

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM040819\
 Data File : BM019825.D
 Acq On : 09 Apr 2019 10:12
 Operator : JU/SJ
 Sample : K2217-12
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BF602

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 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: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032219MA.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	3.122	20	23	33	rVB	40296	65656	2.75%	0.195%
2	3.528	89	92	96	rVB2	8593	11194	0.47%	0.033%
3	3.622	104	108	114	rVV	48663	69310	2.91%	0.206%
4	3.693	117	120	129	rVB5	10483	20675	0.87%	0.061%
5	4.034	175	178	180	rBV4	3506	4254	0.18%	0.013%
6	4.157	196	199	202	rBV3	6383	9865	0.41%	0.029%
7	4.357	231	233	240	rVB5	6477	11504	0.48%	0.034%
8	4.704	288	292	296	rBV3	5812	9840	0.41%	0.029%
9	4.751	298	300	310	rVB4	9870	17674	0.74%	0.053%
10	4.875	316	321	323	rBV4	2820	4164	0.17%	0.012%
11	5.322	394	397	399	rBV3	3557	4439	0.19%	0.013%
12	6.757	635	641	657	rBV	377507	764556	32.06%	2.273%
13	6.916	662	668	686	rBV	341611	602896	25.28%	1.792%
14	7.098	693	699	711	rBV	475925	778995	32.66%	2.316%
15	7.192	714	715	721	rVB3	4238	5087	0.21%	0.015%
16	7.563	771	778	786	rBV	557766	899686	37.72%	2.675%
17	8.286	895	901	915	rBV	294306	594083	24.91%	1.766%
18	8.410	918	922	928	rVB2	15422	27446	1.15%	0.082%
19	8.733	970	977	993	rBV	388653	742225	31.12%	2.207%
20	8.881	997	1002	1007	rVB5	5974	9957	0.42%	0.030%
21	9.045	1026	1030	1037	rVB	22701	31712	1.33%	0.094%
22	9.445	1092	1098	1111	rBV	325274	585421	24.55%	1.740%
