

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
 Data File : BG025728.D
 Acq On : 31 Jan 2017 22:25
 Operator : SJ/MA
 Sample : I1460-12
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BDNS1

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-BG011817.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	3.152	51	53	57	rVB4	11994	11761	0.34%	0.033%
2	3.499	108	112	118	rBV6	17918	33280	0.97%	0.094%
3	3.822	164	167	171	rBV5	6491	12235	0.36%	0.035%
4	4.104	209	215	221	rBV7	8982	16302	0.48%	0.046%
5	4.662	309	310	318	rVB5	5646	10403	0.30%	0.029%
6	4.733	318	322	325	rBV3	4689	8572	0.25%	0.024%
7	5.285	415	416	421	rBV5	5806	8634	0.25%	0.024%
8	6.196	568	571	575	rBV6	6663	11358	0.33%	0.032%
9	6.677	648	653	658	rBV5	5350	13682	0.40%	0.039%
10	7.218	739	745	749	rVB6	6535	10528	0.31%	0.030%
11	7.330	757	764	784	rBV2	347083	854526	24.92%	2.410%
12	7.482	784	790	803	rVB	299504	533888	15.57%	1.506%
13	7.700	820	827	846	rBV2	352458	710552	20.72%	2.004%
14	8.029	879	883	888	rVB3	4611	8964	0.26%	0.025%
15	8.170	900	907	919	rBV	260016	499061	14.55%	1.408%
16	8.734	1001	1003	1008	rVB3	7062	9990	0.29%	0.028%
17	8.810	1008	1016	1020	rBV6	6102	15402	0.45%	0.043%
18	8.887	1020	1029	1042	rBV3	433371	897599	26.18%	2.532%
19	9.357	1099	1109	1125	rBV	389358	772574	22.53%	2.179%
20	9.486	1128	1131	1134	rBV5	7574	10888	0.32%	0.031%
21	9.662	1153	1161	1166	rBV5	11303	18824	0.55%	0.053%
22	10.079	1225	1232	1253	rVV2	350223	706613	20.61%	1.993%
23	10.232	1253	1258	1265	rVV5	5415	11848	0.35%	0.033%
24	10.402	1282	1287	1292	rBV7	7657	18230	0.53%	0.051%
25	10.632	1318	1326	1352	rBV2	382564	932745	27.20%	2.631%
26	10.996	1380	1388	1397	rBV	396131	708720	20.67%	1.999%
27	11.149	1405	1414	1430	rBV2	356439	831804	24.26%	2.346%
28	11.442	1461	1464	1470	rBV4	5363	9337	0.27%	0.026%
29	11.625	1491	1495	1498	rBV4	5189	8839	0.26%	0.025%
30	11.719	1506	1511	1513	rBV3	6287	8509	0.25%	0.024%
31	11.889	1533	1540	1542	rBV4	5573	13114	0.38%	0.037%
32	12.617	1654	1664	1667	rVB6	6395	18059	0.53%	0.051%
33	13.041	1732	1736	1743	rBV8	5853	11032	0.32%	0.031%
34	13.123	1743	1750	1753	rBV5	7811	13586	0.40%	0.038%

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35	13.387	1792	1795	1800	rVB6	5320	10412	0.30%	0.029%
36	13.652	1835	1840	1848	rVB6	12409	20299	0.59%	0.057%
37	14.192	1922	1932	1936	rBV	1021872	1527023	44.53%	4.307%
38	14.239	1936	1940	1954	rVB	326045	549030	16.01%	1.549%
39	14.427	1969	1972	1976	rVB5	6197	8119	0.24%	0.023%
40	14.498	1976	1984	1997	rVB	1030086	1711719	49.92%	4.828%
41	14.592	1997	2000	2004	rBV3	5302	9231	0.27%	0.026%
42	14.639	2004	2008	2012	rBV4	9420	15156	0.44%	0.043%
43	14.797	2026	2035	2045	rBV	660783	1047179	30.54%	2.954%
44	15.044	2070	2077	2095	rBV2	226753	715459	20.87%	2.018%
45	15.185	2097	2101	2107	rVB8	27349	52934	1.54%	0.149%
46	15.326	2123	2125	2133	rVB9	8301	12519	0.37%	0.035%
47	15.538	2156	2161	2165	rVV2	27433	45787	1.34%	0.129%
48	15.579	2165	2168	2175	rVV	39903	54308	1.58%	0.153%
49	15.784	2196	2203	2216	rBV	1390024	2239368	65.31%	6.316%
50	15.937	2223	2229	2241	rBV2	449358	878907	25.63%	2.479%
51	16.025	2241	2244	2251	rVB8	24571	47734	1.39%	0.135%
52	16.119	2258	2260	2266	rVB6	7708	13257	0.39%	0.037%
53	16.307	2288	2292	2293	rBV3	6835	9498	0.28%	0.027%
54	16.442	2308	2315	2323	rBV3	48767	93054	2.71%	0.262%
55	16.583	2337	2339	2343	rVB5	6661	9033	0.26%	0.025%
56	16.789	2368	2374	2380	rBV7	10668	18220	0.53%	0.051%
57	16.924	2390	2397	2398	rBV7	9890	21562	0.63%	0.061%
58	17.018	2409	2413	2418	rVB8	11892	22592	0.66%	0.064%
59	17.071	2418	2422	2426	rBV6	9924	19479	0.57%	0.055%
60	17.124	2429	2431	2436	rBV6	8795	11290	0.33%	0.032%
61	17.230	2444	2449	2453	rBV	69318	87452	2.55%	0.247%
62	17.283	2455	2458	2463	rVB5	22157	30125	0.88%	0.085%
63	17.541	2495	2502	2511	rBV	850100	1367525	39.88%	3.857%
64	17.641	2511	2519	2535	rVB2	1556111	2553352	74.46%	7.202%
65	17.764	2539	2540	2549	rVB7	8885	13820	0.40%	0.039%
66	17.882	2556	2560	2569	rBV10	27120	60552	1.77%	0.171%
67	17.970	2571	2575	2581	rVB	83343	110489	3.22%	0.312%
68	18.152	2602	2606	2611	rVB8	9223	14877	0.43%	0.042%
69	18.381	2641	2645	2656	rBV5	87441	177563	5.18%	0.501%
70	18.464	2657	2659	2664	rVB6	9133	14088	0.41%	0.040%
71	18.657	2687	2692	2696	rBV4	51130	57094	1.67%	0.161%

