

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
 Data File : BM016753.D
 Acq On : 14 Sep 2018 14:58
 Operator : SJ/JU
 Sample : J4868-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DB3Q7

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-BM091018MA.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	3.022	3	6	25	rVB	2438374	2896032	35.08%	3.067%
2	3.270	44	48	55	rBV	81466	100963	1.22%	0.107%
3	3.893	149	154	159	rBV4	19025	31097	0.38%	0.033%
4	4.340	226	230	234	rVB3	12105	14508	0.18%	0.015%
5	4.893	318	324	334	rVB3	12027	21991	0.27%	0.023%
6	5.305	391	394	400	rVB3	9230	12377	0.15%	0.013%
7	5.805	473	479	482	rBV	29769	45379	0.55%	0.048%
8	5.840	482	485	493	rVB	15522	25382	0.31%	0.027%
9	6.399	575	580	586	rVB3	22591	36081	0.44%	0.038%
10	6.722	628	635	642	rBV4	14784	28390	0.34%	0.030%
11	6.846	651	656	658	rBV3	11344	17118	0.21%	0.018%
12	6.899	658	665	675	rVB	292779	481501	5.83%	0.510%
13	7.069	688	694	703	rBV	890984	1360346	16.48%	1.441%
14	7.140	703	706	713	rVB	22743	35846	0.43%	0.038%
15	7.263	720	727	736	rVB	994819	1521641	18.43%	1.611%
16	7.734	800	807	812	rBV	920173	1463825	17.73%	1.550%
17	7.799	812	818	828	rVB	249932	417722	5.06%	0.442%
18	8.346	906	911	915	rBV4	6327	11866	0.14%	0.013%