23	9.710	1135	1143	1150	rBV4	24457	61777	2.59%	0.184%
24	9.986	1182	1190	1214	rBV	434231	914058	38.33%	2.717%
25	10.339	1244	1250	1261	rBV	696714	1190431	49.92%	3.539%
26	10.516	1273	1280	1294	rBV	271549	640584	26.86%	1.904%
27	10.910	1340	1347	1366	rBV2	17977	75401	3.16%	0.224%
28	11.045	1366	1370	1377	rVB5	2269	5209	0.22%	0.015%
29	11.186	1390	1394	1395	rBV3	5466	7177	0.30%	0.021%
30	11.745	1485	1489	1493	rVB4	5161	8277	0.35%	0.025%
31	11.951	1517	1524	1529	rVV3	7359	10967	0.46%	0.033%
32	12.027	1532	1537	1540	rVB3	3223	5518	0.23%	0.016%
33	12.504	1613	1618	1626	rBV2	30328	59613	2.50%	0.177%
34	12.710	1648	1653	1659	rBV7	3421	6218	0.26%	0.018%

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35	12.933	1687	1691	1694	rBV5	2461	3963	0.17%	0.012%
36	13.016	1699	1705	1710	rBV2	7847	12575	0.53%	0.037%
37	13.186	1731	1734	1737	rBV4	3147	3742	0.16%	0.011%
38	13.445	1776	1778	1781	rBV3	4125	4052	0.17%	0.012%
39	13.604	1801	1805	1806	rBV2	6389	6099	0.26%	0.018%
40	13.645	1806	1812	1817	rVV	1017673	1411088	59.17%	4.195%
41	13.692	1817	1820	1829	rVB	158995	237641	9.96%	0.706%
42	13.921	1852	1859	1869	rBV	1183004	1720510	72.14%	5.115%
43	14.027	1873	1877	1883	rVB6	7448	12841	0.54%	0.038%
44	14.104	1887	1890	1895	rVB4	10097	11847	0.50%	0.035%
45	14.157	1897	1899	1904	rBV4	3102	4442	0.19%	0.013%
46	14.227	1904	1911	1921	rBV2	1006218	1506174	63.15%	4.478%
47	14.510	1953	1959	1980	rBV	159679	496516	20.82%	1.476%
48	14.663	1980	1985	1999	rVV	504802	774635	32.48%	2.303%