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72	18.699	2697	2699	2705	rVB7	13669	19870	0.58%	0.056%
73	18.793	2711	2715	2722	rBV9	13587	26945	0.79%	0.076%
74	18.969	2742	2745	2749	rBV6	9649	12693	0.37%	0.036%
75	19.075	2756	2763	2766	rBV6	18416	28836	0.84%	0.081%
76	19.116	2766	2770	2776	rVB6	28517	42277	1.23%	0.119%
77	19.245	2789	2792	2795	rBV4	9091	14472	0.42%	0.041%
78	19.280	2796	2798	2802	rVV3	20451	23944	0.70%	0.068%
79	19.562	2841	2846	2851	rVB	29951	46991	1.37%	0.133%
80	19.645	2855	2860	2865	rBV8	35394	55819	1.63%	0.157%
81	19.703	2868	2870	2874	rVB5	19441	19002	0.55%	0.054%
82	19.809	2885	2888	2893	rBV3	22724	36192	1.06%	0.102%
83	19.921	2899	2907	2920	rVB2	2294059	3420513	99.75%	9.647%
84	20.179	2945	2951	2954	rBV	423394	462432	13.49%	1.304%
85	20.220	2954	2958	2963	rVB	674690	784274	22.87%	2.212%
86	20.914	3073	3076	3080	rBV4	18297	18696	0.55%	0.053%
87	21.172	3116	3120	3123	rBV	183965	236271	6.89%	0.666%
88	21.207	3123	3126	3133	rVB	315613	387945	11.31%	1.094%
89	21.407	3154	3160	3173	rBV	58879	193568	5.65%	0.546%
90	21.830	3225	3232	3243	rBV	1053239	1927605	56.22%	5.437%
91	22.289	3306	3310	3314	rBV4	68059	108856	3.17%	0.307%
92	22.336	3314	3318	3329	rVB2	122024	206083	6.01%	0.581%
93	23.217	3463	3468	3473	rBV7	42423	70714	2.06%	0.199%
94	23.270	3474	3477	3485	rVB10	35495	70315	2.05%	0.198%
95	23.722	3550	3554	3559	rBV4	53929	107643	3.14%	0.304%
96	23.781	3559	3564	3576	rVB3	111880	249286	7.27%	0.703%
97	24.098	3613	3618	3625	rVB5	34808	74476	2.17%	0.210%
98	24.974	3757	3767	3780	rBV2	1189347	3428984	100.00%	9.671%
99	25.062	3780	3782	3793	rVB8	45263	98744	2.88%	0.279%
100	25.209	3797	3807	3824	rVB2	580832	1870015	54.54%	5.274%

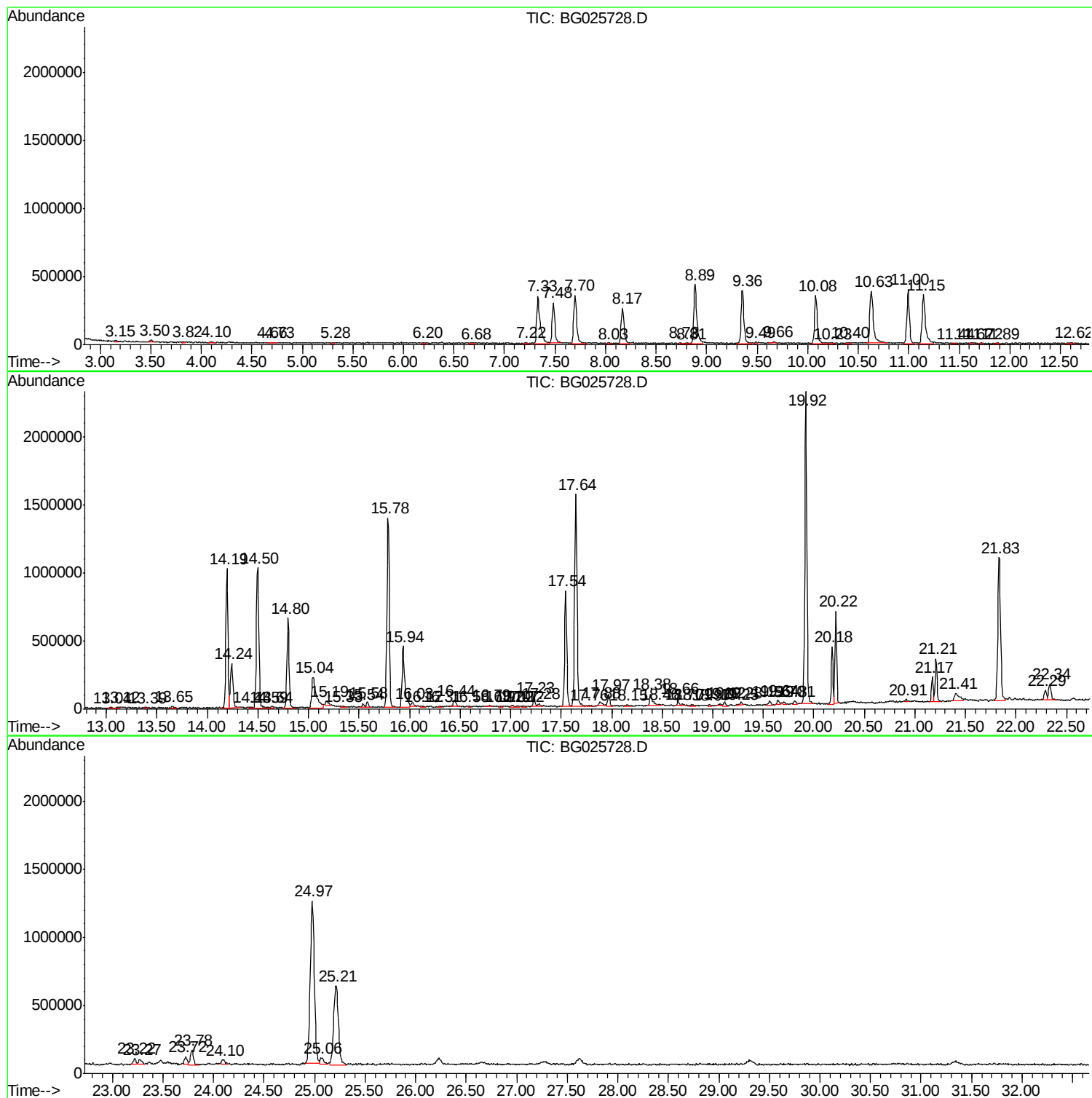
Sum of corrected areas: 35455026

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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



