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	59



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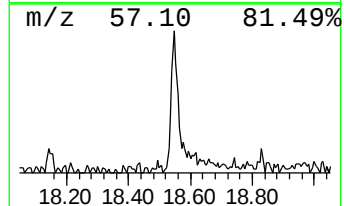
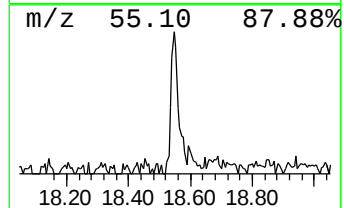
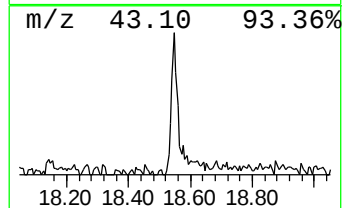
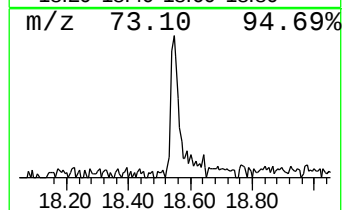
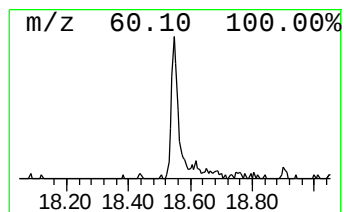
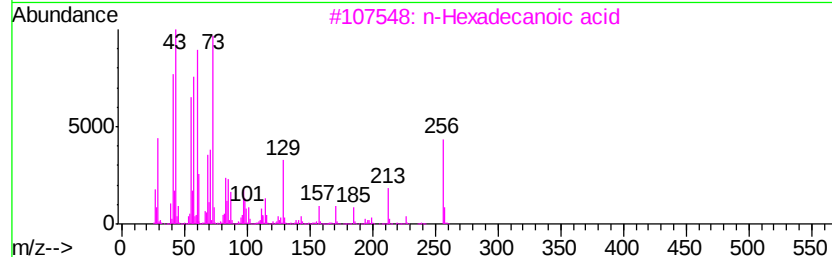
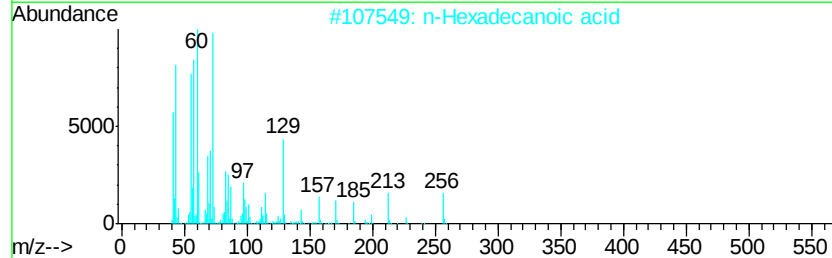
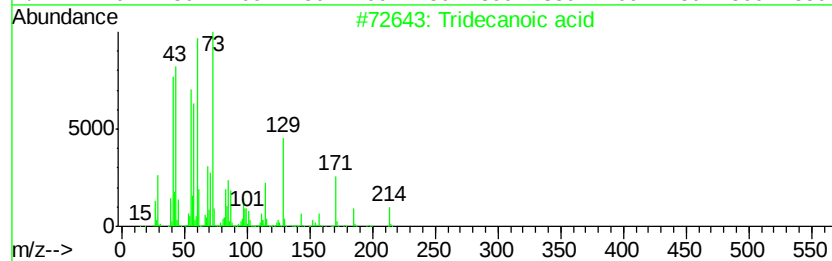
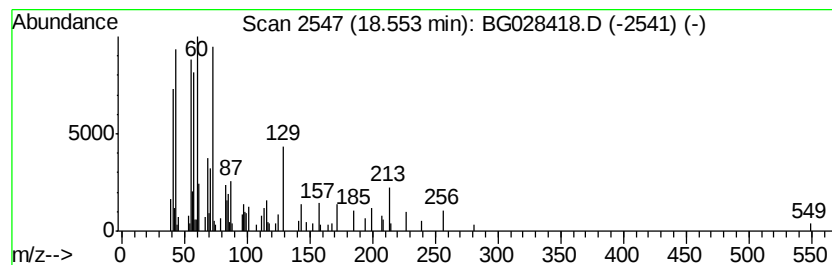
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	3.23 ng/ul	117283	Phenanthrene-d10	17.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	89
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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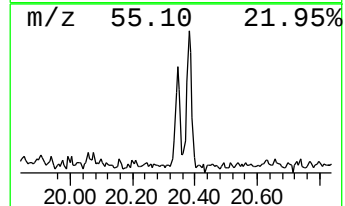
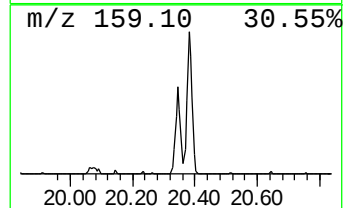