19	8.428	919	925	937	rVV	738659	1183978	14.34%	1.254%
20	8.546	937	945	952	rVB2	31839	64872	0.79%	0.069%
21	8.822	986	992	996	rBV	160300	255153	3.09%	0.270%
22	8.881	996	1002	1014	rVV	1082085	1746799	21.16%	1.850%
23	8.975	1014	1018	1025	rVV6	9741	19523	0.24%	0.021%
24	9.051	1025	1031	1036	rVB3	18230	27693	0.34%	0.029%
25	9.316	1071	1076	1081	rBV	47962	67440	0.82%	0.071%
26	9.440	1090	1097	1103	rBV5	5140	10736	0.13%	0.011%
27	9.599	1117	1124	1132	rBV	725716	1150506	13.94%	1.218%
28	9.728	1140	1146	1151	rBV2	16434	28300	0.34%	0.030%
29	9.787	1151	1156	1159	rVV4	6792	13185	0.16%	0.014%
30	9.822	1159	1162	1167	rVB5	8078	12953	0.16%	0.014%
31	10.046	1194	1200	1207	rVB4	12200	23791	0.29%	0.025%
32	10.128	1207	1214	1225	rBV	1300814	2140034	25.92%	2.266%
33	10.298	1238	1243	1249	rBV2	31420	47907	0.58%	0.051%
34	10.381	1253	1257	1261	rVV4	7828	13153	0.16%	0.014%

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Integrator: RTE
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Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM091018MA.M
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35	10.422	1261	1264	1272	rVB9	9379	18159	0.22%	0.019%
36	10.510	1272	1279	1286	rBV	1249795	2085254	25.26%	2.208%
37	10.575	1286	1290	1294	rVB3	16195	23788	0.29%	0.025%