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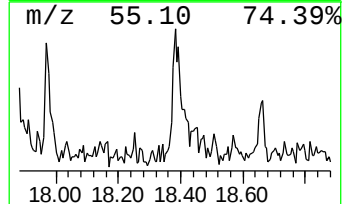
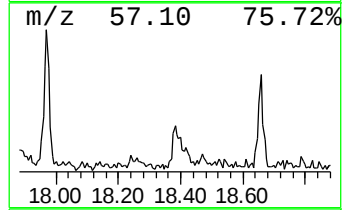
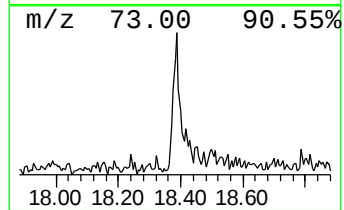
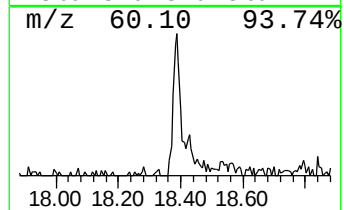
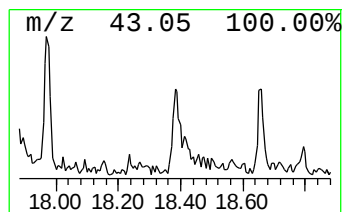
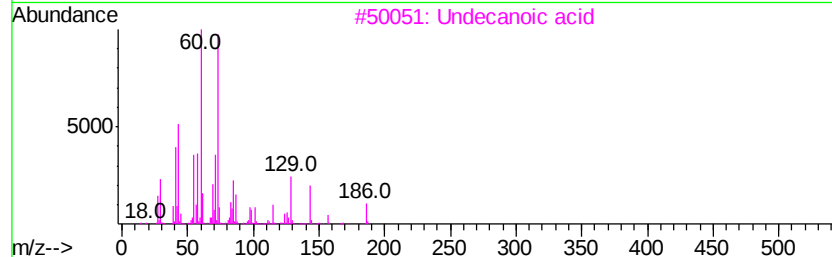
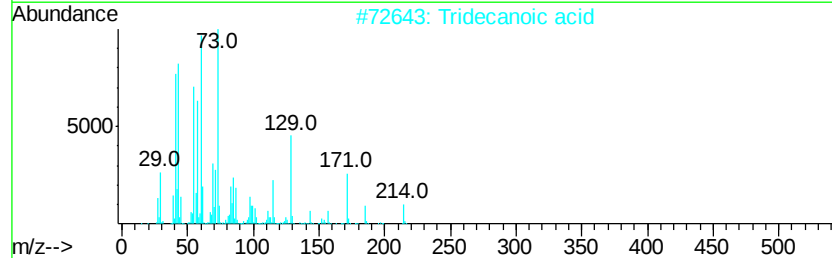
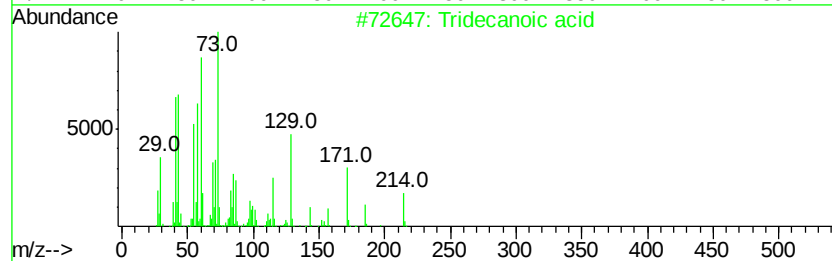
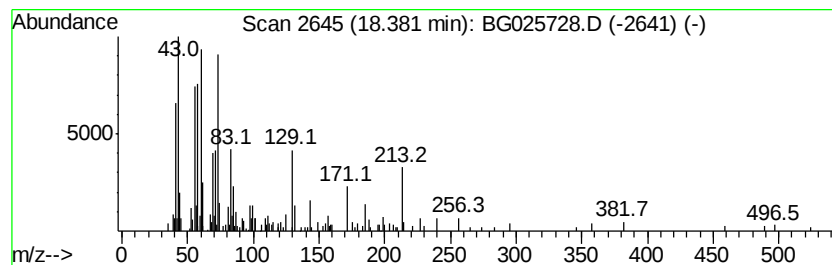
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.60 ng/ul	177563	Phenanthrene-d10	17.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanoic acid	214	C13H26O2	000638-53-9	62
2		Tridecanoic acid	214	C13H26O2	000638-53-9	59
3		Undecanoic acid	186	C11H22O2	000112-37-8	47
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
5		n-Decanoic acid	172	C10H20O2	000334-48-5	38



