

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
 Data File : BG024279.D
 Acq On : 12 Oct 2016 00:05
 Operator : UM/SJ
 Sample : H5113-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BDP54

Integration Parameters: LSCINT.P

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

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

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

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.642	135	137	146	rVB4	32473	38548	0.86%	0.066%
2	4.142	220	222	231	rBV7	11540	23284	0.52%	0.040%
3	4.342	254	256	261	rVB4	12903	17846	0.40%	0.031%
4	4.418	264	269	273	rVV7	22639	31345	0.70%	0.054%
5	4.712	316	319	321	rBV4	12504	16677	0.37%	0.029%
6	5.029	366	373	375	rBV8	14027	18092	0.40%	0.031%
7	5.399	433	436	439	rBV5	12619	16922	0.38%	0.029%
8	5.905	514	522	528	rBV10	21685	64332	1.43%	0.111%
9	6.269	583	584	590	rVB5	16570	22540	0.50%	0.039%
10	6.322	590	593	595	rBV4	11794	17633	0.39%	0.030%
11	6.850	681	683	686	rVB4	17417	17616	0.39%	0.030%
12	6.886	686	689	691	rBV4	11789	15988	0.36%	0.028%
13	7.209	740	744	751	rVB6	11405	26901	0.60%	0.046%
14	7.356	766	769	771	rBV3	14871	16831	0.38%	0.029%
15	7.415	772	779	791	rVB	690442	1299702	28.96%	2.239%
16	7.603	804	811	822	rBV	485712	885637	19.73%	1.526%
17	7.814	839	847	856	rBV2	663282	1163928	25.93%	2.005%
18	8.290	921	928	939	rVB	689920	1195283	26.63%	2.059%
19	8.660	989	991	998	rVV6	9202	21121	0.47%	0.036%
20	8.736	1003	1004	1011	rBV7	9310	19701	0.44%	0.034%
21	8.977	1037	1045	1056	rVB	807221	1448776	32.28%	2.496%
22	9.465	1118	1128	1135	rBV	666865	1253524	27.93%	2.159%
23	10.188	1243	1251	1263	rVB	567279	1058258	23.58%	1.823%
24	10.722	1333	1342	1353	rBV	825117	1524021	33.96%	2.625%
25	11.122	1401	1410	1421	rBV	873189	1655871	36.90%	2.852%
26	11.251	1424	1432	1442	rBV2	339359	643249	14.33%	1.108%
27	12.685	1667	1676	1683	rVB6	28530	60457	1.35%	0.104%
28	12.826	1695	1700	1705	rBV5	8732	16515	0.37%	0.028%
29	12.937	1711	1719	1721	rVB8	9621	15763	0.35%	0.027%
30	13.255	1771	1773	1780	rBV7	11601	22376	0.50%	0.039%
31	13.507	1812	1816	1819	rVB5	21193	24648	0.55%	0.042%
32	13.572	1824	1827	1832	rBV6	10560	16103	0.36%	0.028%
33	13.772	1857	1861	1868	rBV7	31620	63906	1.42%	0.110%
34	14.107	1912	1918	1922	rVB9	13886	25560	0.57%	0.044%

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35	14.177	1927	1930	1934	rVB4	12481	18929	0.42%	0.033%
36	14.301	1943	1951	1955	rVV	1505764	2303423	51.32%	3.968%
37	14.348	1955	1959	1970	rVV	1262559	1874182	41.76%	3.228%
38	14.465	1977	1979	1985	rVB6	8356	16357	0.36%	0.028%
39	14.600	1992	2002	2010	rBV	1576510	2603161	58.00%	4.484%
40	14.759	2025	2029	2035	rVB5	33463	56038	1.25%	0.097%
41	14.823	2035	2040	2045	rBV8	7753	17652	0.39%	0.030%
42	14.906	2045	2054	2063	rBV	1427282	2234947	49.80%	3.850%
43	15.064	2072	2081	2091	rBV	783781	1258732	28.05%	2.168%
44	15.200	2101	2104	2109	rBV6	14178	27968	0.62%	0.048%
45	15.270	2111	2116	2120	rVB8	25036	40895	0.91%	0.070%
46	15.323	2120	2125	2129	rVV8	12806	27362	0.61%	0.047%
47	15.376	2129	2134	2141	rVB8	17853	34549	0.77%	0.060%
48	15.446	2143	2146	2153	rBV7	11145	23101	0.51%	0.040%
49	15.534	2158	2161	2166	rVB6	13261	26231	0.58%	0.045%
50	15.581	2166	2169	2172	rBV5	12041	21180	0.47%	0.036%
51	15.623	2172	2176	2179	rVV6	11993	19636	0.44%	0.034%
52	15.670	2179	2184	2185	rVV5	15291	21463	0.48%	0.037%
53	15.705	2185	2190	2196	rVB	101204	146194	3.26%	0.252%
54	15.769	2197	2201	2206	rVV8	11053	20870	0.47%	0.036%
55	15.893	2215	2222	2232	rBV	2181976	3390764	75.55%	5.841%
56	15.993	2232	2239	2249	rVB	678161	1053134	23.47%	1.814%
57	16.122	2253	2261	2270	rVB8	40940	121660	2.71%	0.210%
58	16.210	2273	2276	2281	rVB6	23074	37221	0.83%	0.064%
59	16.275	2281	2287	2290	rBV6	23999	52328	1.17%	0.090%
60	16.328	2293	2296	2302	rVB6	18323	20428	0.46%	0.035%
61	16.463	2316	2319	2322	rBV4	14126	16055	0.36%	0.028%
62	16.569	2332	2337	2346	rVB3	126005	243341	5.42%	0.419%
63	16.639	2346	2349	2351	rBV4	15278	18093	0.40%	0.031%
64	16.745	2364	2367	2373	rBV8	14709	31071	0.69%	0.054%
65	16.909	2392	2395	2399	rBV6	24402	33223	0.74%	0.057%
66	16.997	2408	2410	2419	rVV9	18213	39417	0.88%	0.068%
67	17.068	2419	2422	2429	rVB7	23157	38380	0.86%	0.066%
68	17.138	2431	2434	2438	rBV6	13864	21045	0.47%	0.036%
69	17.362	2467	2472	2477	rBV3	87557	133505	2.97%	0.230%
70	17.409	2477	2480	2488	rVB9	27159	59888	1.33%	0.103%
71	17.644	2512	2520	2528	rBV2	1679067	2745435	61.17%	4.729%