38	10.646	1299	1302	1311	rVB3	16778	31409	0.38%	0.033%
39	10.816	1328	1331	1338	rVB4	7680	10486	0.13%	0.011%
40	11.298	1409	1413	1420	rBV3	15853	24471	0.30%	0.026%
41	11.687	1473	1479	1483	rBV3	7356	11174	0.14%	0.012%
42	11.810	1496	1500	1504	rBV	30122	44200	0.54%	0.047%
43	12.022	1530	1536	1542	rVB4	5420	12060	0.15%	0.013%
44	12.104	1545	1550	1554	rBV2	20753	31856	0.39%	0.034%
45	12.728	1650	1656	1662	rBV	113549	174003	2.11%	0.184%
46	12.981	1691	1699	1709	rBV	189436	268010	3.25%	0.284%
47	13.281	1744	1750	1757	rBV	209712	326253	3.95%	0.346%
48	13.786	1829	1836	1847	rBV	2348570	3169031	38.39%	3.356%
49	13.892	1847	1854	1861	rVB5	29462	64415	0.78%	0.068%
50	14.063	1874	1883	1889	rBV	2639220	3937788	47.70%	4.170%
51	14.369	1928	1935	1943	rVB2	1731634	2604760	31.55%	2.758%
52	14.457	1947	1950	1956	rVB4	9558	13772	0.17%	0.015%
53	14.557	1962	1967	1976	rBV	176822	268105	3.25%	0.284%
54	14.798	2004	2008	2012	rBV3	16511	23457	0.28%	0.025%
55	14.975	2034	2038	2043	rBV2	23870	33248	0.40%	0.035%
56	15.057	2046	2052	2056	rVV2	19398	31393	0.38%	0.033%
57	15.098	2056	2059	2068	rVB2	18656	32813	0.40%	0.035%
58	15.192	2070	2075	2082	rBV2	30085	56869	0.69%	0.060%
59	15.369	2097	2105	2111	rBV	3330533	4973224	60.25%	5.267%