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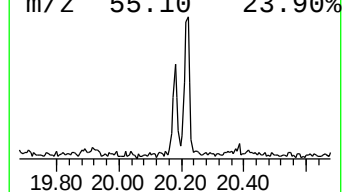
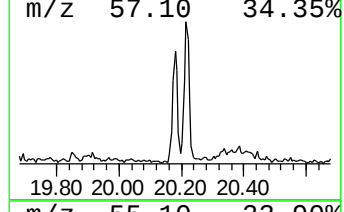
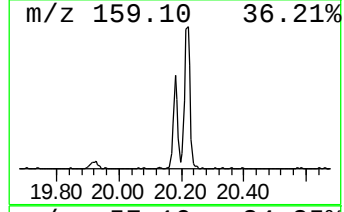
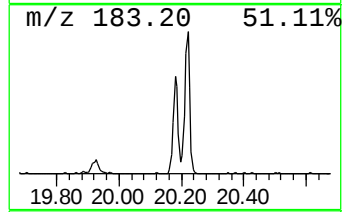
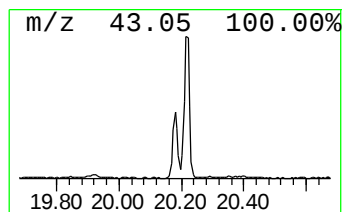
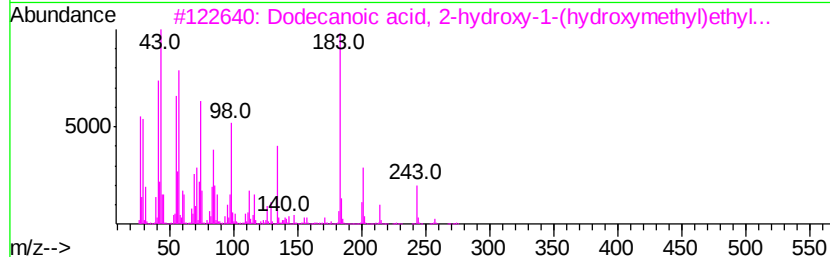
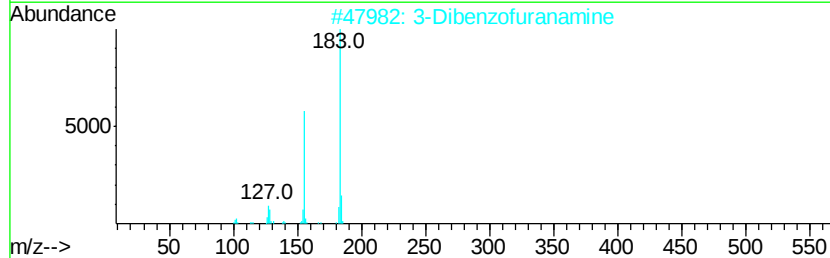
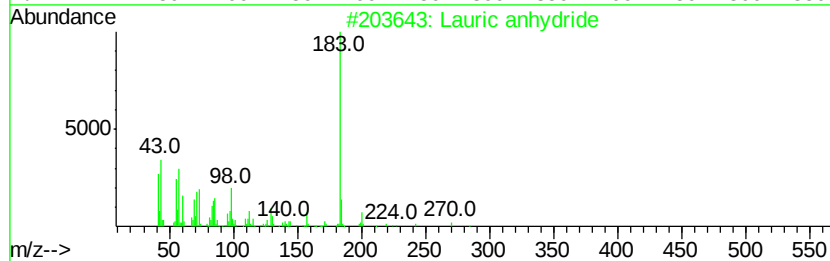
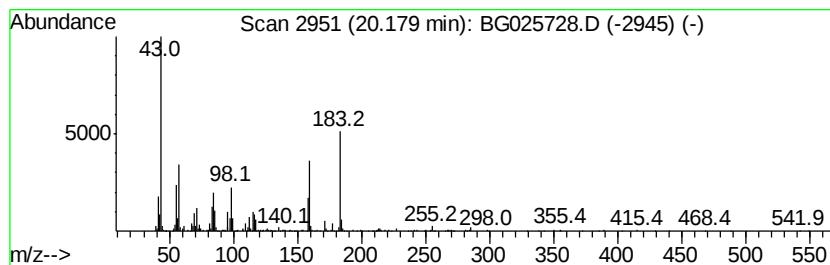
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Lauric anhydride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.18	4.80 ng/ul	462432	Chrysene-d12	21.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Lauric anhydride	382 C24H46O3	000645-66-9	50
2	3-Dibenzofuranamine	183 C12H9NO	004106-66-5	43
3	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274 C15H30O4	001678-45-1	42
4	Fumaric acid, cyclobutyl isohexyl...	254 C14H22O4	1000345-03-5	32
5	Fumaric acid, di(3-hexyl) ester	284 C16H28O4	1000348-61-9	27



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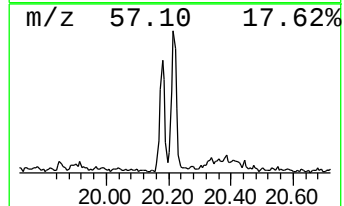
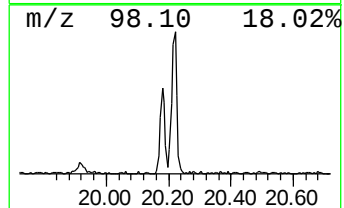
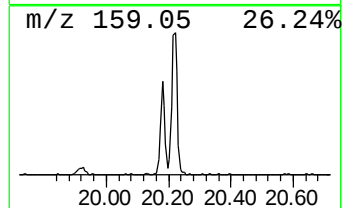
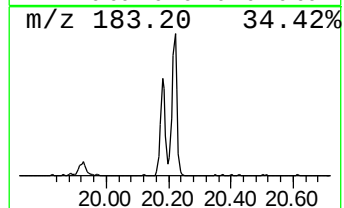
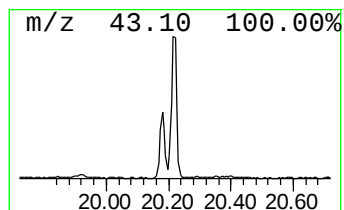
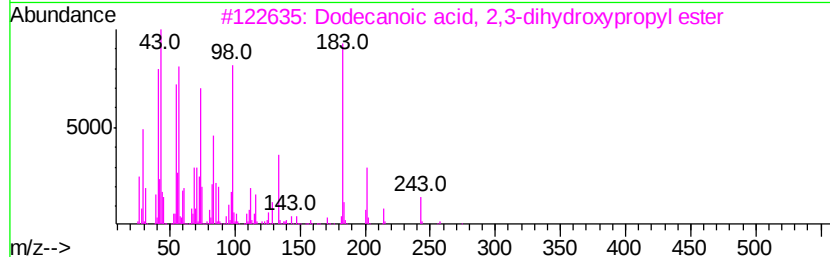
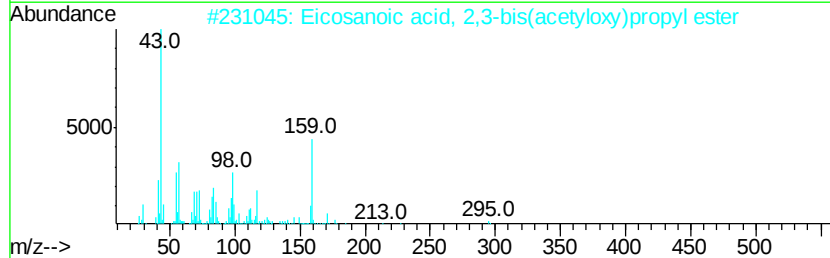
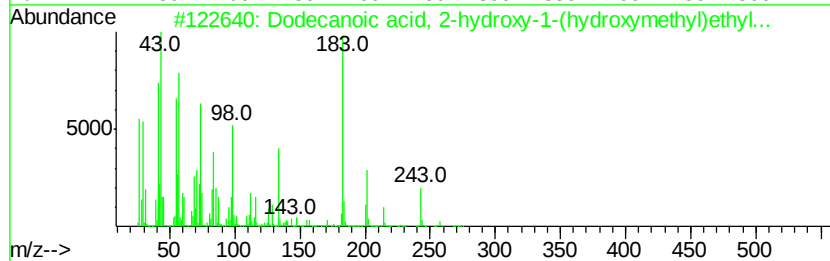
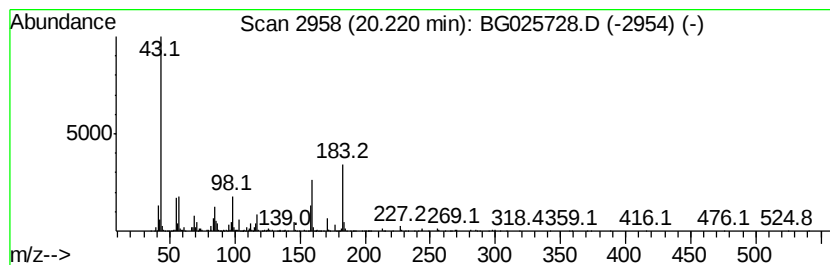
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	8.14 ng/ul	784274	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	38
2		Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	37
3		Dodecanoic acid, 2,3-dihydroxypropyl ester	274	C15H30O4	000142-18-7	32
4		Eicosanoic acid, 2-(acetyloxy)-1-(hydroxymethyl)ethyl ester	470	C27H50O6	055429-68-0	12
5		Acetamide, N-(2-methyl-3-oxo-4-iodophenyl)-	158	C6H10N2O3	014617-48-2	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BDNS1