49	14.992	2038	2041	2048	rBV7	10668	18960	0.80%	0.056%
50	15.063	2049	2053	2058	rBV5	12463	21755	0.91%	0.065%
51	15.233	2075	2082	2090	rBV	1350809	1989892	83.44%	5.916%
52	15.404	2108	2111	2117	rBV7	14071	24193	1.01%	0.072%
53	15.468	2119	2122	2130	rVB4	22961	34979	1.47%	0.104%
54	15.521	2130	2131	2132	rBV	6983	4763	0.20%	0.014%
55	15.798	2174	2178	2182	rVB6	10581	18128	0.76%	0.054%
56	15.857	2183	2188	2191	rBV5	17313	26574	1.11%	0.079%
57	15.951	2197	2204	2207	rBV4	30226	73340	3.08%	0.218%
58	16.121	2230	2233	2239	rBV4	20741	34400	1.44%	0.102%
59	16.392	2274	2279	2286	rBV2	231327	364368	15.28%	1.083%
60	16.992	2375	2381	2389	rBV	1162606	1651948	69.27%	4.911%
61	17.092	2393	2398	2404	rVB	1526715	2025633	84.94%	6.022%
62	17.274	2425	2429	2432	rBV	135699	154941	6.50%	0.461%
63	17.321	2433	2437	2441	rVB	232504	265696	11.14%	0.790%
64	17.880	2528	2532	2541	rBV	450568	759546	31.85%	2.258%
65	18.639	2659	2661	2665	rVB	156006	156911	6.58%	0.466%
66	19.174	2749	2752	2758	rBV	364780	554847	23.27%	1.649%
67	19.403	2786	2791	2798	rBV	1697391	2384889	100.00%	7.090%
68	19.733	2843	2847	2850	rBV	1009666	1165053	48.85%	3.464%
69	19.768	2850	2853	2859	rVB	1223698	1383753	58.02%	4.114%
70	20.709	3011	3013	3016	rBV	312508	303425	12.72%	0.902%
71	21.103	3077	3080	3084	rVB	1205054	1205907	50.56%	3.585%

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72	21.203	3093	3097	3103	rBV	1746358	2199114	92.21%	6.538%
73	23.415	3469	3473	3482	rVB2	1305503	2352687	98.65%	6.994%

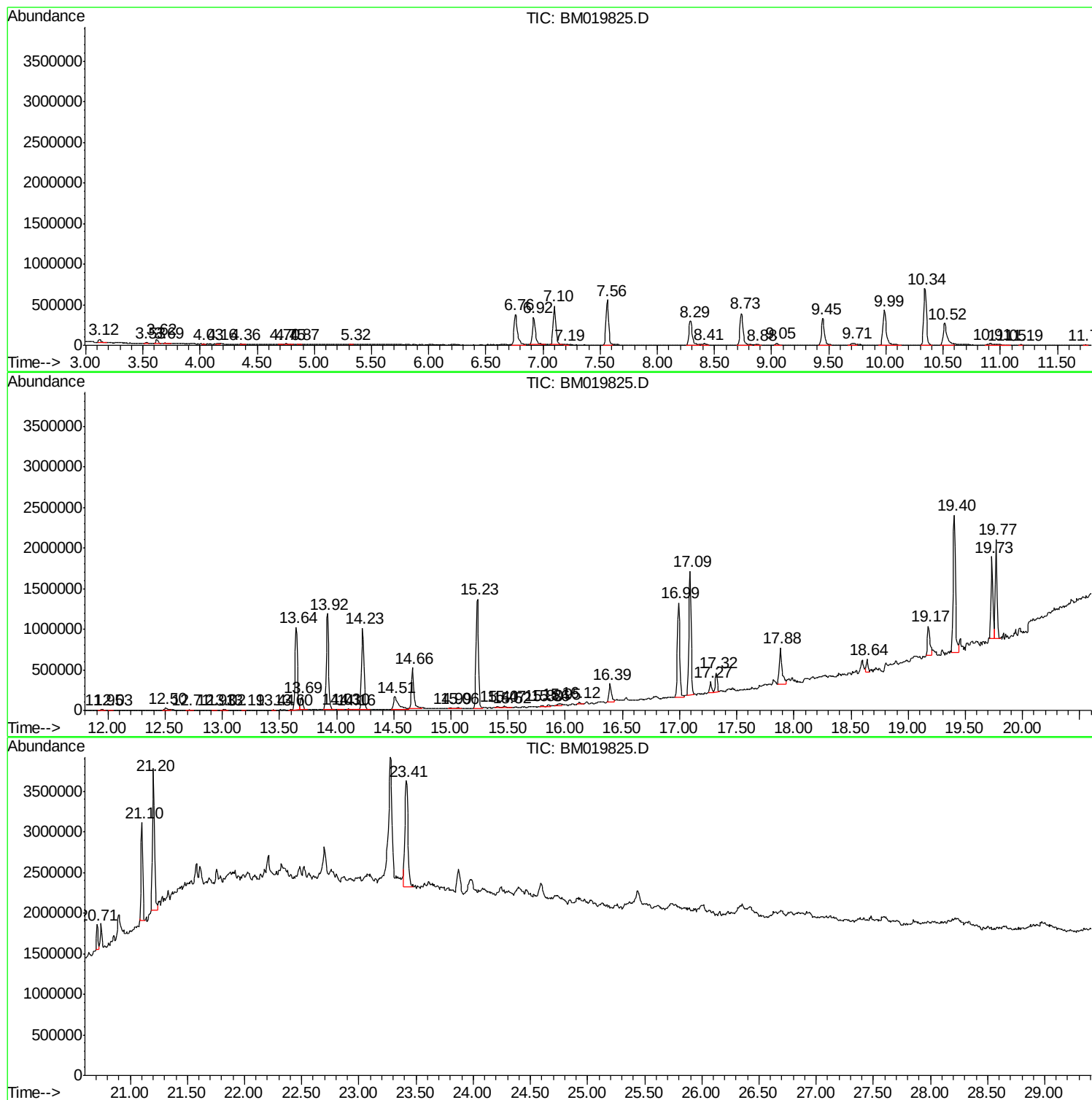