60	15.480	2117	2124	2136	rBV	702609	980396	11.88%	1.038%
61	15.604	2141	2145	2150	rVV	38210	48517	0.59%	0.051%
62	15.739	2163	2168	2172	rBV4	20423	27694	0.34%	0.029%
63	16.175	2235	2242	2248	rBV	84487	118176	1.43%	0.125%
64	16.386	2273	2278	2285	rVB	32043	42864	0.52%	0.045%
65	16.492	2292	2296	2300	rBV3	25078	34466	0.42%	0.036%
66	16.533	2300	2303	2309	rVB4	12849	21016	0.25%	0.022%
67	16.904	2361	2366	2369	rBV	9781	15381	0.19%	0.016%
68	17.116	2395	2402	2410	rBV2	2177431	2951595	35.76%	3.126%
69	17.216	2413	2419	2433	rBV	3845223	5315804	64.40%	5.629%
70	17.422	2449	2454	2458	rBV	337999	400391	4.85%	0.424%
71	17.469	2458	2462	2471	rVB	699888	884656	10.72%	0.937%

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72	17.798	2512	2518	2525	rBV2	283942	371938	4.51%	0.394%
73	18.027	2552	2557	2565	rBV	181576	256678	3.11%	0.272%
74	18.098	2565	2569	2574	rVB4	14682	29498	0.36%	0.031%
75	18.274	2596	2599	2605	rVB5	10949	16769	0.20%	0.018%
76	18.363	2611	2614	2619	rVB6	14296	19859	0.24%	0.021%
77	18.745	2674	2679	2682	rBV	367434	413375	5.01%	0.438%
78	18.786	2682	2686	2696	rVB	805767	926425	11.22%	0.981%
79	19.145	2742	2747	2752	rVB	45759	60649	0.73%	0.064%
80	19.316	2771	2776	2786	rBV	482858	703508	8.52%	0.745%
81	19.398	2787	2790	2796	rVB2	42642	69230	0.84%	0.073%