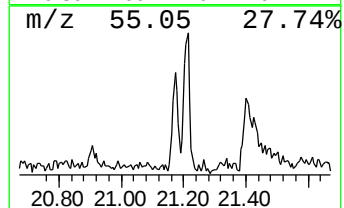
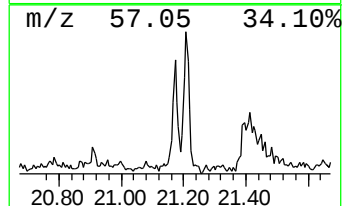
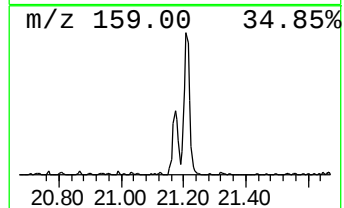
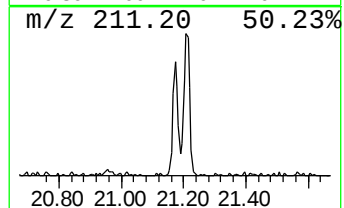
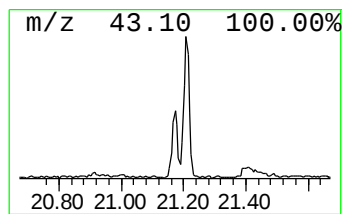
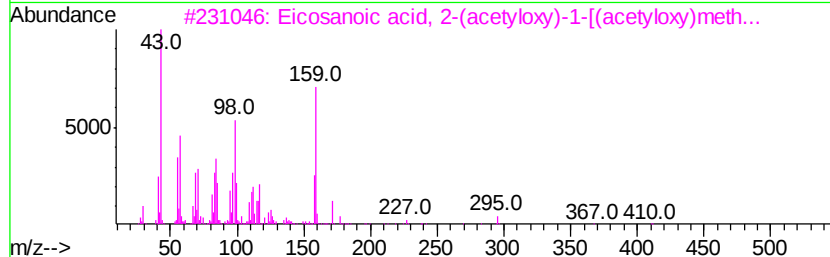
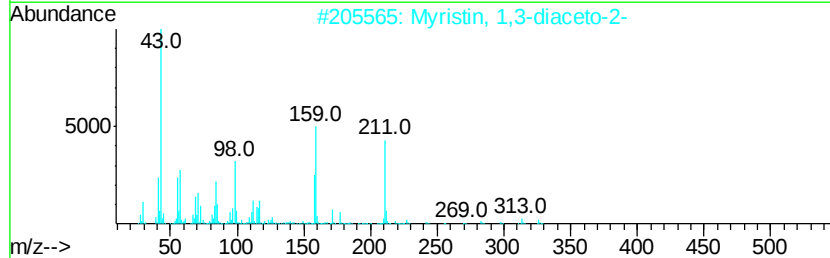
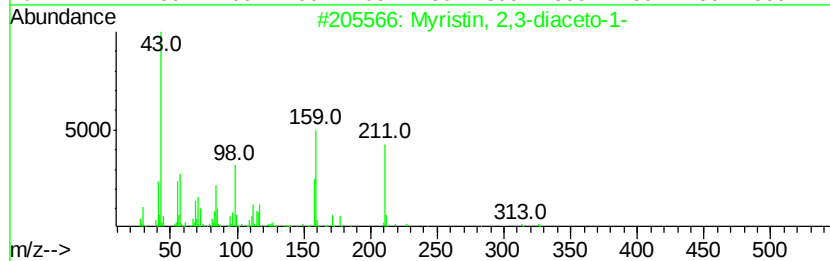
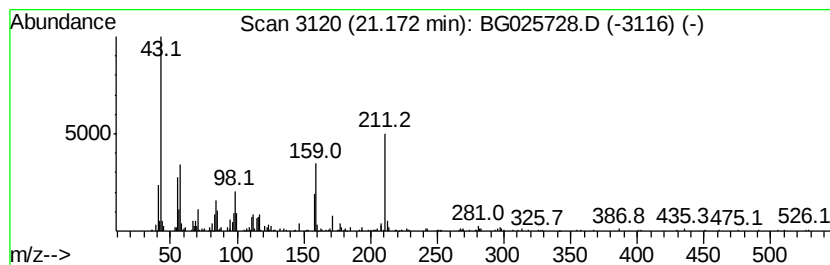
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Myristin, 2,3-diaceto-1- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	2.45 ng/ul	236271	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	62
2		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	62
3		Eicosanoic acid, 2-(acetvloxv)-1...	470	C27H50O6	055429-68-0	38
4		Milrinone	211	C12H9N3O	078415-72-2	22
5		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	14