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72	17.744	2530	2537	2550	rVB	2375324	3725944	83.02%	6.418%
73	17.885	2557	2561	2564	rBV3	40247	51490	1.15%	0.089%
74	17.932	2566	2569	2575	rVB	98722	121130	2.70%	0.209%
75	17.984	2575	2578	2582	rBV6	28337	40158	0.89%	0.069%
76	18.102	2593	2598	2601	rBV6	38293	45880	1.02%	0.079%
77	18.366	2640	2643	2655	rBV6	26266	61640	1.37%	0.106%
78	18.490	2658	2664	2675	rBV	461590	715444	15.94%	1.232%
79	18.578	2677	2679	2687	rVB9	18780	21731	0.48%	0.037%
80	18.819	2718	2720	2723	rVB3	19408	16146	0.36%	0.028%
81	18.919	2734	2737	2740	rVB5	20841	23612	0.53%	0.041%
82	19.189	2778	2783	2786	rBV2	69647	77028	1.72%	0.133%
83	19.230	2786	2790	2795	rVB	150746	173111	3.86%	0.298%
84	19.641	2856	2860	2868	rVB4	67294	144811	3.23%	0.249%
85	19.747	2874	2878	2885	rBV	295726	401399	8.94%	0.691%
86	19.900	2902	2904	2910	rVB5	41362	55811	1.24%	0.096%
87	20.012	2916	2923	2931	rVB	2924164	4488057	100.00%	7.731%
88	20.294	2967	2971	2974	rBV	704635	810566	18.06%	1.396%
89	20.335	2974	2978	2983	rVB	1475013	1687370	37.60%	2.907%
90	21.304	3138	3143	3146	rBV	278535	364109	8.11%	0.627%
91	21.345	3146	3150	3156	rVB	548327	743751	16.57%	1.281%
92	21.533	3177	3182	3194	rVB	461398	773682	17.24%	1.333%
93	21.945	3245	3252	3260	rVB	1825805	3268333	72.82%	5.630%
94	22.462	3336	3340	3344	rBV4	125662	195791	4.36%	0.337%
95	22.514	3344	3349	3354	rVB2	214847	350738	7.81%	0.604%
96	23.713	3547	3553	3559	rVB4	144132	308847	6.88%	0.532%
97	23.960	3592	3595	3600	rVB5	74852	107231	2.39%	0.185%
98	24.024	3601	3606	3613	rVB4	192894	384257	8.56%	0.662%
99	25.153	3787	3798	3813	rVB2	1308265	4002940	89.19%	6.895%
100	25.388	3828	3838	3852	rVB3	1071021	3284435	73.18%	5.658%

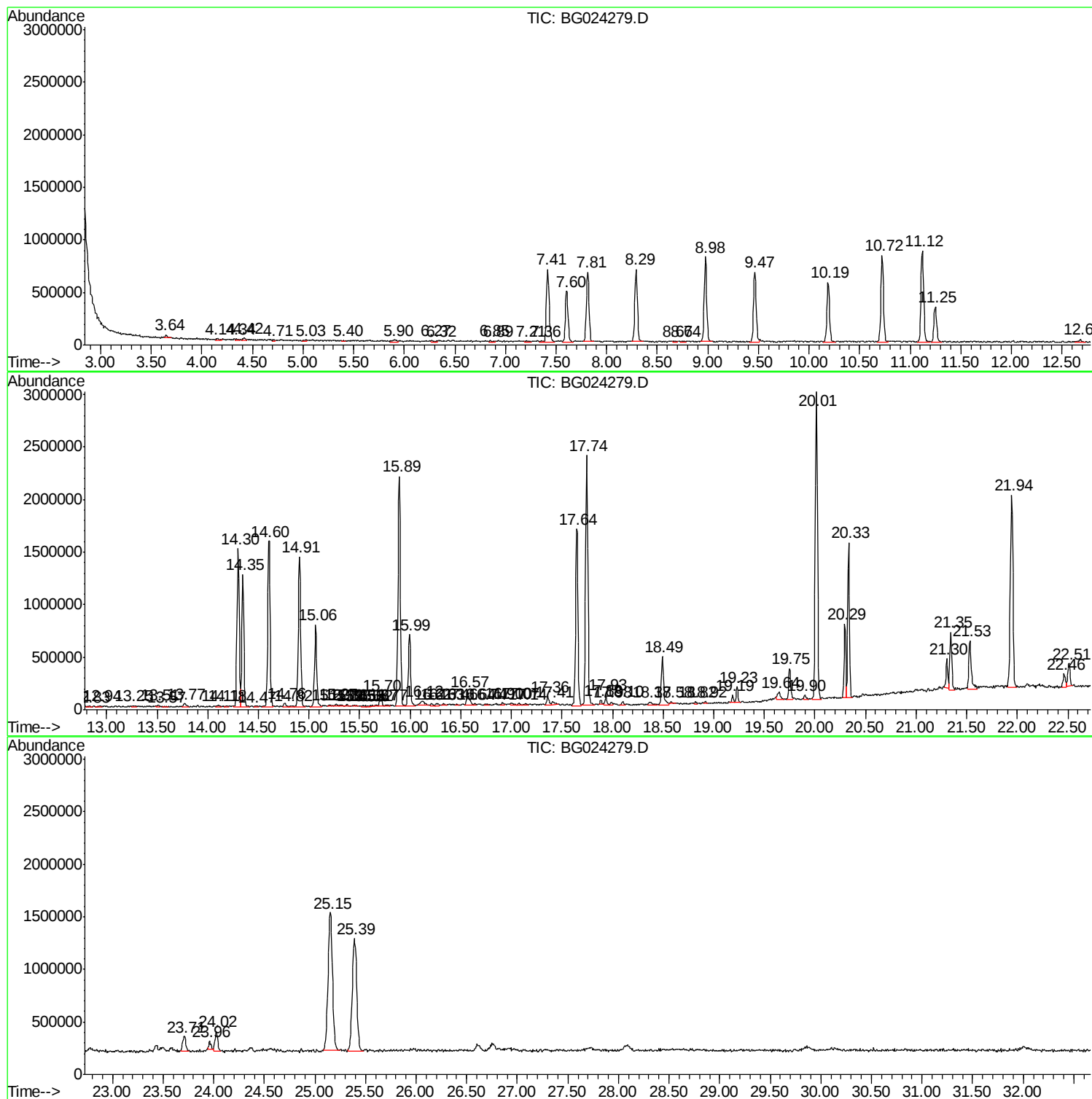
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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