82	19.510	2803	2809	2816	rBV2	4671750	6310496	76.45%	6.683%
83	19.586	2816	2822	2830	rVB	309013	516118	6.25%	0.547%
84	19.874	2866	2871	2874	rBV	3725277	3946718	47.81%	4.180%
85	19.915	2874	2878	2891	rVB	7257610	8254733	100.00%	8.742%
86	20.410	2959	2962	2966	rVB5	33676	34675	0.42%	0.037%
87	20.633	2993	3000	3004	rBV3	94402	168370	2.04%	0.178%
88	20.851	3033	3037	3040	rBV	1738234	1903969	23.07%	2.016%
89	20.886	3040	3043	3052	rVB	3791430	3930203	47.61%	4.162%
90	21.098	3076	3079	3083	rVB	84164	97089	1.18%	0.103%
91	21.239	3101	3103	3107	rVB2	47896	52801	0.64%	0.056%
92	21.304	3109	3114	3122	rVV	3118298	3738360	45.29%	3.959%
93	21.721	3181	3185	3188	rBV	807061	1000971	12.13%	1.060%
94	21.757	3188	3191	3203	rVB	1839846	2145402	25.99%	2.272%
95	22.345	3287	3291	3296	rBV	280568	388178	4.70%	0.411%
96	22.439	3304	3307	3311	rVB3	103693	123371	1.49%	0.131%
97	22.668	3341	3346	3348	rBV	778674	1099451	13.32%	1.164%
98	22.704	3348	3352	3359	rVB	1740993	2454459	29.73%	2.599%
99	23.404	3464	3471	3479	rVB	3811452	6945841	84.14%	7.356%
100	23.545	3488	3495	3504	rVB	2091242	4009850	48.58%	4.246%

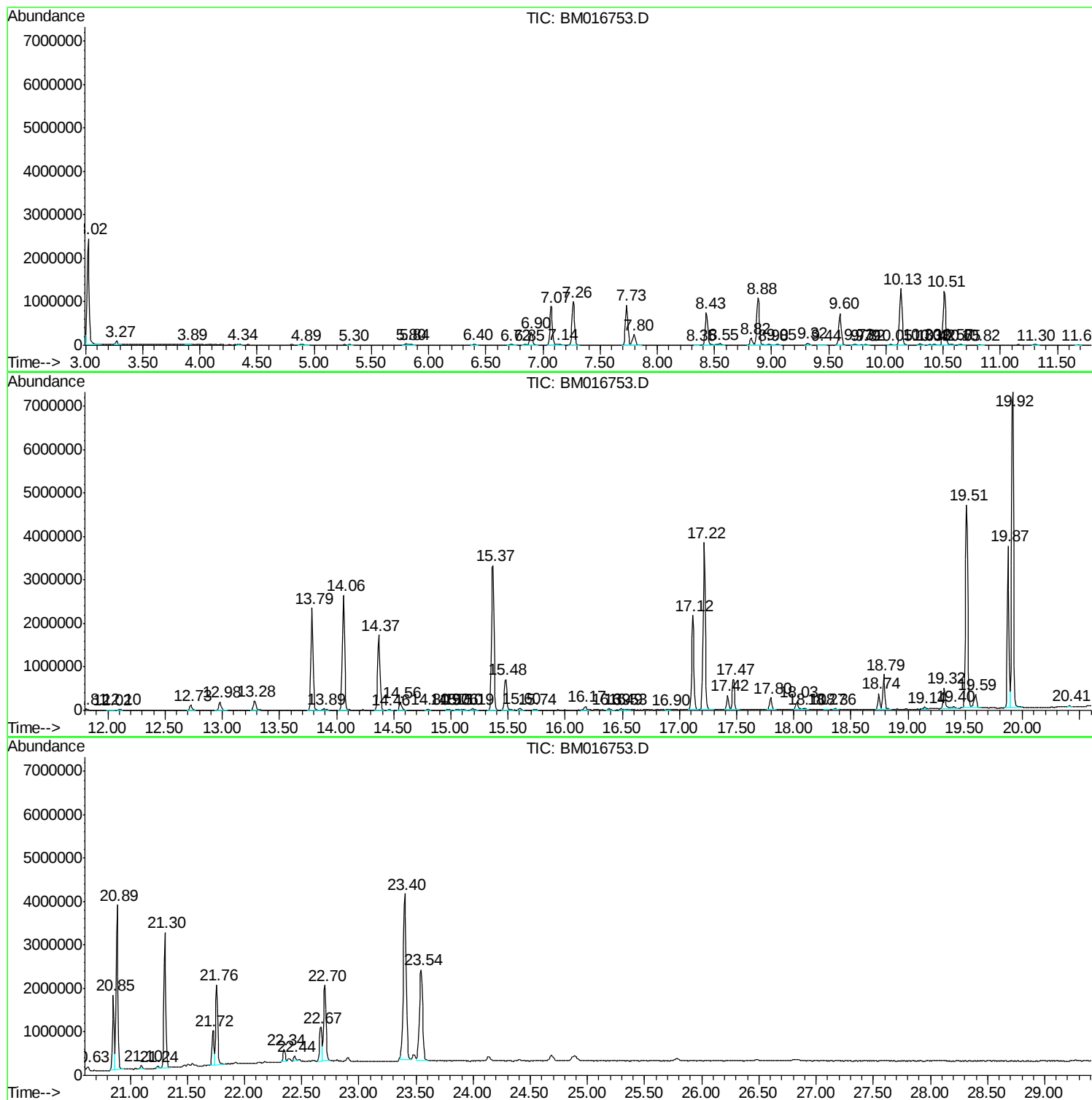
Sum of corrected areas: 94428026

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM091018MA.M