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNS1

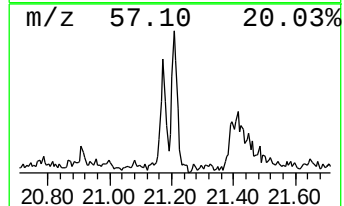
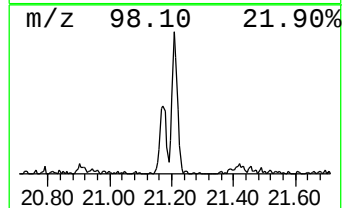
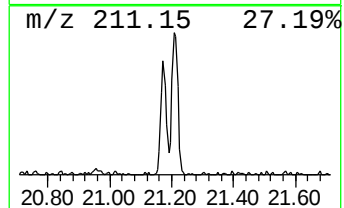
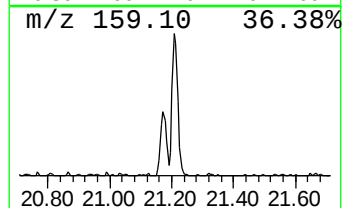
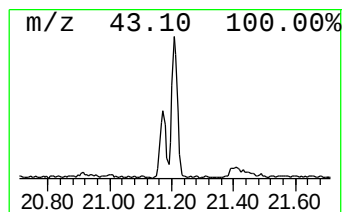
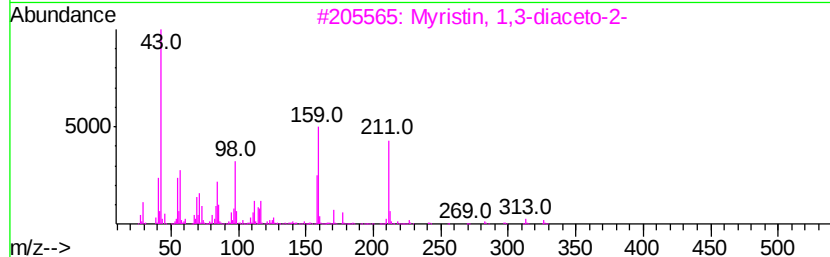
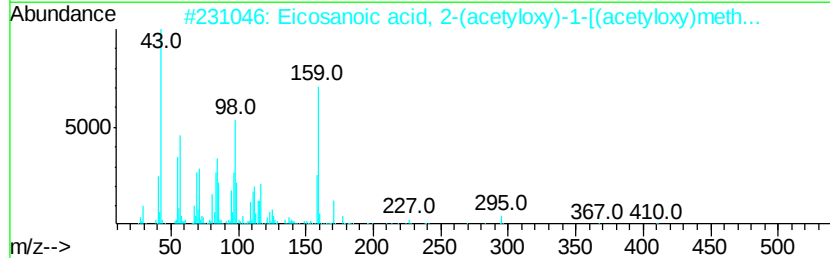
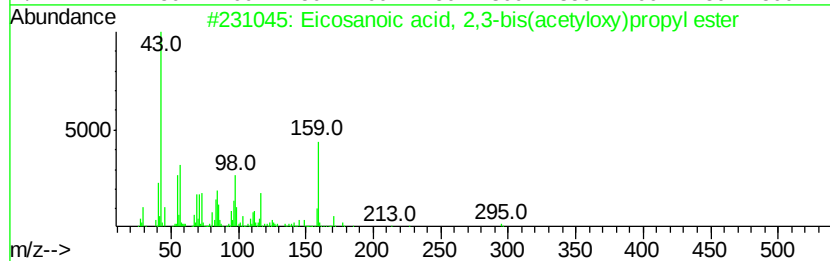
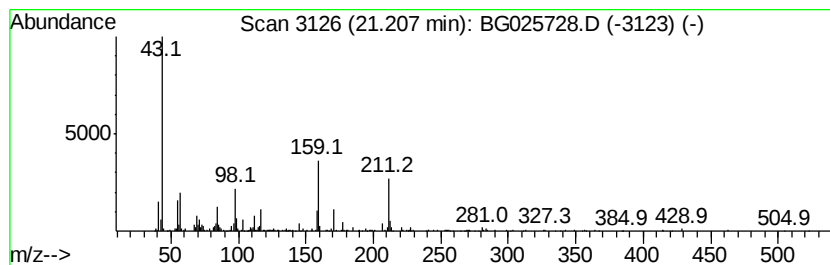
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	4.03 ng/ul	387945	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	42
2		Eicosanoic acid, 2-(acetyloxv)-1...	470	C27H50O6	055429-68-0	38
3		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	32
4		Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	32
5		2-Propanone, 1-[2,5-dihydro-1-[(...	241	C10H15N3O2S	1000317-27-6	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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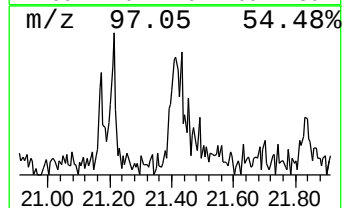
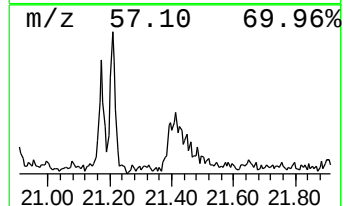
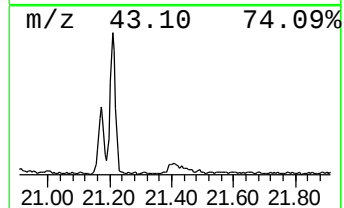
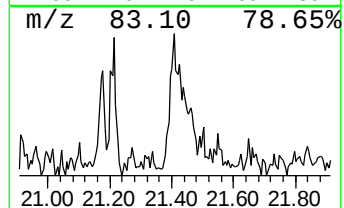
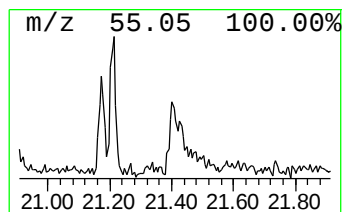
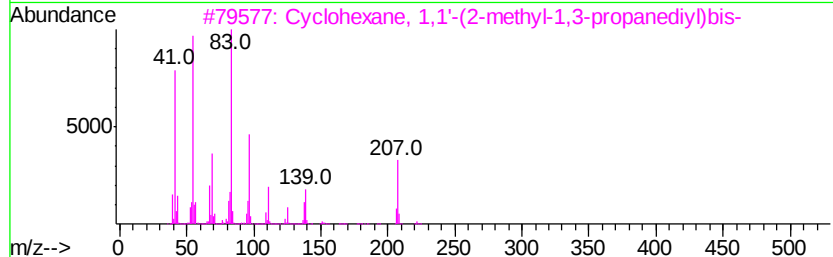
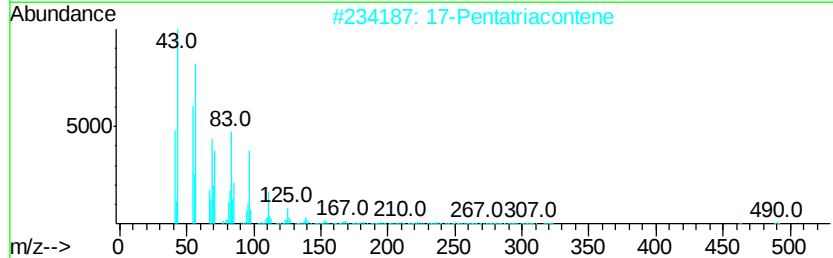
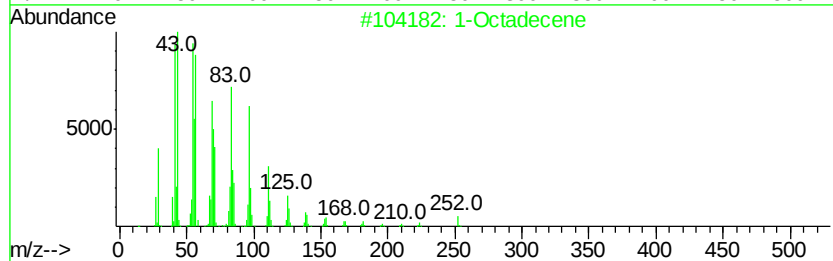
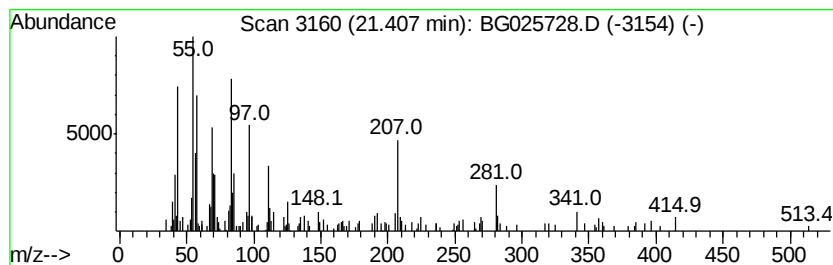
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Cyclic21.41 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	2.01 ng/ul	193568	Chrysene-d12	21.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	49
2			17-Pentatriacontene	491	C35H70	006971-40-0	49
3			Cyclohexane, 1,1'-(2-methyl-1,3-...	222	C16H30	002883-08-1	46
4			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	43
5			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl303	1000314-56-3	42