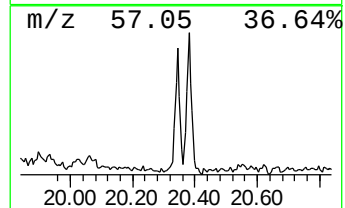
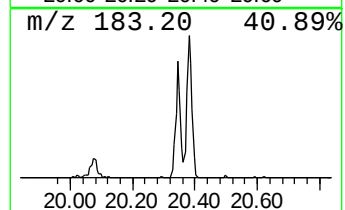
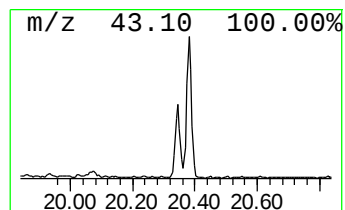
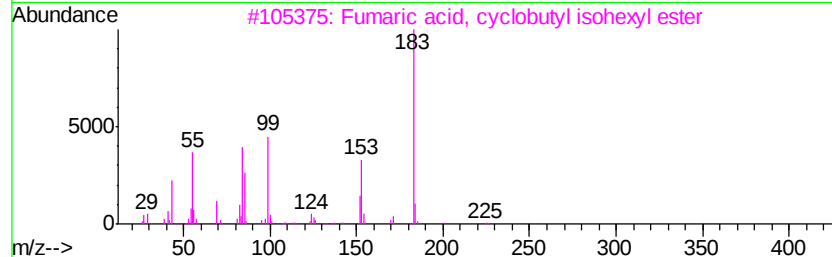
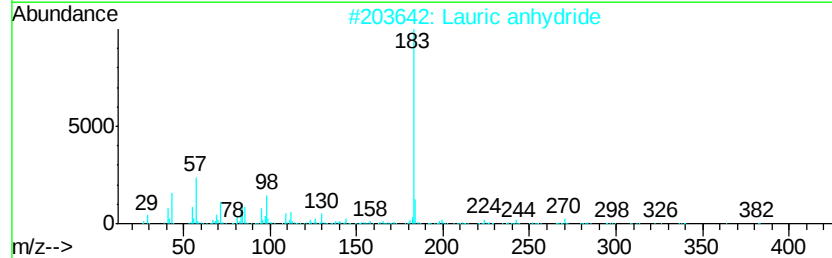
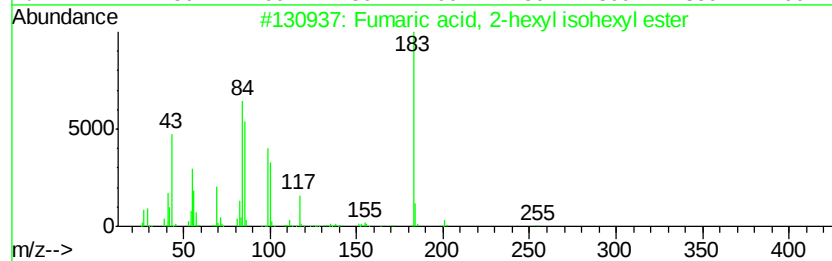
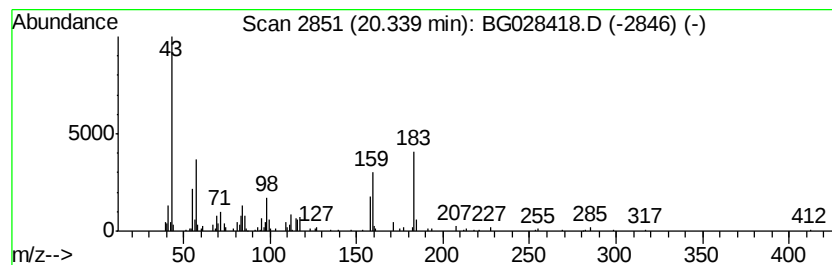
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.34	3.45 ng/ul	142076	Chrysene-d12	22.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, 2-hexyl isohexyl e...	284	C16H28O4	1000348-74-4	47
2		Lauric anhydride	382	C24H46O3	000645-66-9	43
3		Fumaric acid, cyclobutyl isohexy...	254	C14H22O4	1000345-03-5	38
4		Fumaric acid, hexyl 2-methylpent...	284	C16H28O4	1000348-76-3	38
5		Fumaric acid, hexyl 3-hexyl ester	284	C16H28O4	1000348-60-5	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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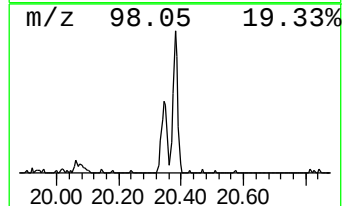