Quant Title : SVOA CALIBRATION

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



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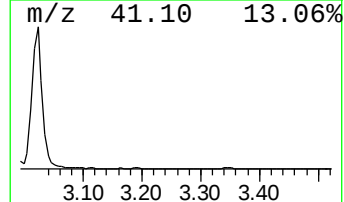
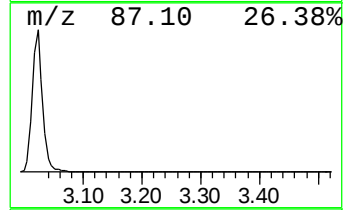
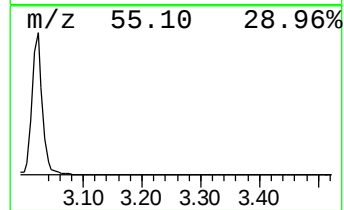
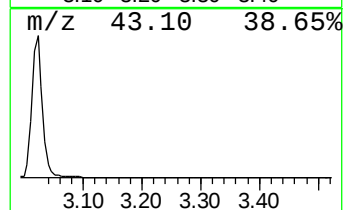
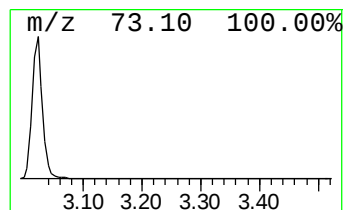
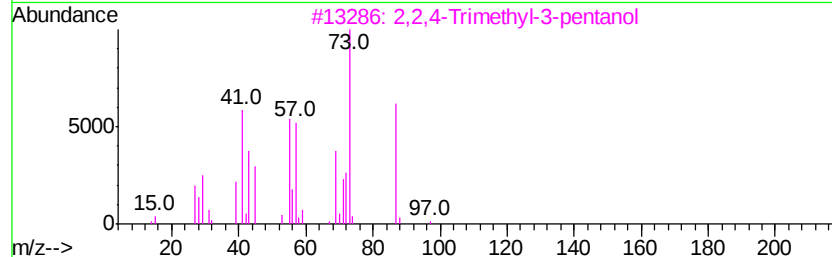
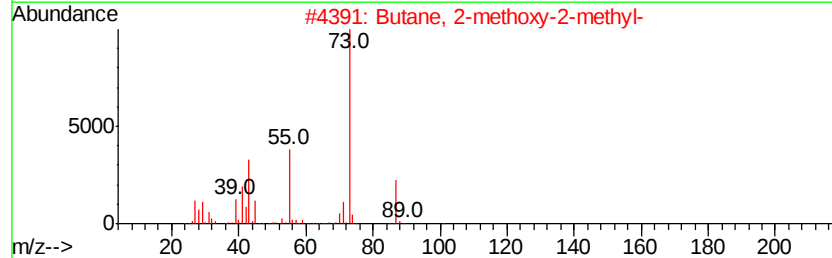
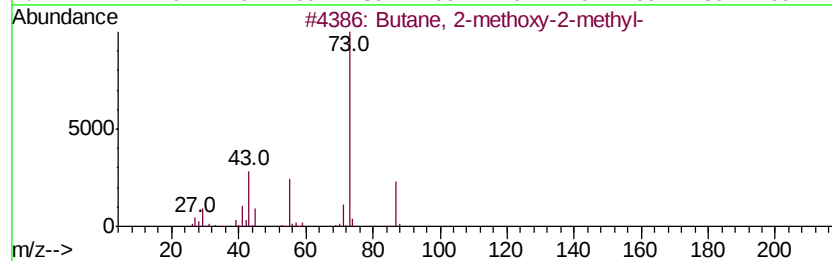
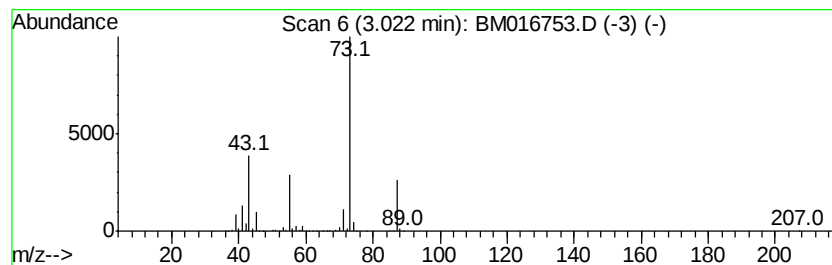
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM091018MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	39.57 ng/ul	2896030	1,4-Dichlorobenzene-d4	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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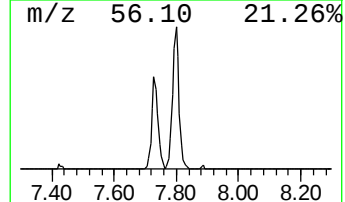
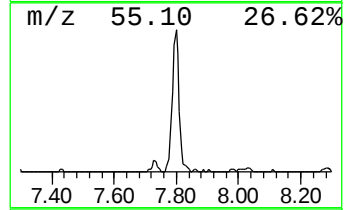
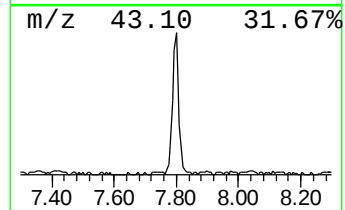
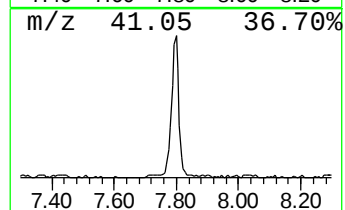
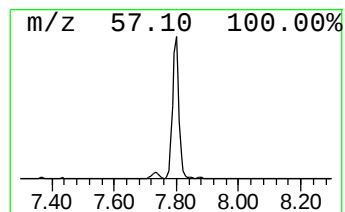
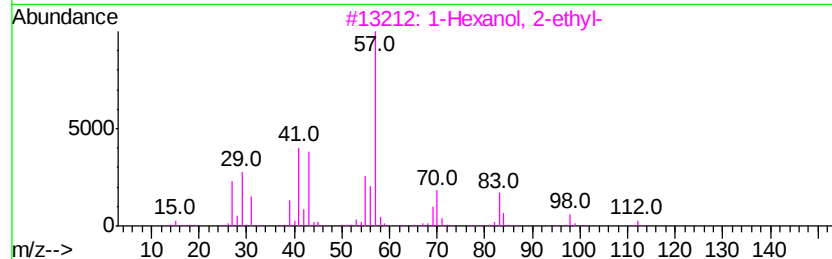
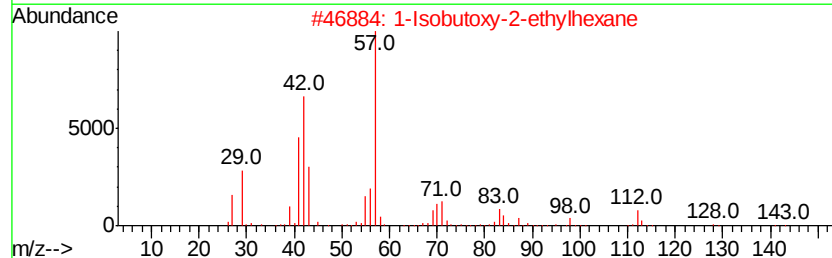
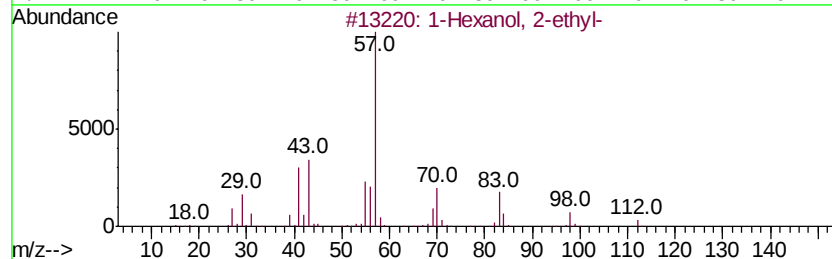
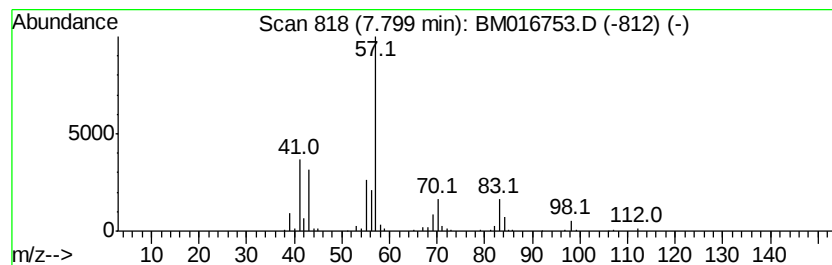
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	5.71 ng/ul	417722	1,4-Dichlorobenzene-d4	7.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