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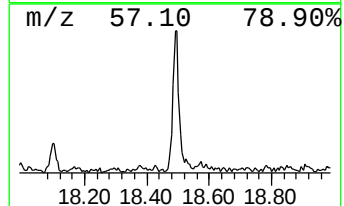
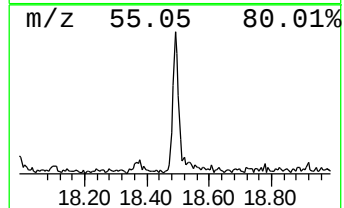
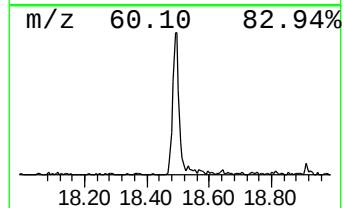
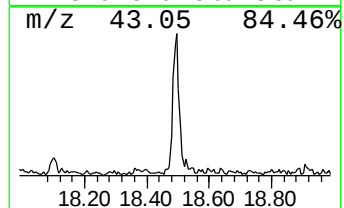
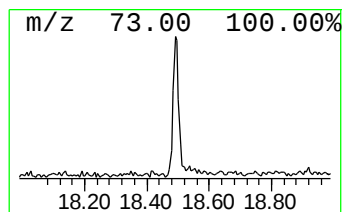
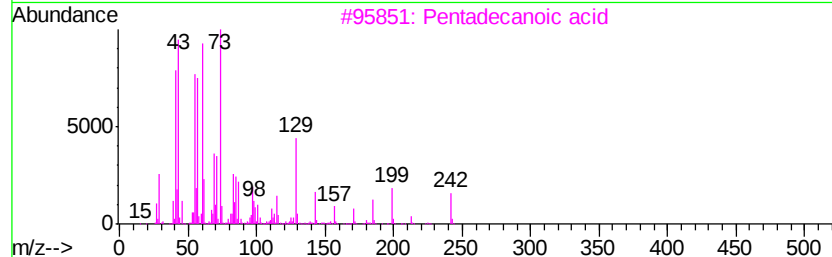
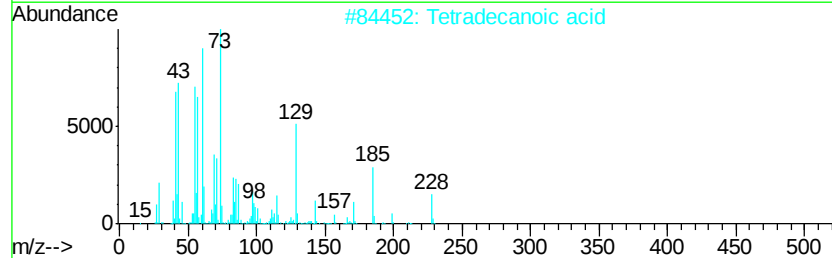
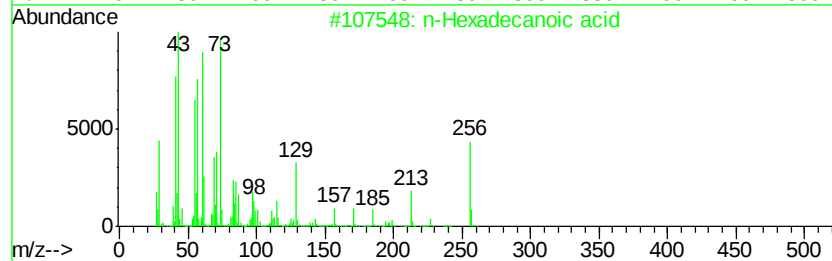
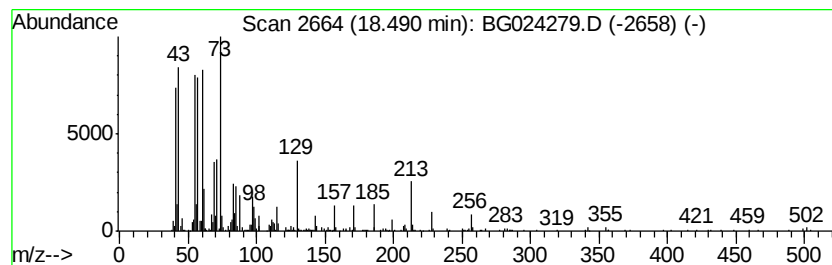
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	5.21 ng/ul	715444	Phenanthrene-d10	17.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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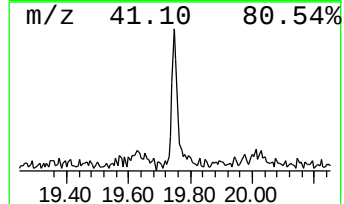
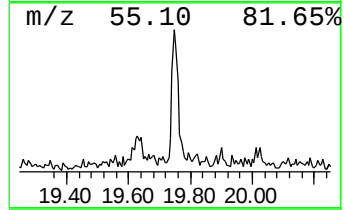
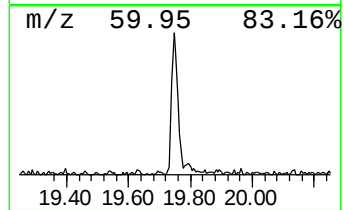
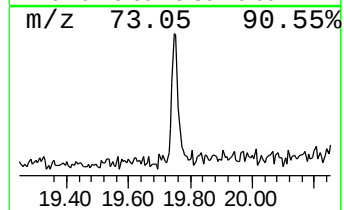
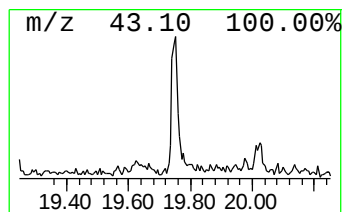
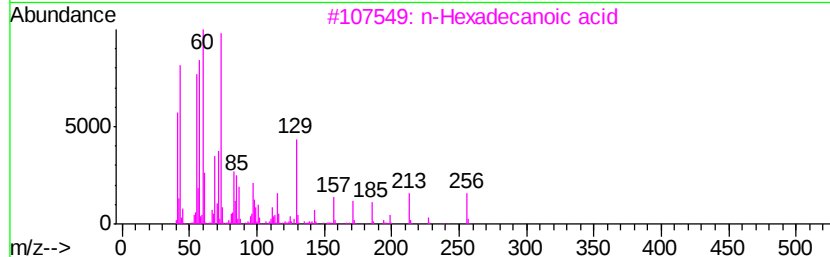
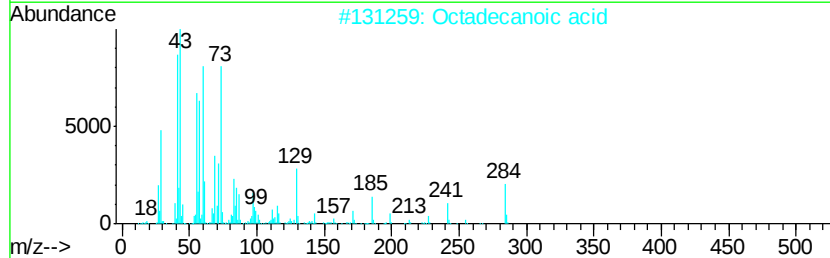
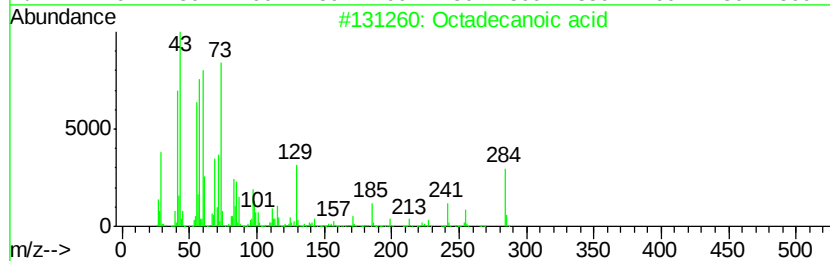
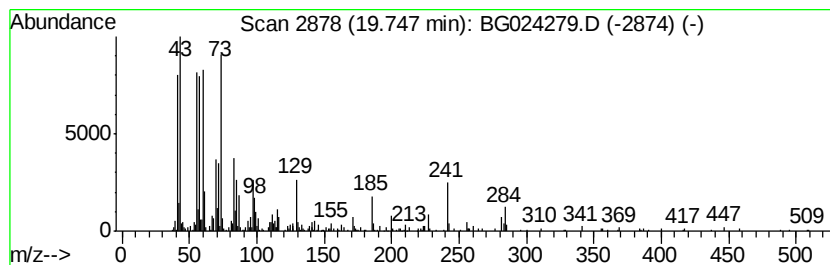
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	2.92 ng/ul	401399	Phenanthrene-d10	17.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Octadecanoic acid	284	C18H36O2	000057-11-4	95
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	89