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNS1

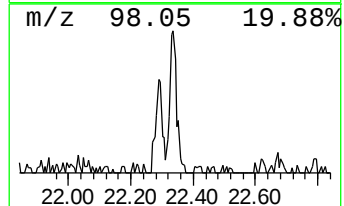
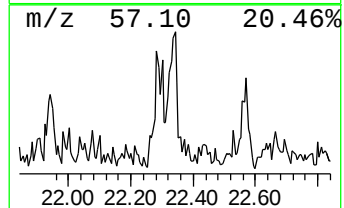
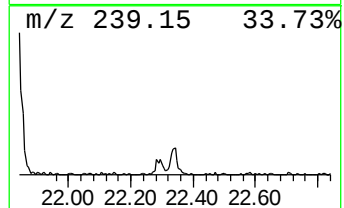
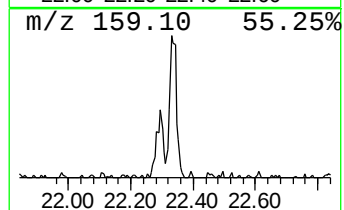
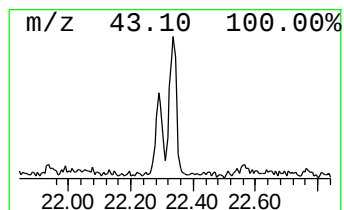
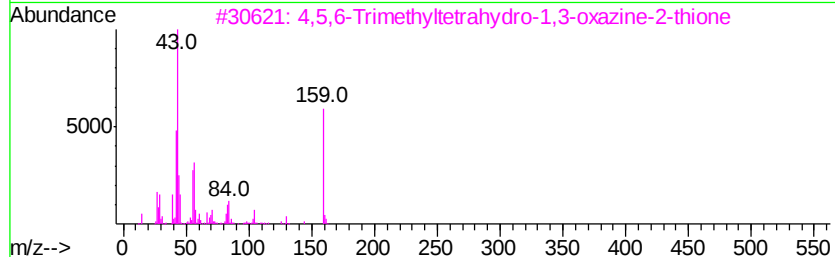
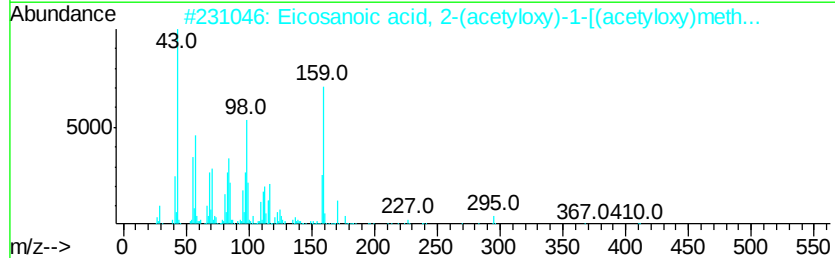
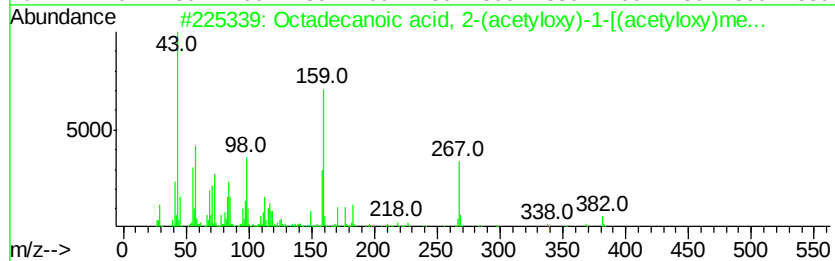
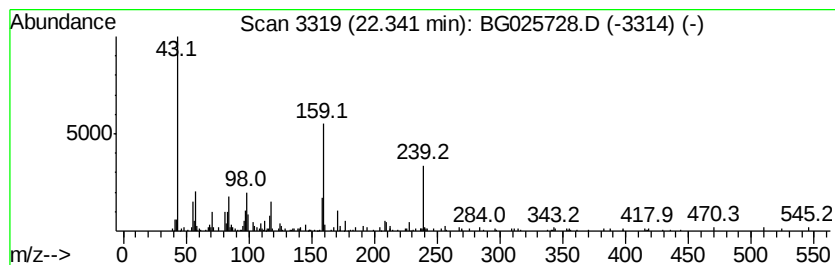
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	2.14 ng/ul	206083	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	33
2		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	33
3		4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	12
4		Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	10
5		1,2-Propanediol, 3-[[2-(acetylox...	458	C25H46O7	056599-36-1	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNS1