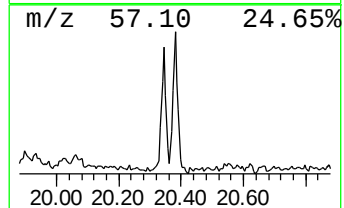
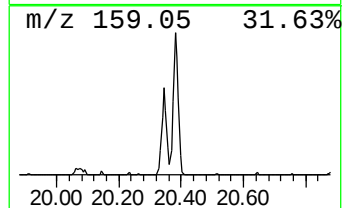
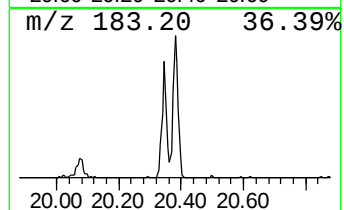
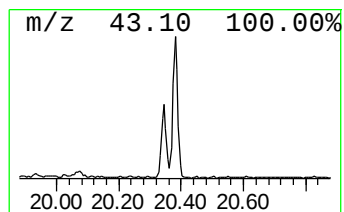
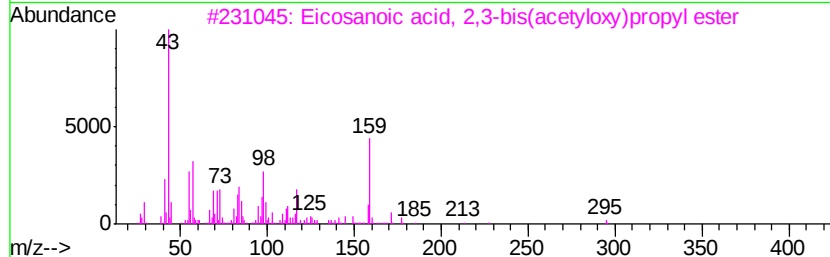
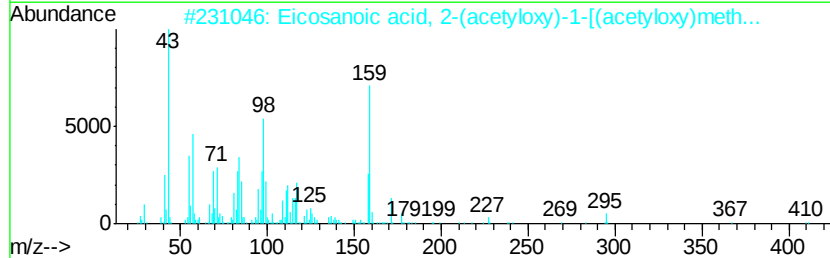
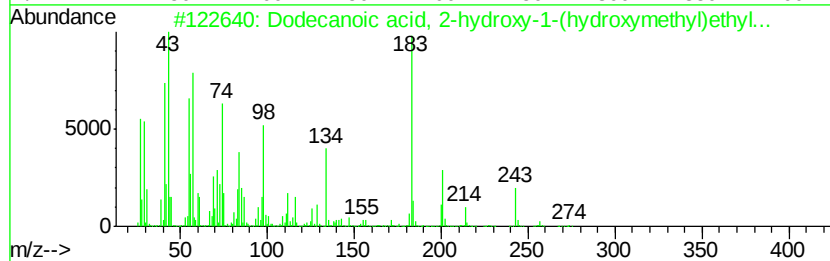
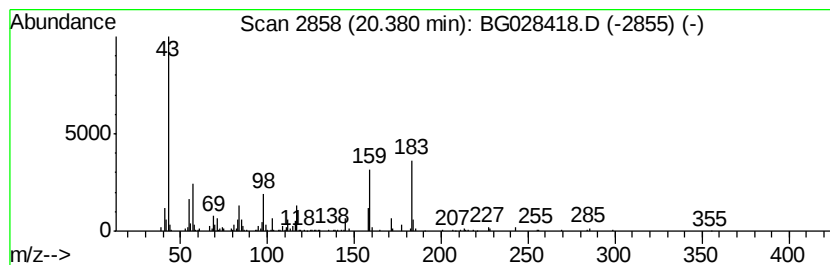
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.38	5.26 ng/ul	216691	Chrysene-d12	22.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	38
2		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	30
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	10
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9
5		3,5-Di-O-acetyl-1,4-anhydro-2-O-...	232	C10H16O6	1000366-02-8	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