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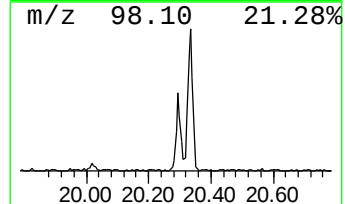
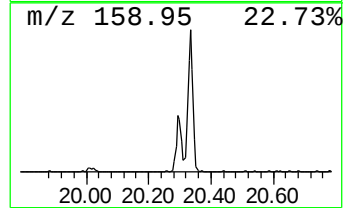
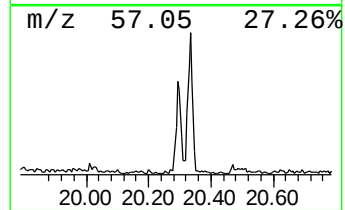
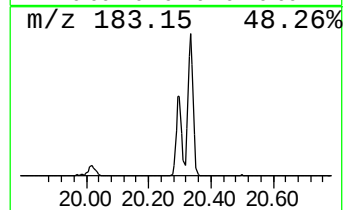
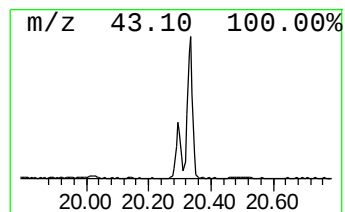
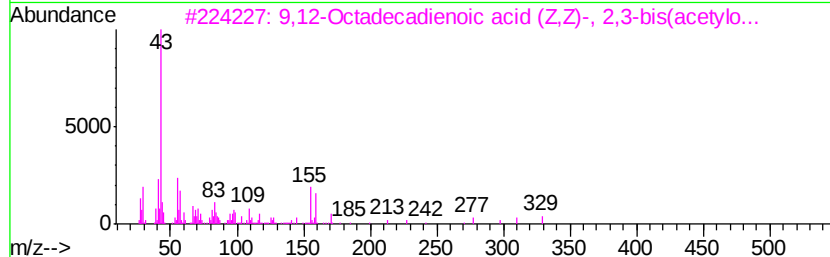
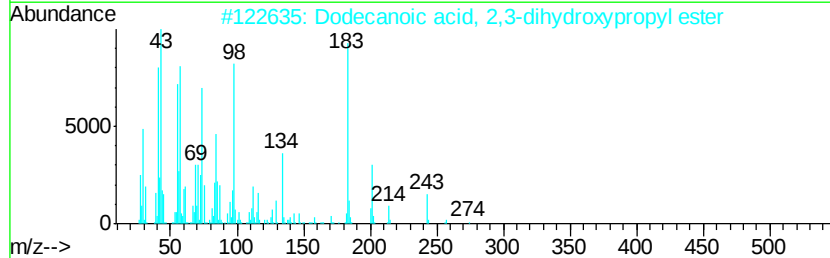
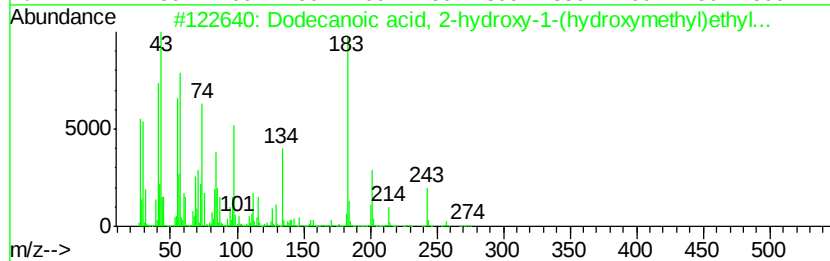
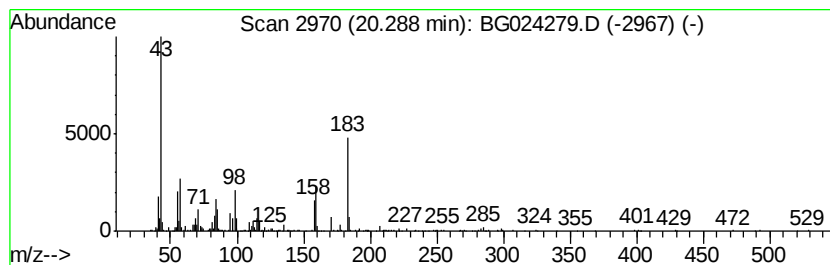
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Peak Number 3 Dodecanoic acid, 2-hydroxy-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	4.96 ng/ul	810566	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	53
2		Dodecanoic acid, 2,3-dihydroxypropyl ester	274	C15H30O4	000142-18-7	38
3		9,12-Octadecadienoic acid (Z,Z)-, 2,3-bis(acetyloxy)propyl ester	438	C25H42O6	055320-04-2	12
4		Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	10
5		Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDP54