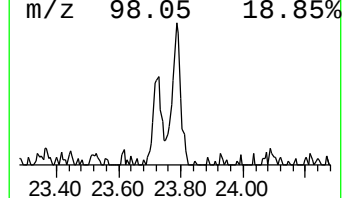
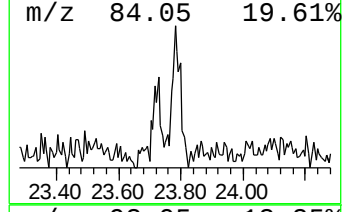
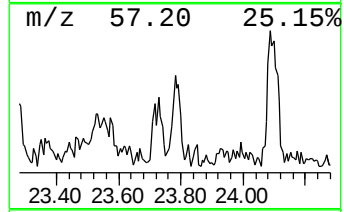
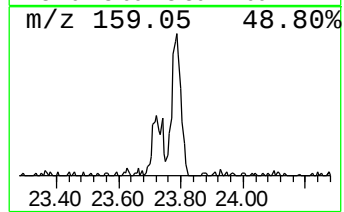
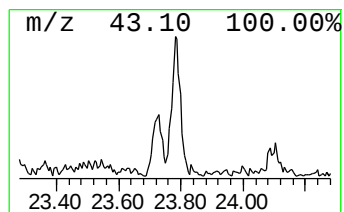
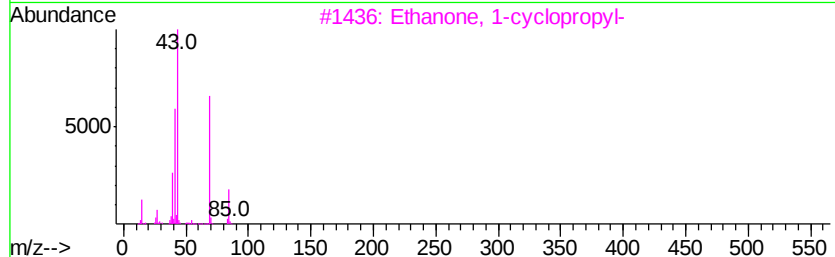
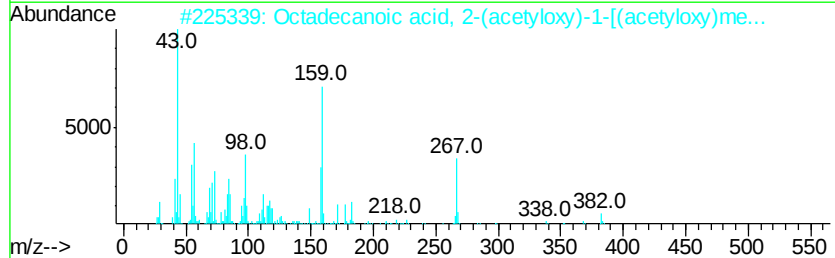
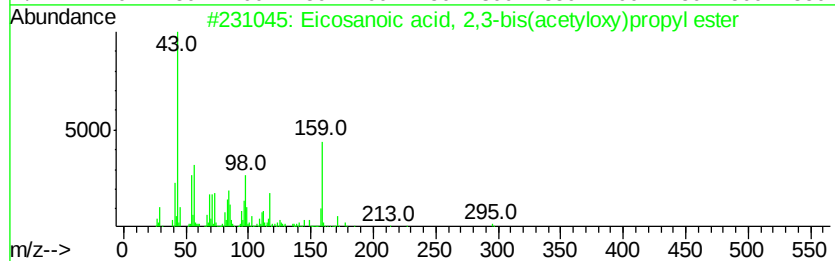
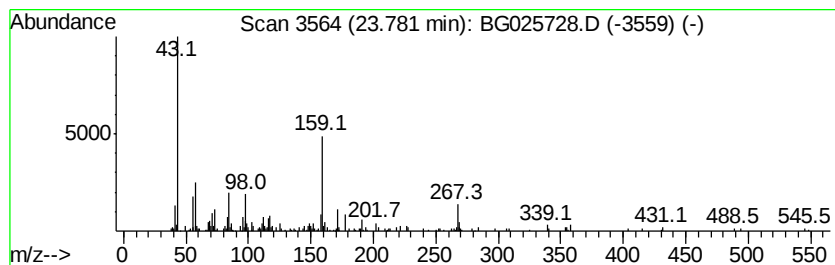
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.78	2.67 ng/ul	249286	Perylene-d12	25.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	25
2		Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	10
3		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	9
4		Ethanethioic acid, S-(1-ethylbut...	160	C8H16OS	055590-84-6	9
5		Ketone, methyl 2,2,3-trimethylcy...	154	C10H18O	017983-22-1	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG013117\
Data File : BG025728.D
Acq On : 31 Jan 2017 22:25
Operator : SJ/MA
Sample : I1460-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNS1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG011817.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
Tridecanoic acid	18.38	2.6	ng/ul	177563	4	17.54	1367530	20.0
Lauric anhydride	20.18	4.8	ng/ul	462432	5	21.83	1927610	20.0
unknown-01	20.22	8.1	ng/ul	784274	5	21.83	1927610	20.0
Myristin, 2,3-dia...	21.17	2.5	ng/ul	236271	5	21.83	1927610	20.0
unknown-02	21.21	4.0	ng/ul	387945	5	21.83	1927610	20.0
(DEL) Alkane: Cyc...	21.41	2.0	ng/ul	193568	5	21.83	1927610	20.0
unknown-03	22.34	2.1	ng/ul	206083	5	21.83	1927610	20.0
unknown-04	23.78	2.7	ng/ul	249286	6	25.21	1870020	20.0