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Instrument :
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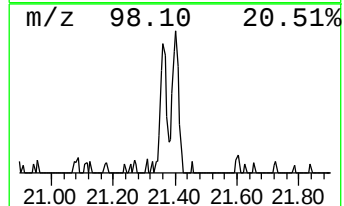
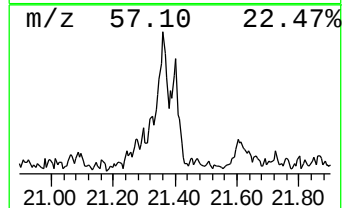
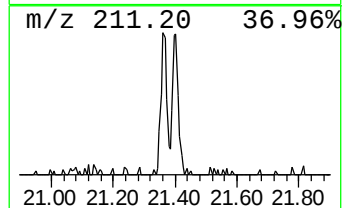
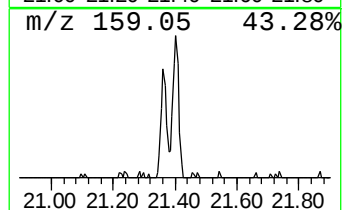
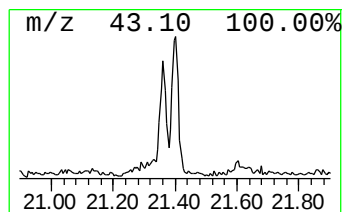
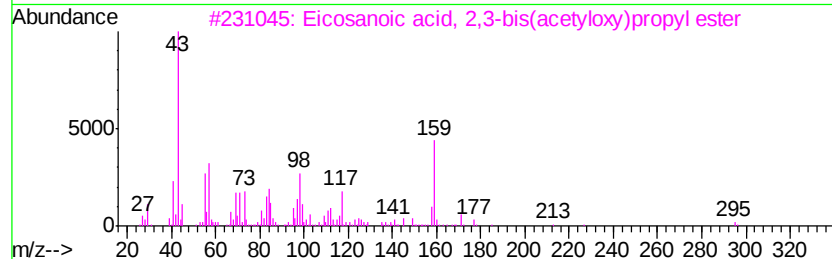
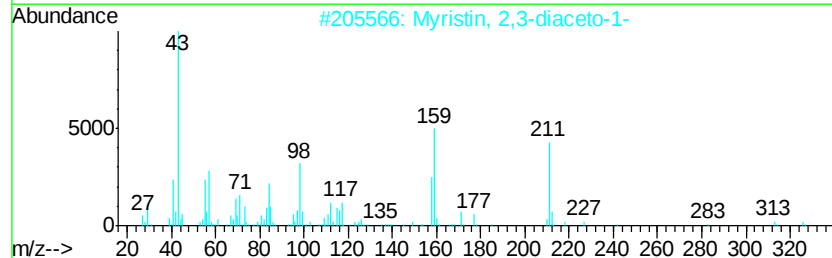
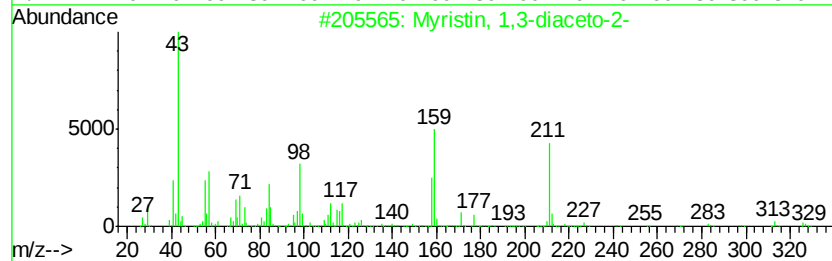
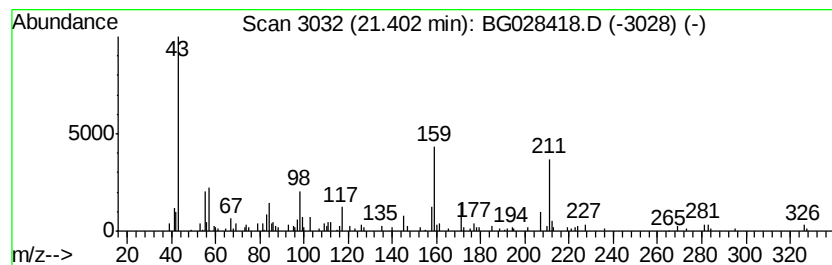
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.76 ng/ul	113541	Chrysene-d12	22.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	42
2		Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	35
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	12