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032219MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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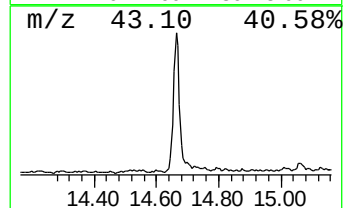
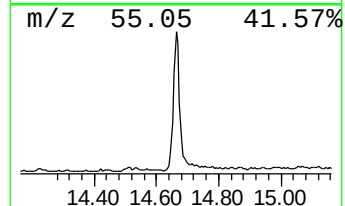
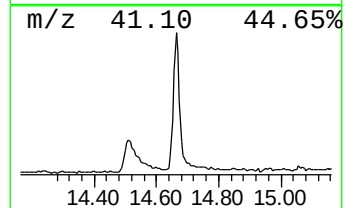
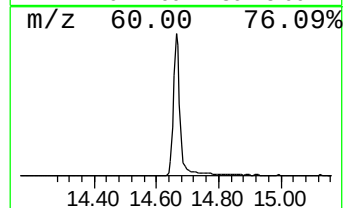
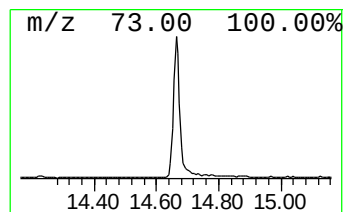
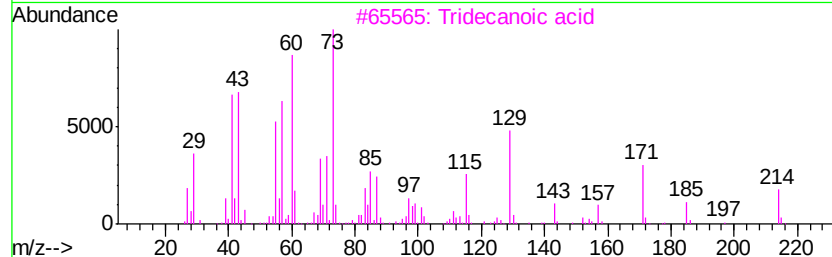
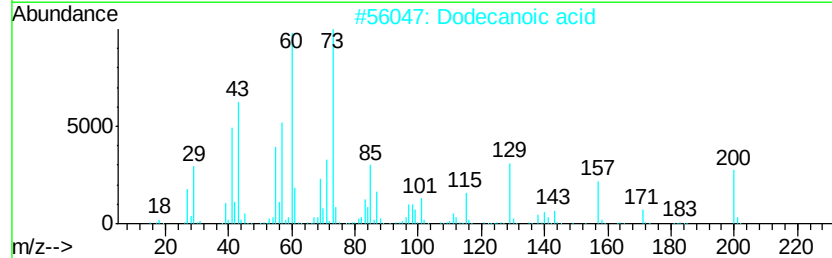
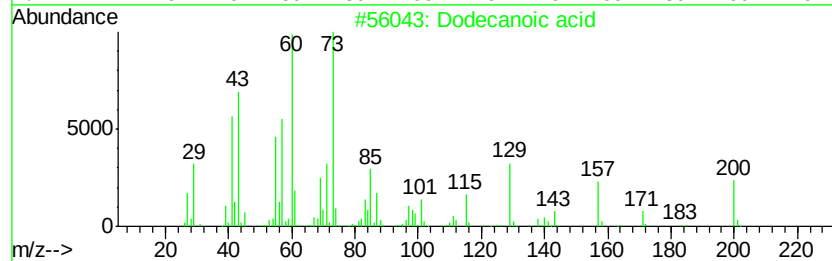
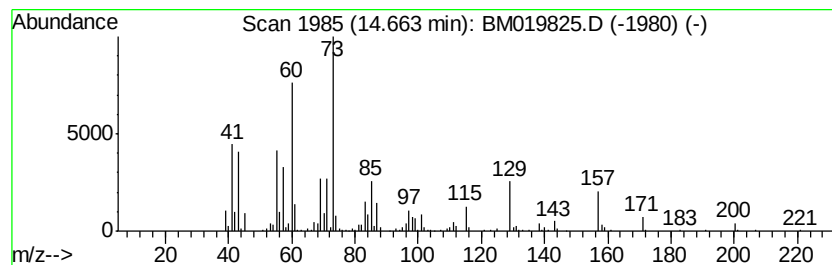
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	10.29 ng/ul	774635	Acenaphthene-d10	14.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid	200 C12H24O2	000143-07-7	94
2	Dodecanoic acid	200 C12H24O2	000143-07-7	93
3	Tridecanoic acid	214 C13H26O2	000638-53-9	83
4	Undecanoic acid	186 C11H22O2	000112-37-8	80
5	Tridecanoic acid	214 C13H26O2	000638-53-9	64



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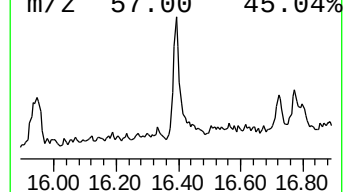
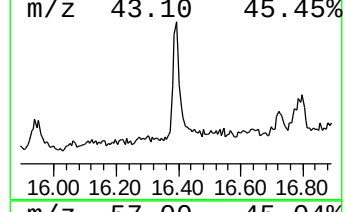
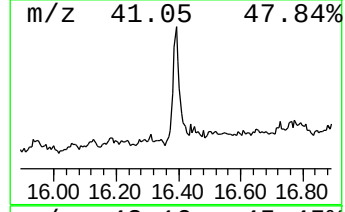
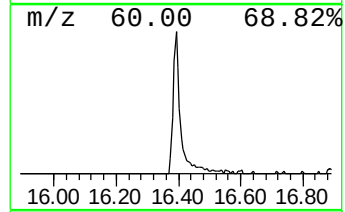
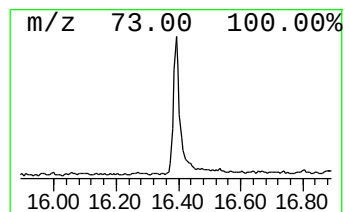
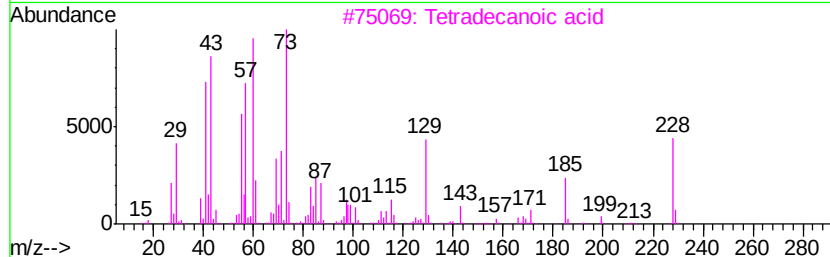
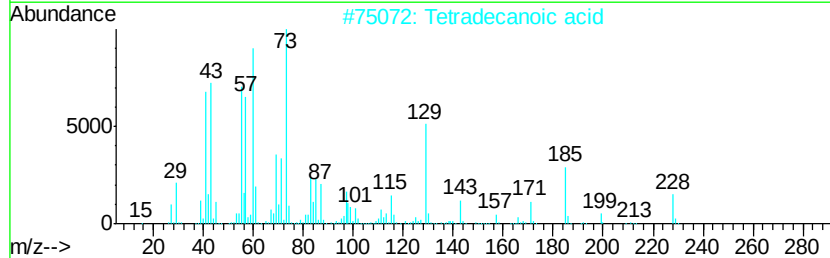
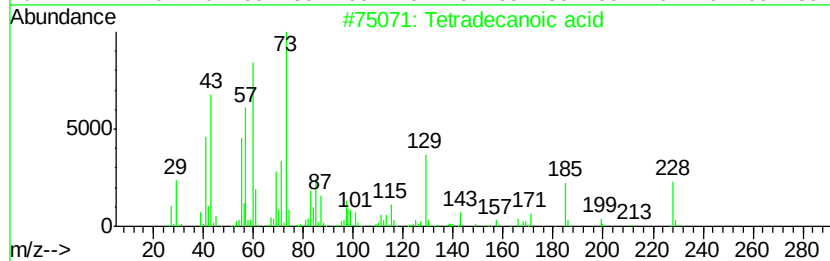
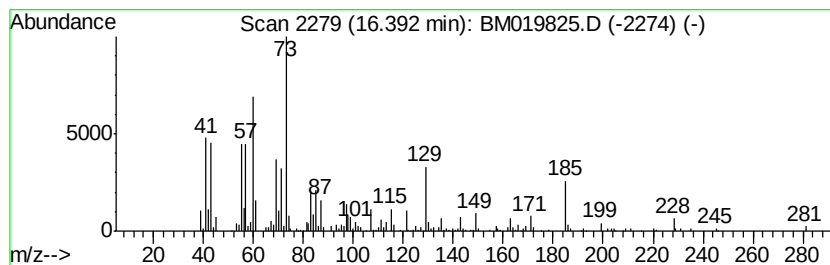
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032219MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.39	4.41 ng/ul	364368	Phenanthrene-d10		16.99		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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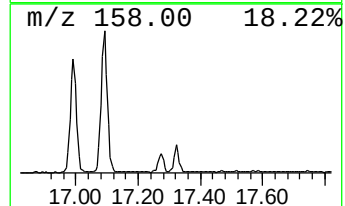