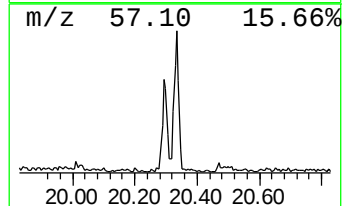
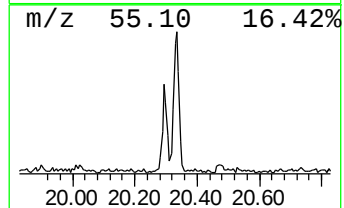
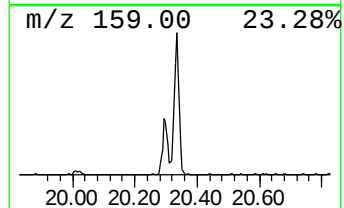
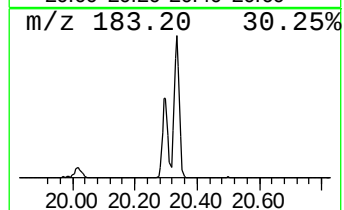
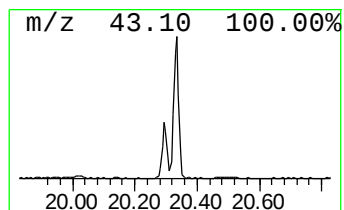
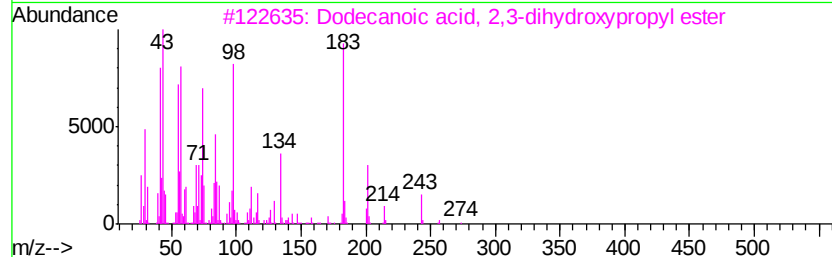
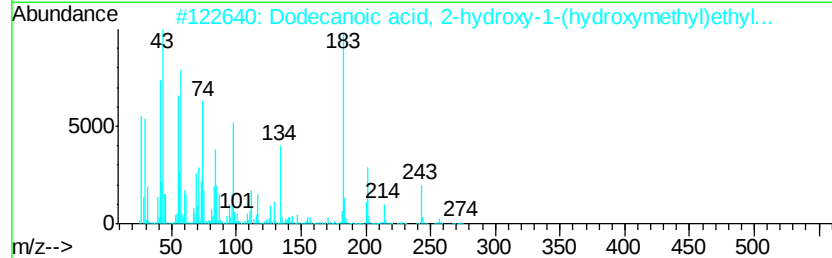
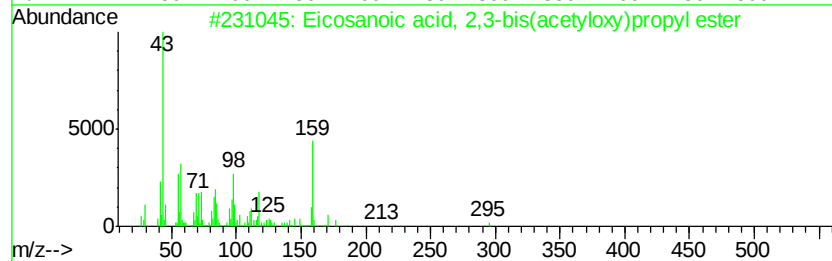
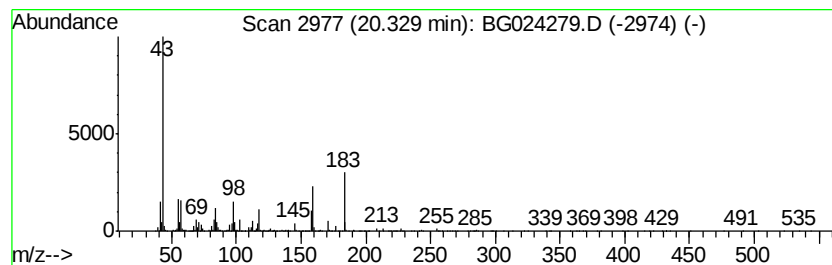
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.33	10.33 ng/ul	1687370	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	32
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	32
3		Dodecanoic acid, 2,3-dihydroxyp...	274	C15H30O4	000142-18-7	16
4		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12
5		9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDP54

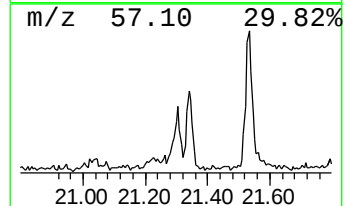
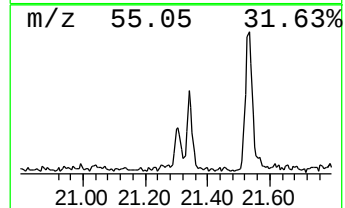
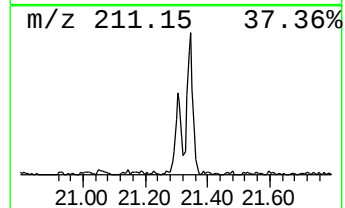
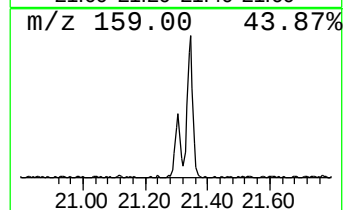
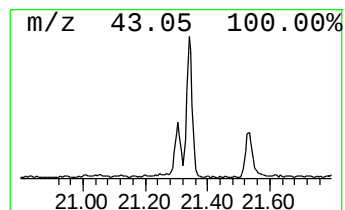
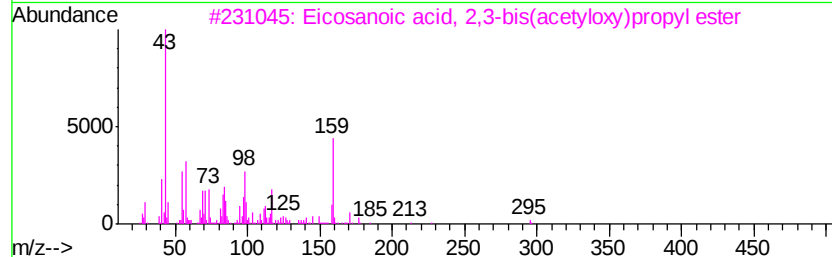
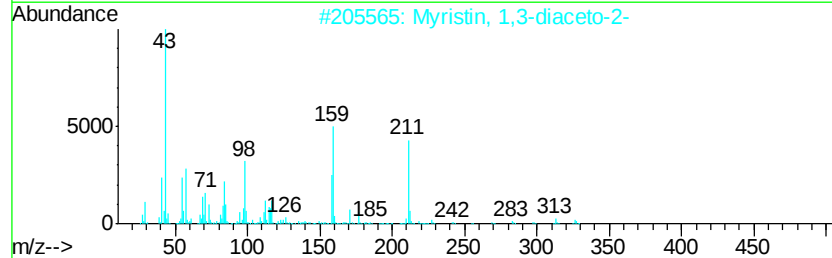
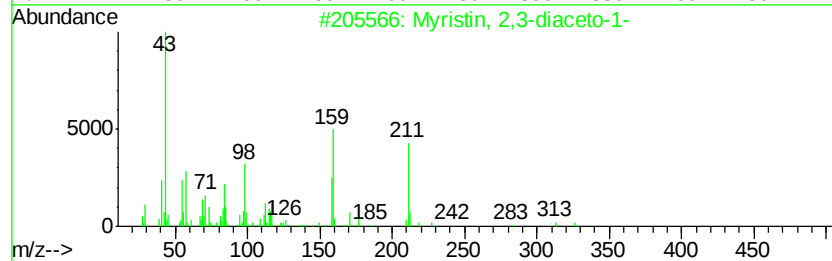
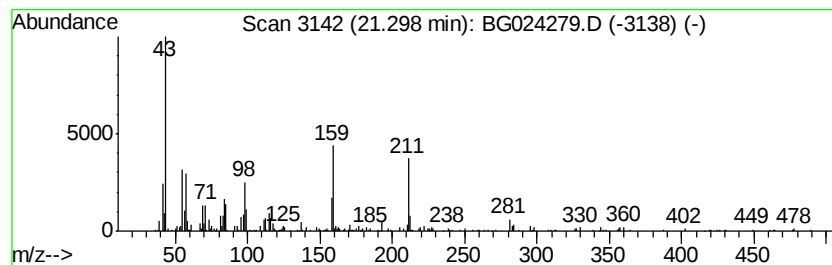
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.23 ng/ul	364109	Chrysene-d12	21.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	90	
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	78	
3	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	38	
4	Tetradecanoic acid, 2-hydroxy-1-...	302	C17H34O4	003443-83-2	27	
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	25	