4		2-Chloro-5-acetylthiomethylpyridine	201	C8H8ClNOS	1000306-87-6	9
5		4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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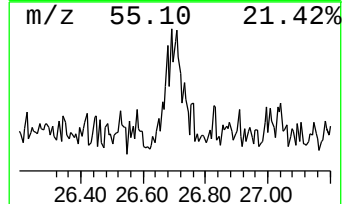
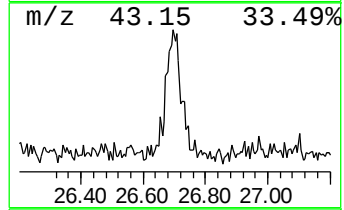
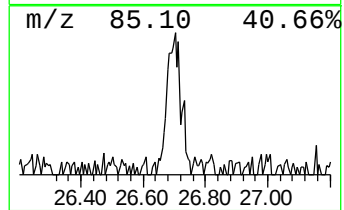
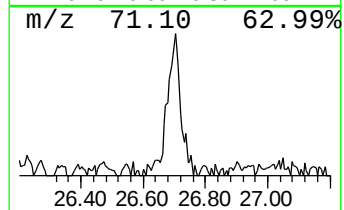
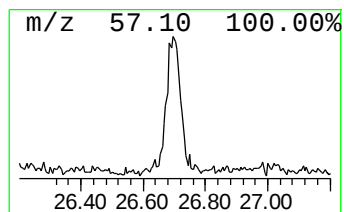
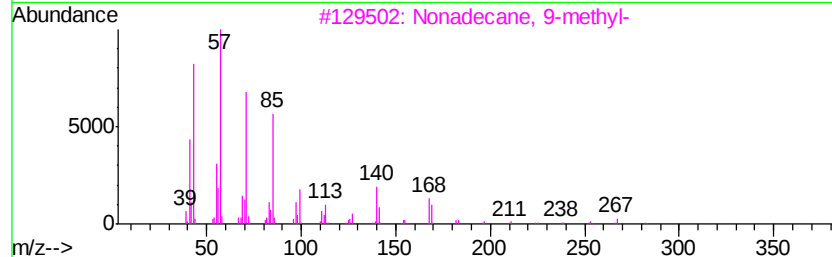
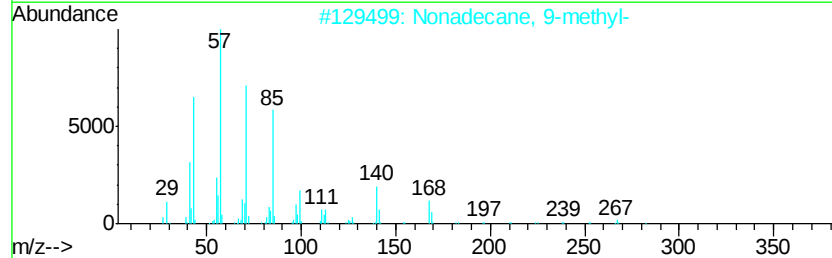
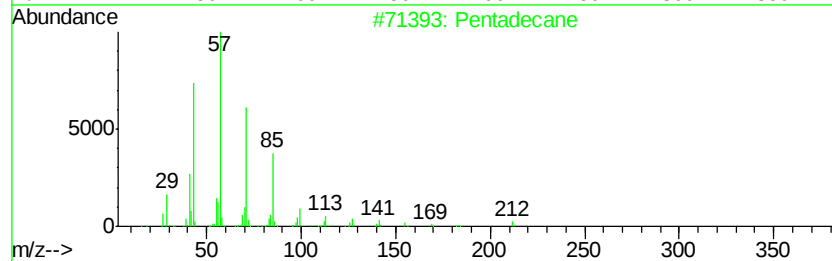
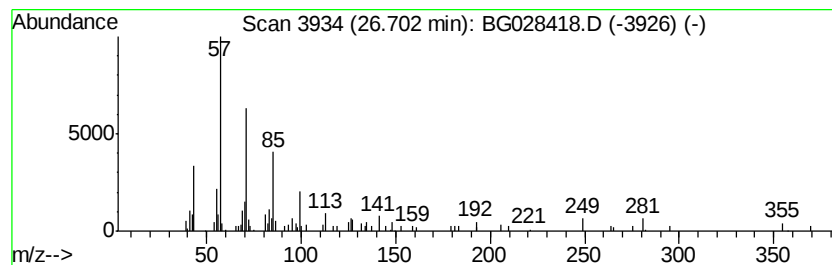
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.70	2.49 ng/ul	108554	Perylene-d12	25.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	81
2			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	81
3			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	76