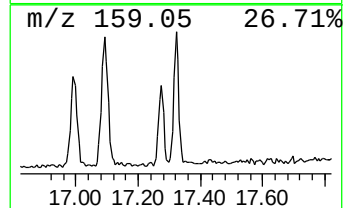
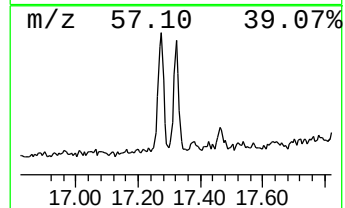
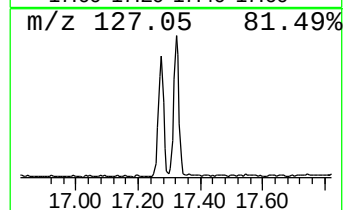
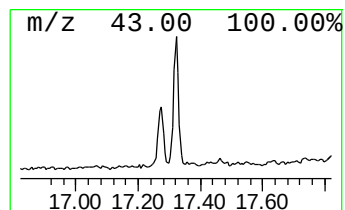
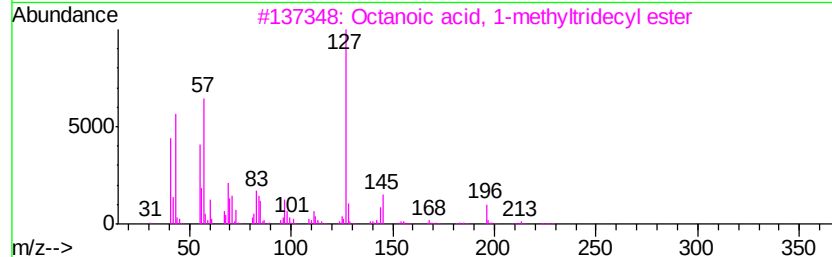
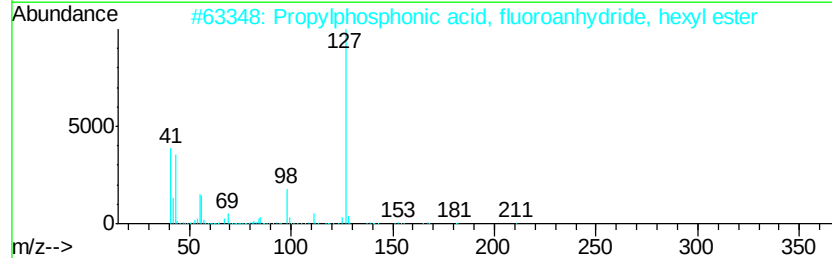
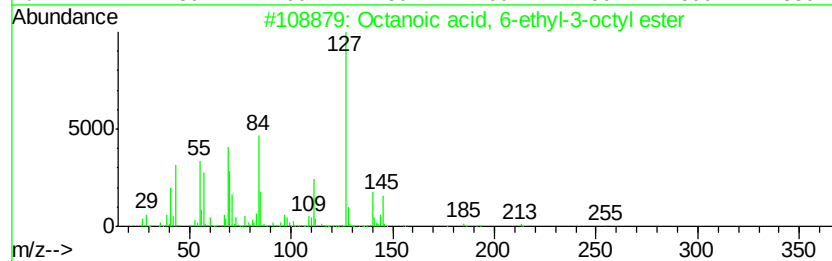
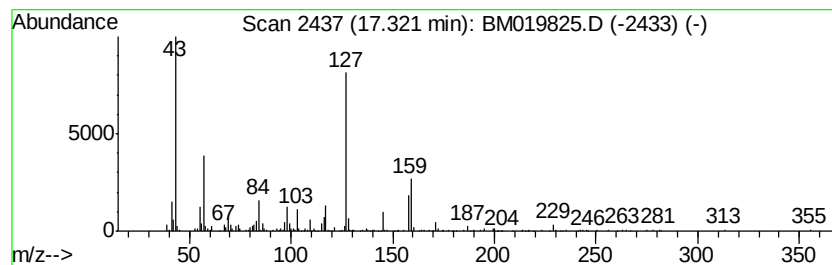
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.32	3.22 ng/ul	265696	Phenanthrene-d10	16.99		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octanoic acid, 6-ethyl-3-octyl e...	284	C18H36O2	1000282-67-8	47
2		Propylphosphonic acid, fluoroanh...	210	C9H20FO2P	333416-18-5	43
3		Octanoic acid, 1-methyltridecyl ...	340	C22H44O2	055193-79-8	38
4		1-(4-Fluoro-benzenesulfonyl)-pip...	286	C12H15FN2O3S	1000295-13-0	38
5		Octanoic acid, cyclobutyl ester	198	C12H22O2	1000282-86-6	37



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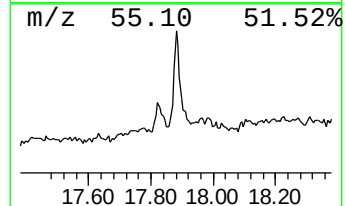
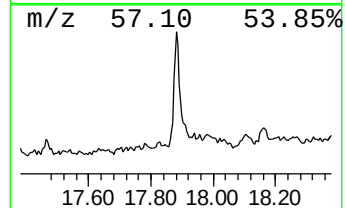
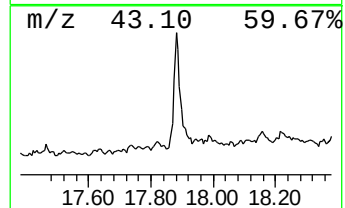
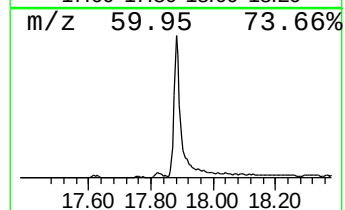
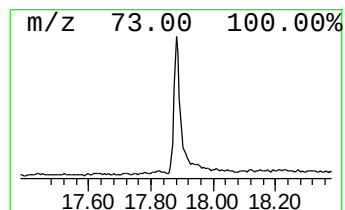
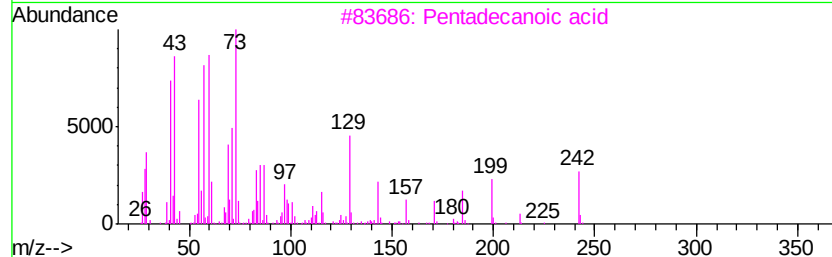
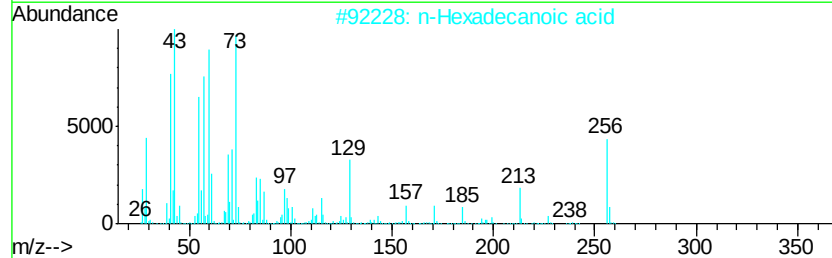
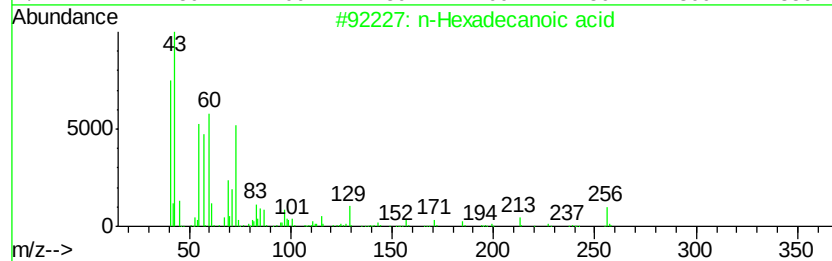
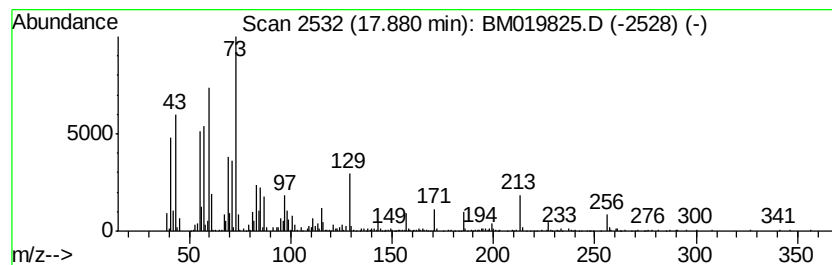
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032219MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	9.20 ng/ul	759546	Phenanthrene-d10	16.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96	