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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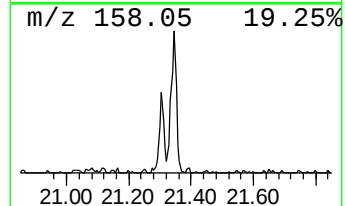
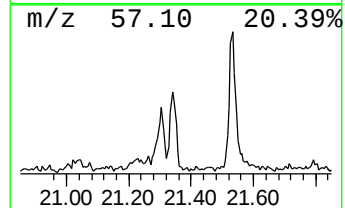
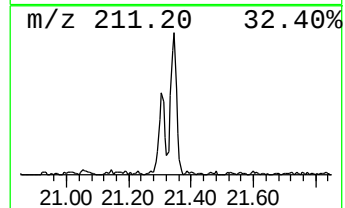
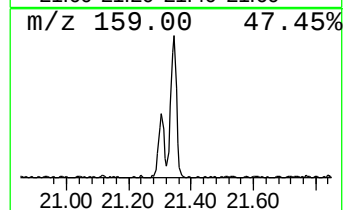
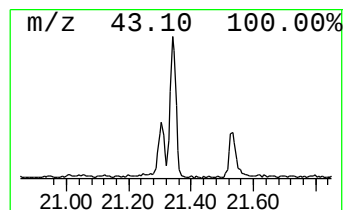
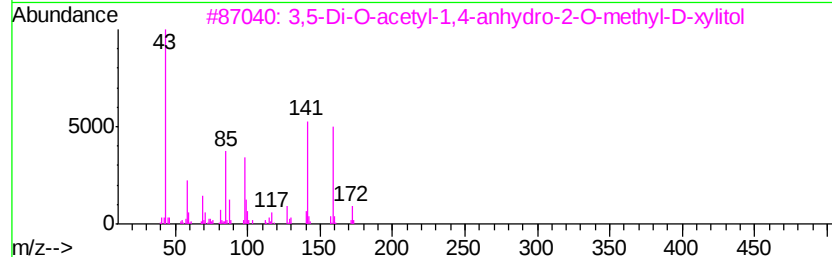
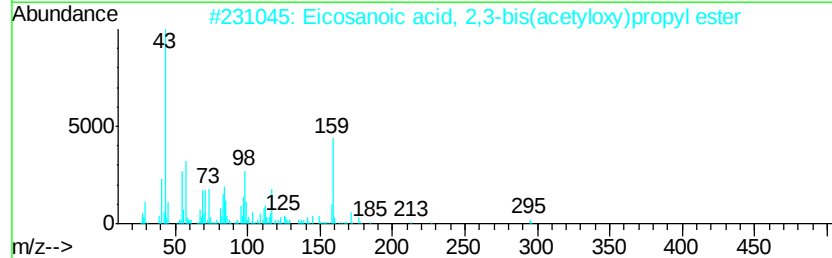
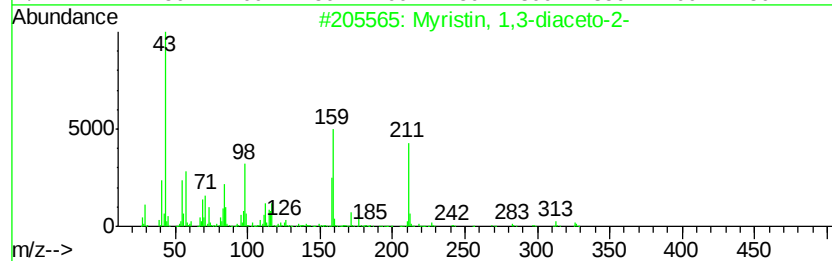
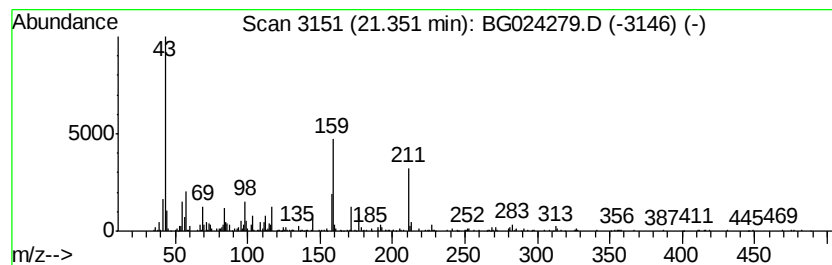
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	4.55 ng/ul	743751	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	27
2		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	16
3		3,5-Di-O-acetyl-1,4-anhydro-2-O-...	232	C10H16O6	1000366-02-8	13
4		Tetradecanoic acid, 2-hydroxyeth...	272	C16H32O3	022122-18-5	12
5		Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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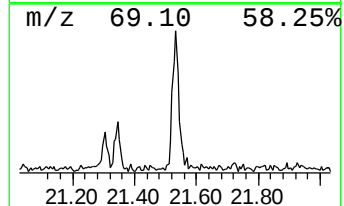
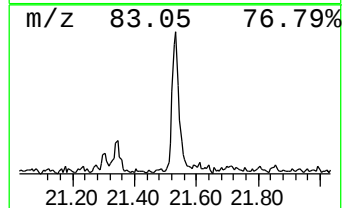
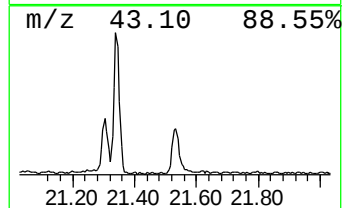
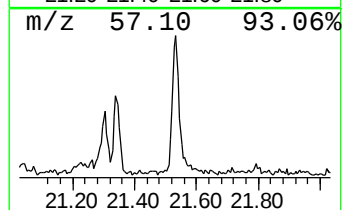
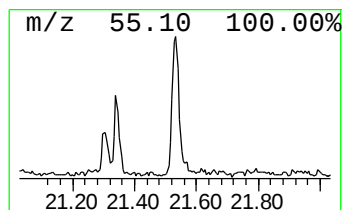
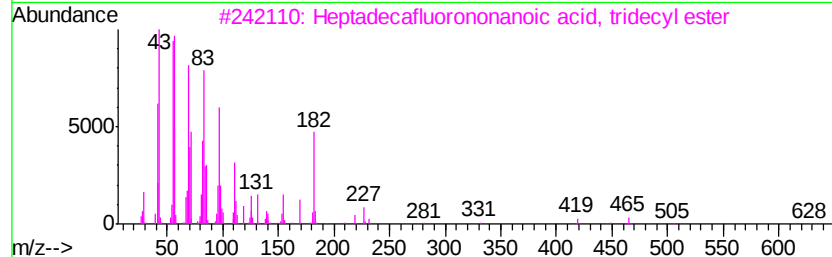
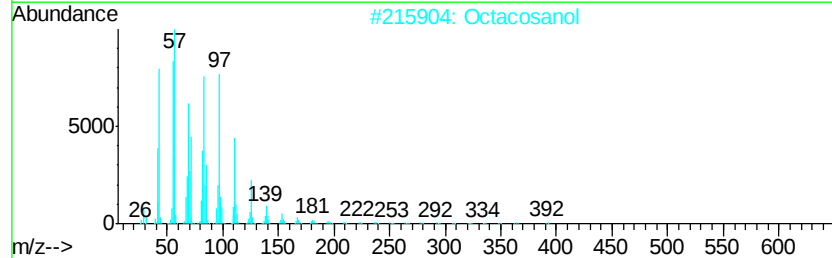
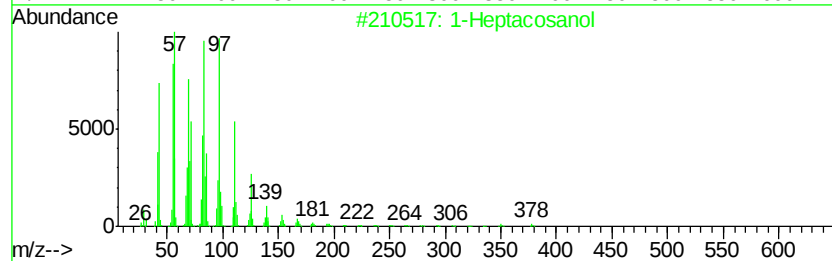
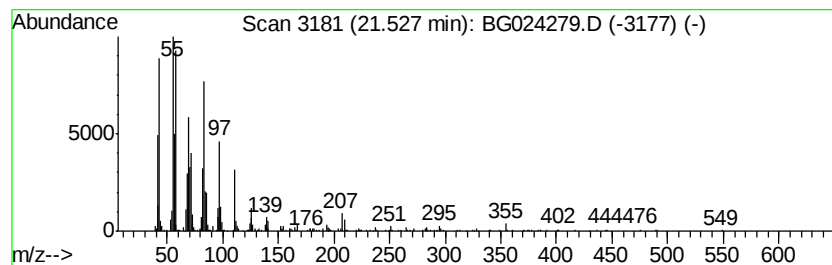
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.53	4.73 ng/ul	773682	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	91
2		Octacosanol	410	C28H58O	000557-61-9	91
3		Heptadecafluorononanoic acid, tr...	646	C22H27F17O2	1000356-02-9	90
4		17-Pentatriacontene	491	C35H70	006971-40-0	89
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	87