4			Pentadecane	212	C15H32	000629-62-9	74
5			Hentriacontane	437	C31H64	000630-04-6	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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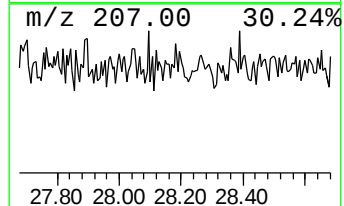
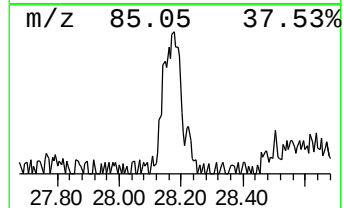
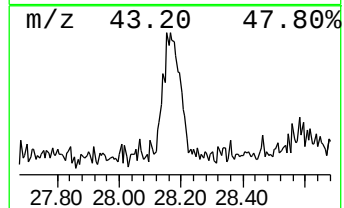
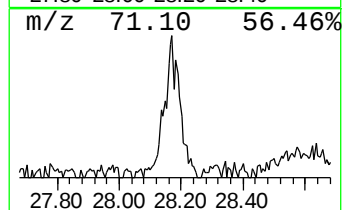
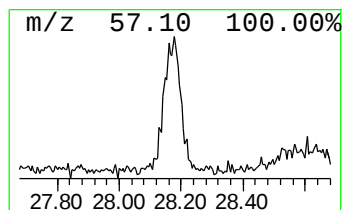
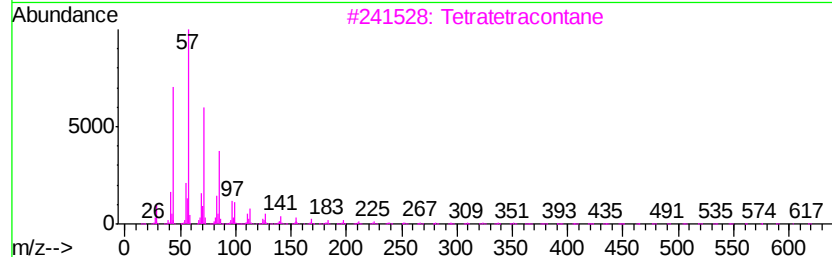
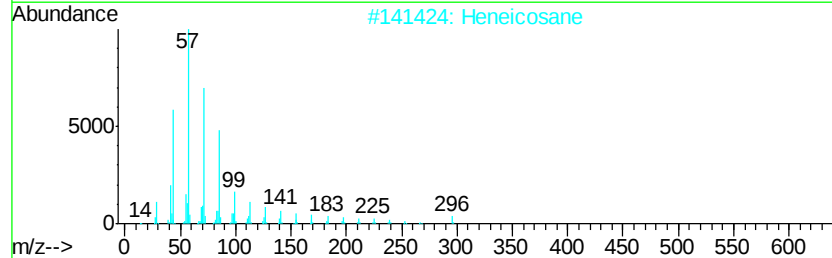
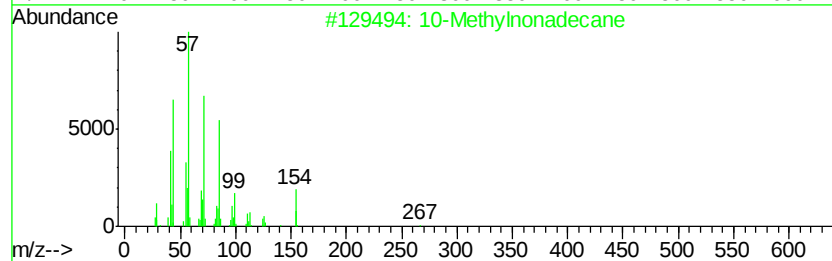
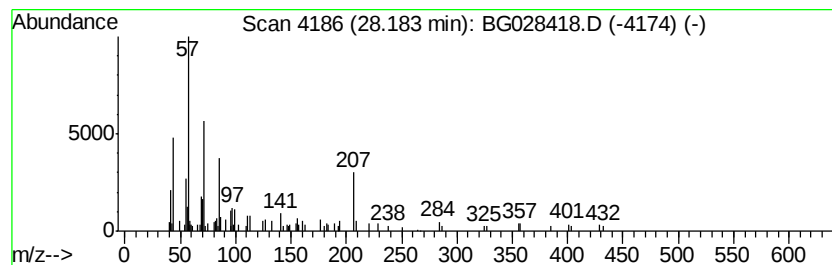
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.18	2.83 ng/ul	123640	Perylene-d12	25.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Methylnonadecane	282	C20H42	056862-62-5	46
2			Heneicosane	296	C21H44	000629-94-7	46