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87	
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87	
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64	



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Data File : BM019825.D
Acq On : 09 Apr 2019 10:12
Operator : JU/SJ
Sample : K2217-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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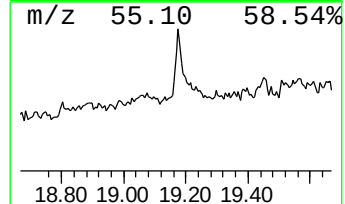
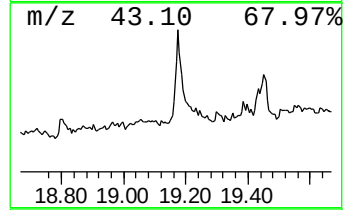
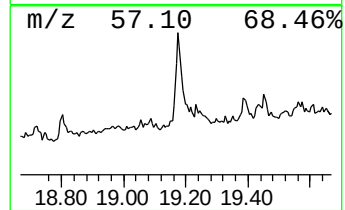
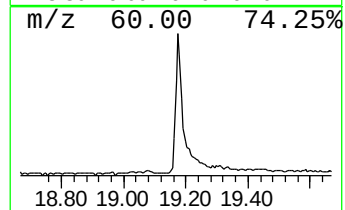
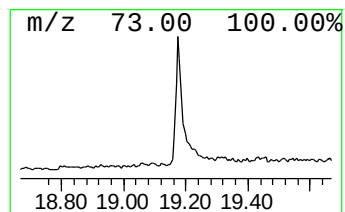
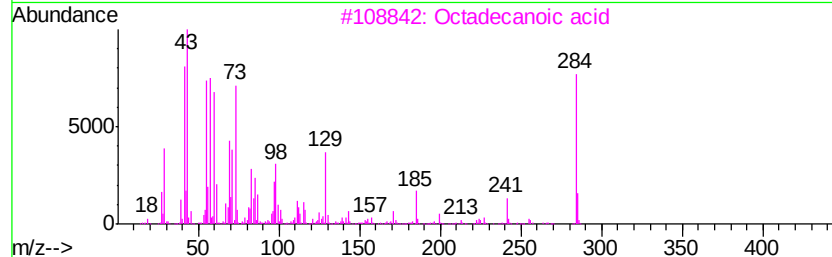
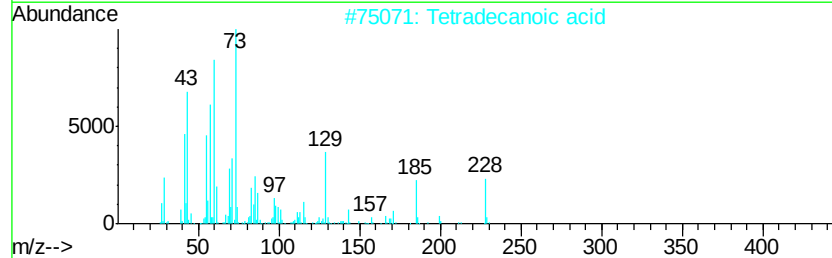
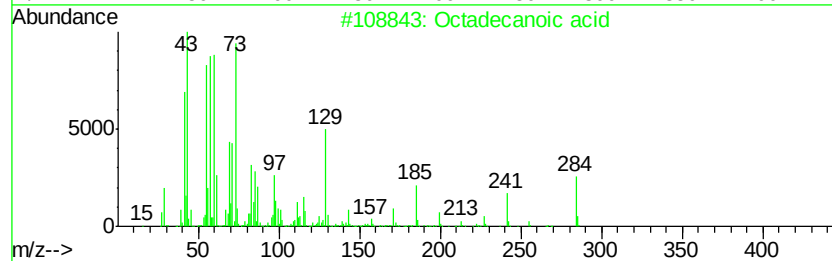
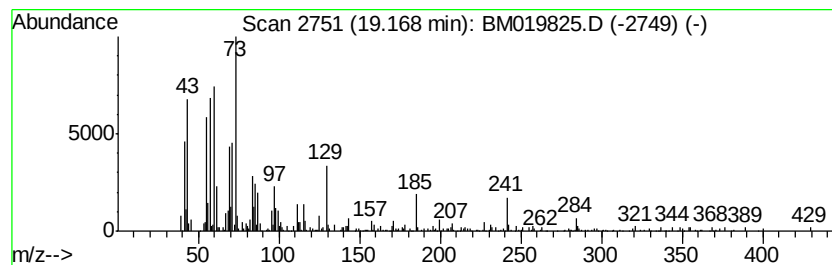
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	5.05 ng/ul	554847	Chrysene-d12	21.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95	
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93	
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90	
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83	
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	76	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM040819\
Data File : BM019825.D
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Sample : K2217-12
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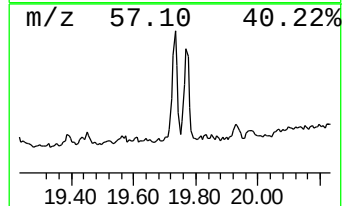
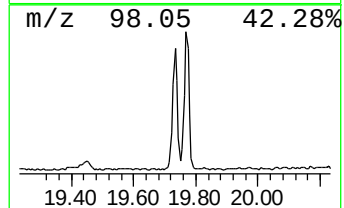
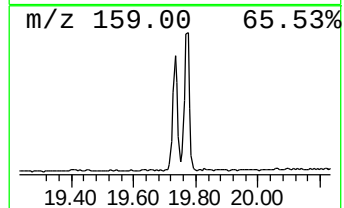