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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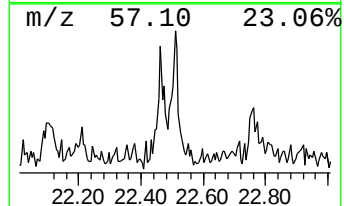
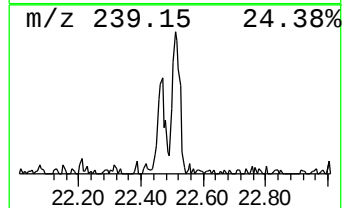
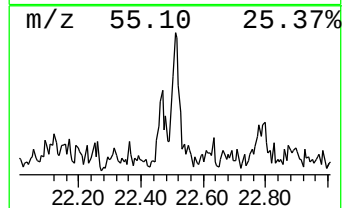
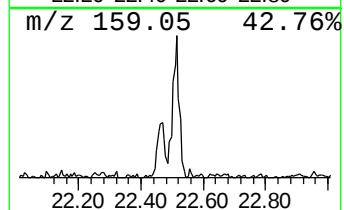
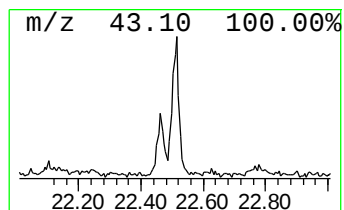
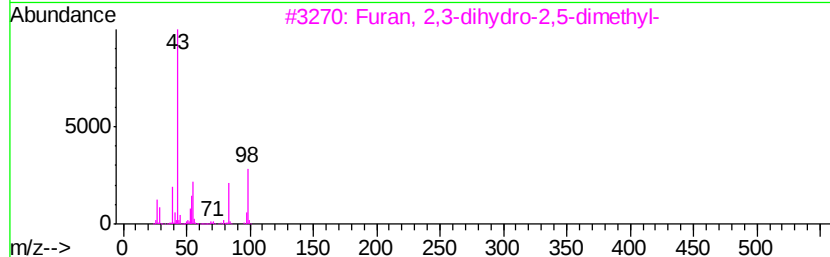
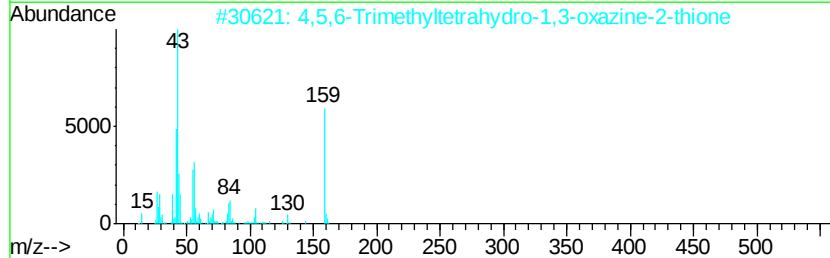
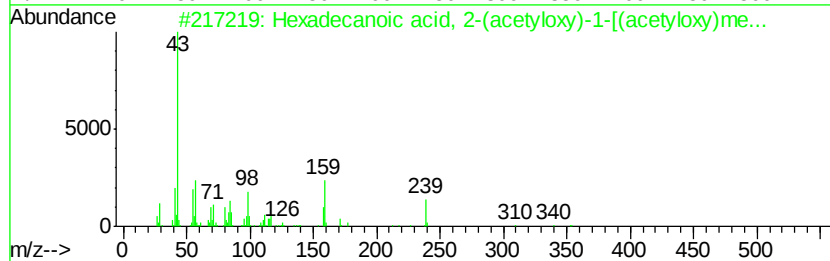
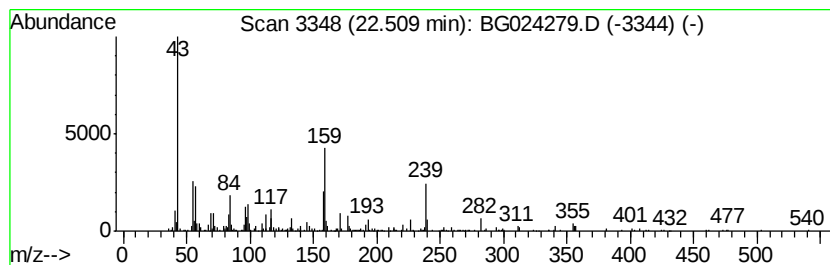
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-03 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	2.15 ng/ul	350738	Chrysene-d12	21.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	32
2		4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	12
3		Furan, 2,3-dihydro-2,5-dimethyl-	98	C6H10O	017108-52-0	10
4		2H-Pyran, 3,4-dihydro-6-methyl-	98	C6H10O	016015-11-5	9
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101116\
Data File : BG024279.D
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Operator : UM/SJ
Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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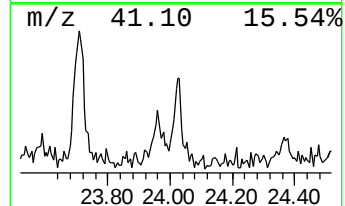
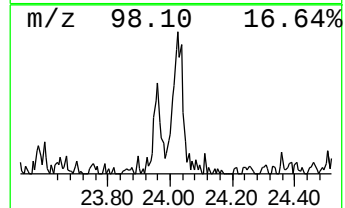
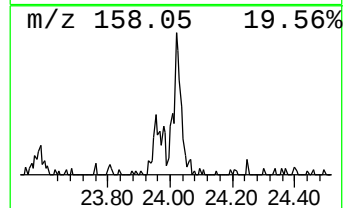
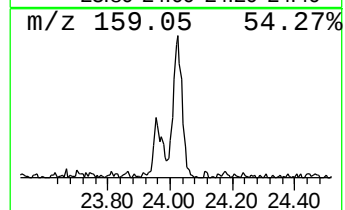
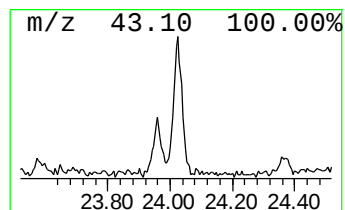
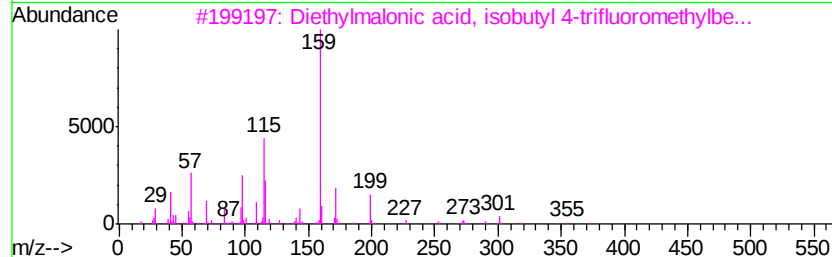
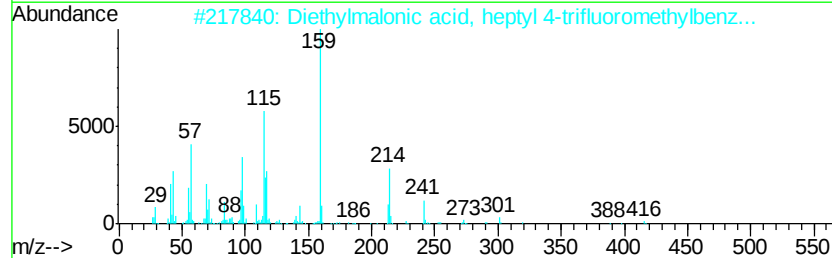
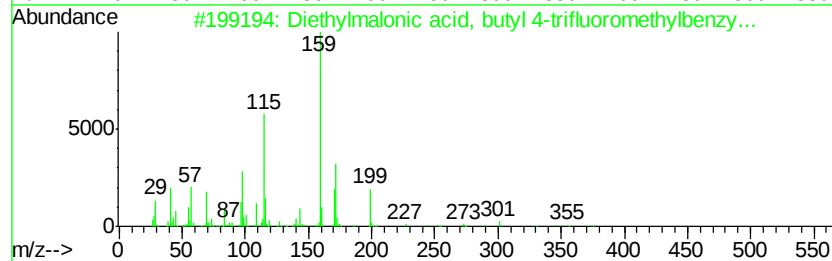