3			Tetratetracontane	619	C44H90	007098-22-8	46
4			Hentriacontane	437	C31H64	000630-04-6	46
5			Tricosane	324	C23H48	000638-67-5	46



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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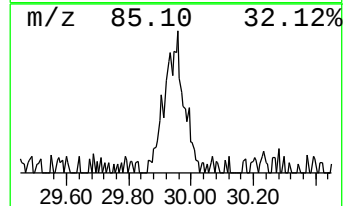
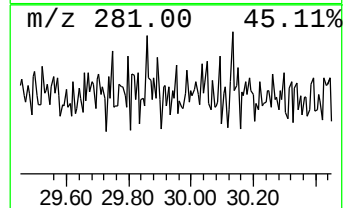
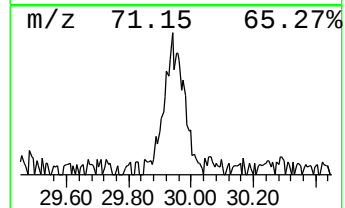
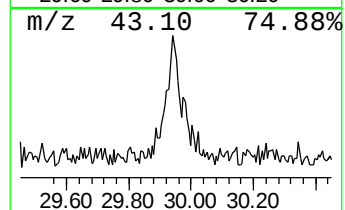
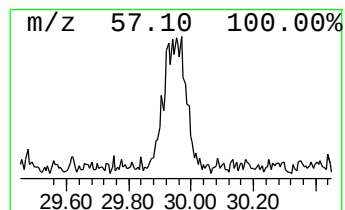
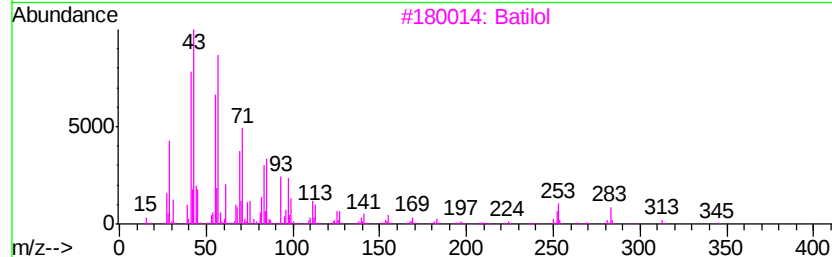
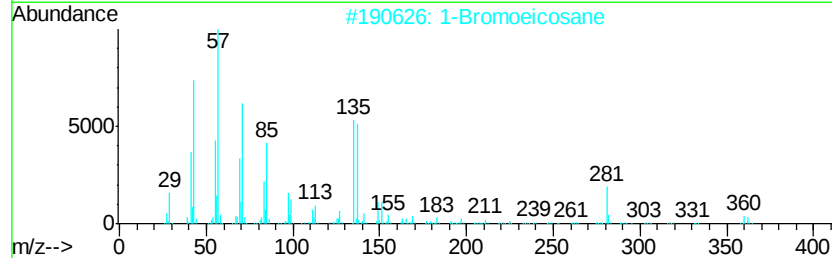
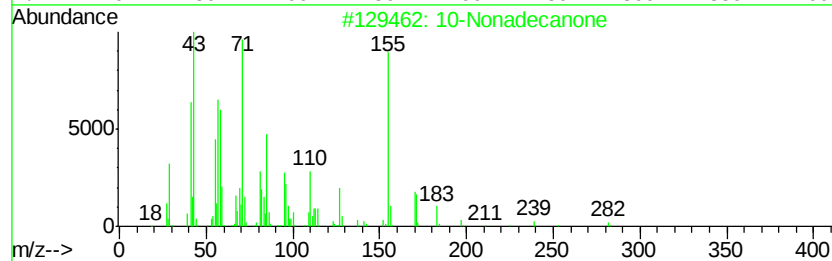
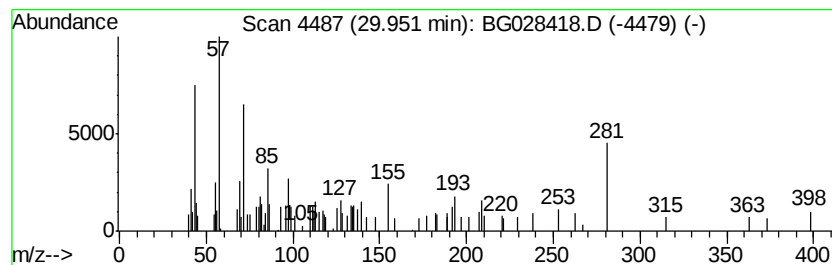
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.95	2.27 ng/ul	99053	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Nonadecanone	282	C19H38O	000504-57-4	35
2		1-Bromoeicosane	360	C20H41Br	004276-49-7	25
3		Batilol	344	C21H44O3	000544-62-7	25
4		Heneicosane, 3-methyl-	310	C22H46	006418-47-9	25
5		Docosane, 7-hexyl-	394	C28H58	055373-86-9	22



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082217\
Data File : BG028418.D
Acq On : 22 Aug 2017 14:40
Operator : SJ/JU
Sample : I4827-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Dodecanoic acid	15.33	3.6	ng/ul	98181	3	14.95	545720	20.0
Tridecanoic acid	18.55	3.2	ng/ul	117283	4	17.70	725336	20.0
unknown-02	20.34	3.5	ng/ul	142076	5	22.03	823377	20.0
unknown-03	20.38	5.3	ng/ul	216691	5	22.03	823377	20.0
unknown-04	21.40	2.8	ng/ul	113541	5	22.03	823377	20.0
(DEL) Alkane: Str...	26.70	2.5	ng/ul	108554	6	25.53	872978	20.0
(DEL) Alkane: Str...	28.18	2.8	ng/ul	123640	6	25.53	872978	20.0
unknown-05	29.95	2.3	ng/ul	99053	6	25.53	872978	20.0