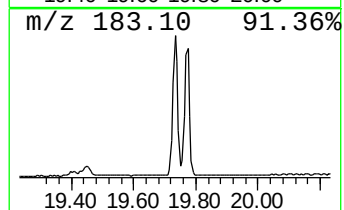
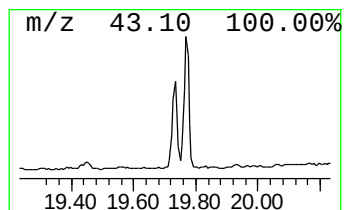
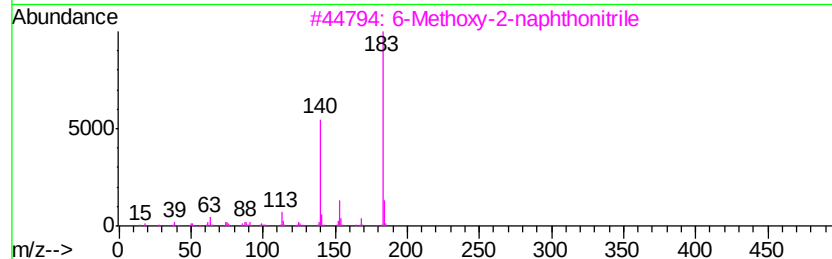
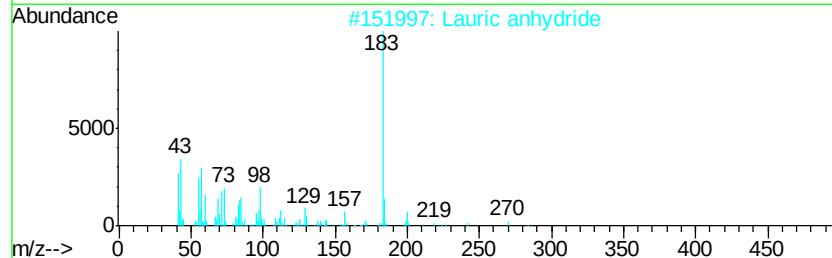
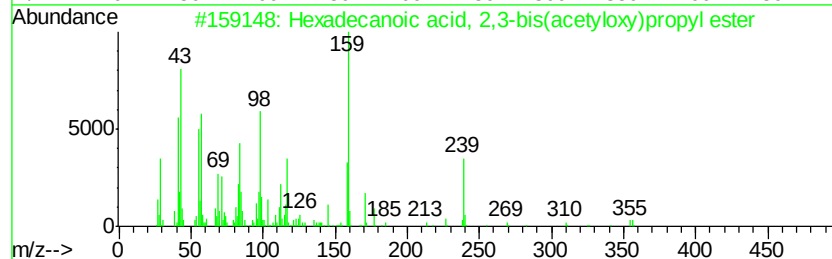
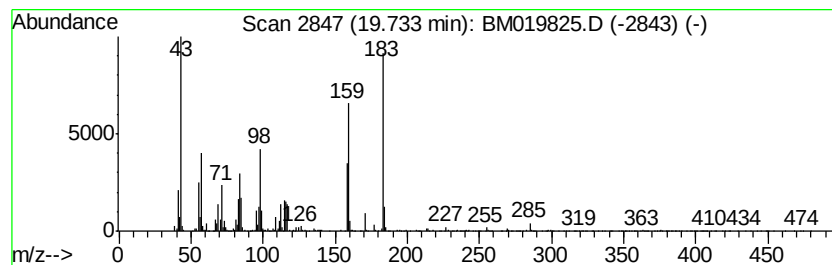
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	10.60 ng/ul	1165050	Chrysene-d12	21.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	37
2		Lauric anhydride	382	C24H46O3	000645-66-9	35
3		6-Methoxy-2-naphthonitrile	183	C12H9NO	067886-70-8	25
4		4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	25
5		4-Hydroxy-3-nitrobenzoic acid	183	C7H5NO5	000616-82-0	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM040819\
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Sample : K2217-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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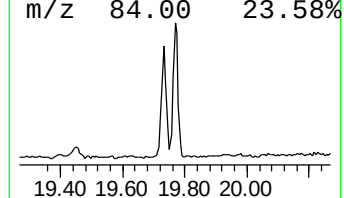
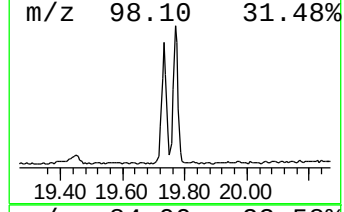
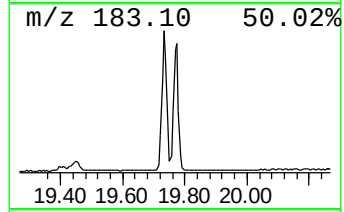
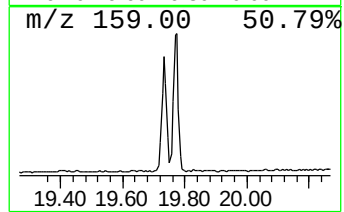
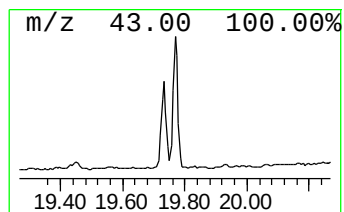
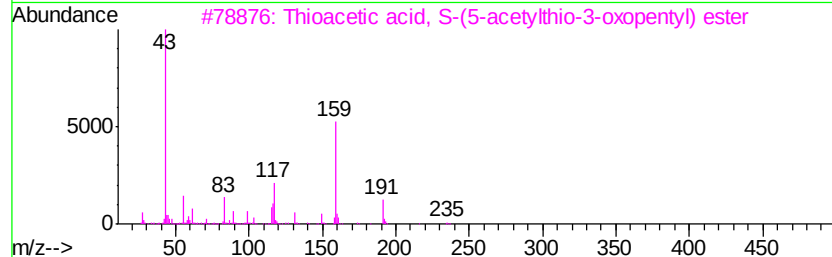
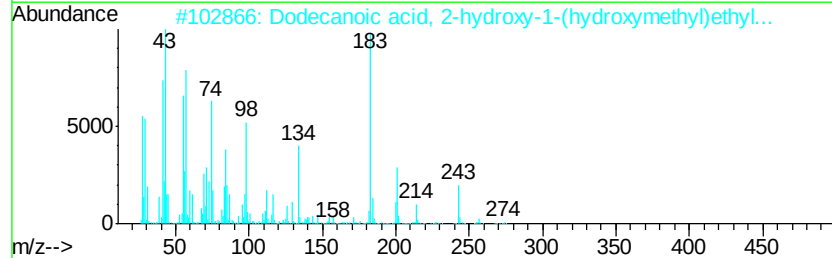
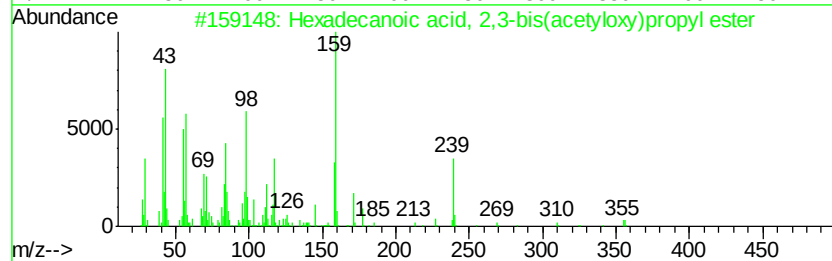
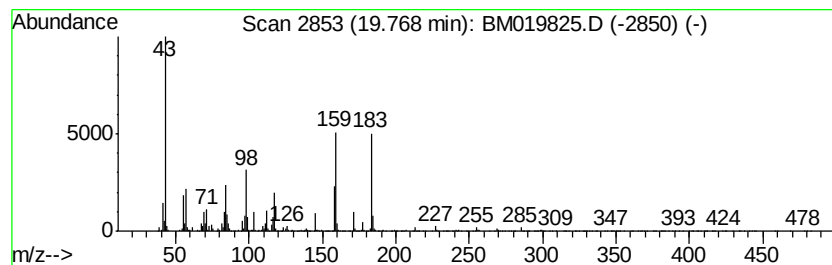
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	12.58 ng/ul	1383750	Chrysene-d12	21.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	58
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	25
3		Thioacetic acid, S-(5-acetylthio...	234	C9H14O3S2	1000185-15-4	18