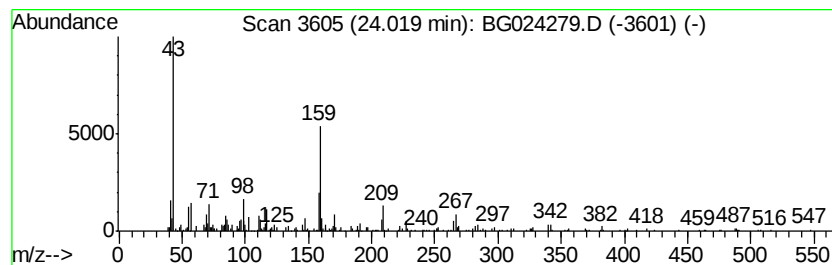
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Diethylmalonic acid, butyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.02	2.34 ng/ul	384257	Perylene-d12	25.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylmalonic acid, butyl 4-tri...	374	C19H25F3O4	1000368-40-2	60
2		Diethylmalonic acid, heptyl 4-tr...	416	C22H31F3O4	1000368-40-5	49
3		Diethylmalonic acid, isobutyl 4-...	374	C19H25F3O4	1000368-40-1	47
4		2H-1,4-Ethanoquinoline, 3,4-dihy...	159	C11H13N	004363-25-1	47
5		2,4-Difluorobenzoic acid, eicosy...	438	C27H44F2O2	1000338-79-8	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101116\
Data File : BG024279.D
Acq On : 12 Oct 2016 00:05
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Sample : H5113-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG0100716.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	18.49	5.2	ng/ul	715444	4	17.64	2745440	20.0
Octadecanoic acid	19.75	2.9	ng/ul	401399	4	17.64	2745440	20.0
Dodecanoic acid, ...	20.29	5.0	ng/ul	810566	5	21.94	3268330	20.0
unknown-01	20.33	10.3	ng/ul	1687370	5	21.94	3268330	20.0
Myristin, 2,3-dia...	21.30	2.2	ng/ul	364109	5	21.94	3268330	20.0
unknown-02	21.35	4.5	ng/ul	743751	5	21.94	3268330	20.0
1-Heptacosanol	21.53	4.7	ng/ul	773682	5	21.94	3268330	20.0
unknown-03	22.51	2.1	ng/ul	350738	5	21.94	3268330	20.0
Diethylmalonic ac...	24.02	2.3	ng/ul	384257	6	25.39	3284440	20.0