4		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12
5		2,3,4-Trifluorobenzoic acid, 2-o...	288	C15H19F3O2	1000282-58-1	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM040819\
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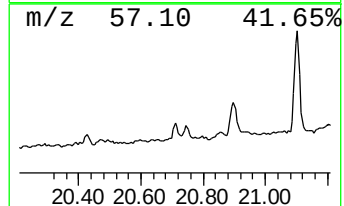
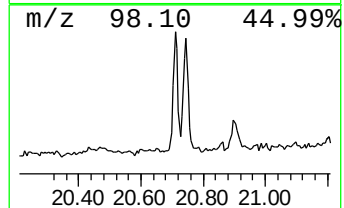
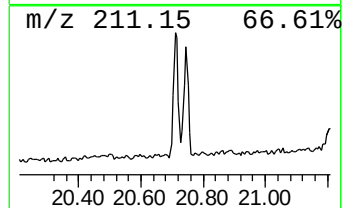
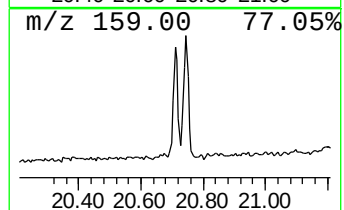
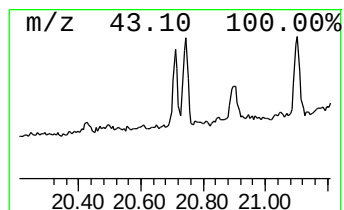
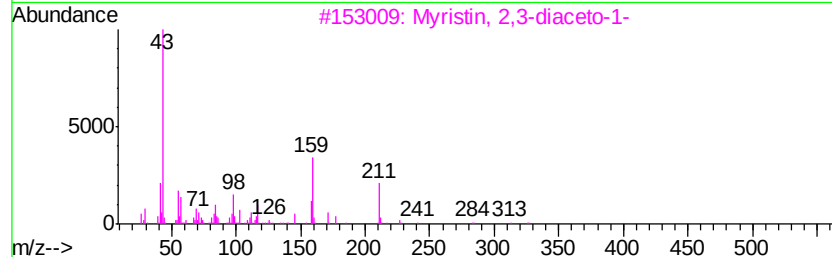
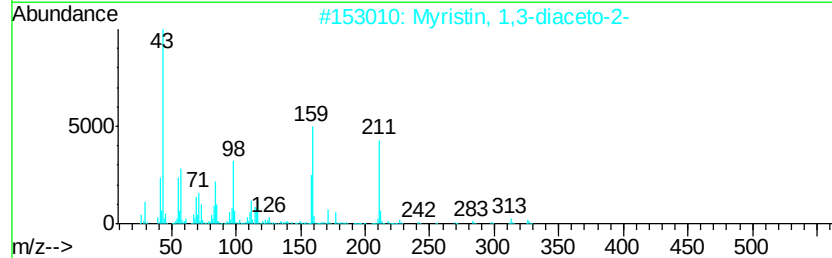
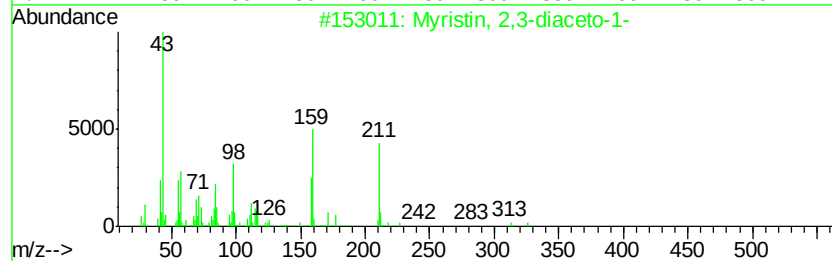
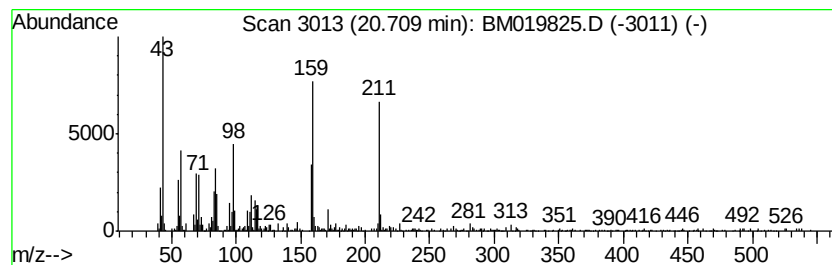
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.71	2.76 ng/ul	303425	Chrysene-d12	21.20		
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	87
3	Myristin,	2,3-diaceto-1-	386	C21H38O6	014473-55-3	40
4	1-Methyl-2-	formylindole	159	C10H9NO	027421-51-8	38
5	4-(Methylamino)	quinazoline	159	C9H9N3	007154-47-4	38



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Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecanoic acid	14.66	10.3	ng/ul	774635	3	14.23	1506170	20.0
Tetradecanoic acid	16.39	4.4	ng/ul	364368	4	16.99	1651950	20.0
unknown-01	17.32	3.2	ng/ul	265696	4	16.99	1651950	20.0
n-Hexadecanoic acid	17.88	9.2	ng/ul	759546	4	16.99	1651950	20.0
Octadecanoic acid	19.17	5.0	ng/ul	554847	5	21.20	2199110	20.0
unknown-02	19.73	10.6	ng/ul	1165050	5	21.20	2199110	20.0
Hexadecanoic acid...	19.77	12.6	ng/ul	1383750	5	21.20	2199110	20.0
Myristin, 2,3-dia...	20.71	2.8	ng/ul	303425	5	21.20	2199110	20.0