5			dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	53



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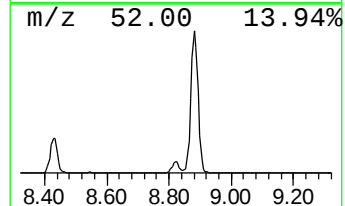
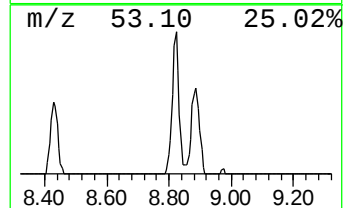
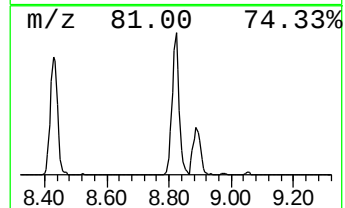
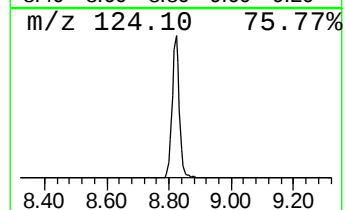
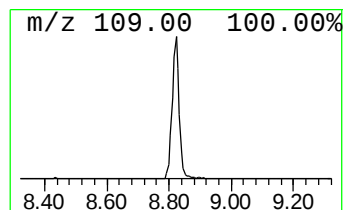
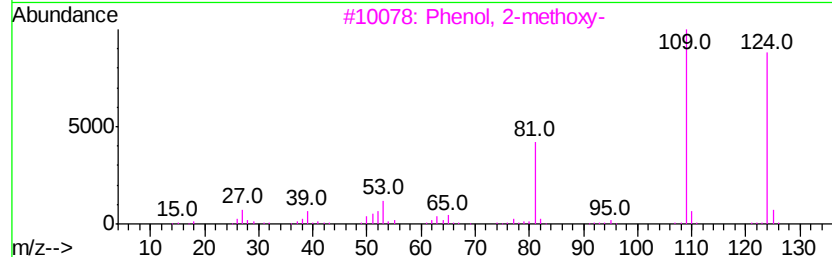
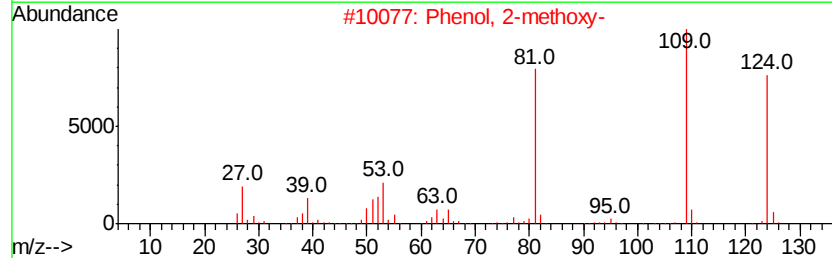
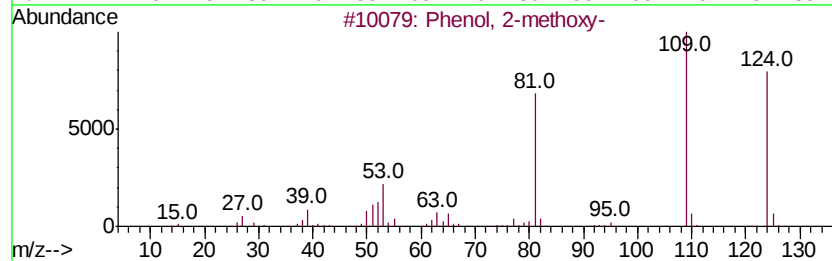
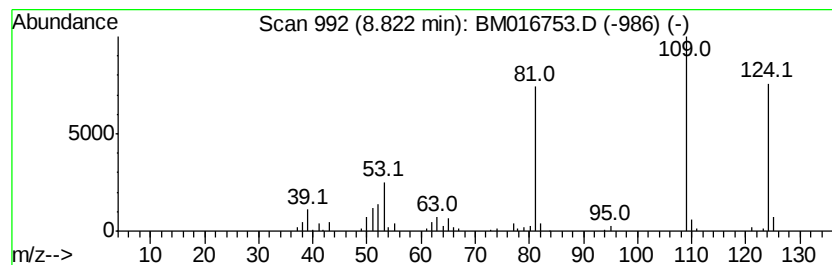
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Phenol, 2-methoxy- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	3.49 ng/ul	255153	1,4-Dichlorobenzene-d4	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
2		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
3		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
4		Mequinol	124	C7H8O2	000150-76-5	94
5		Mequinol	124	C7H8O2	000150-76-5	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
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Instrument :
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ClientSampleId :
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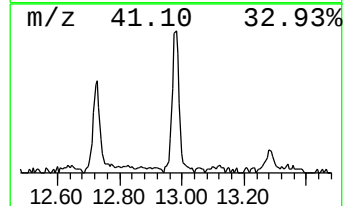
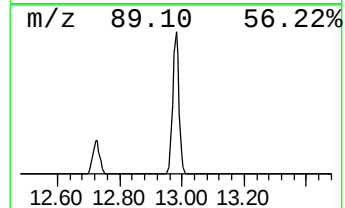
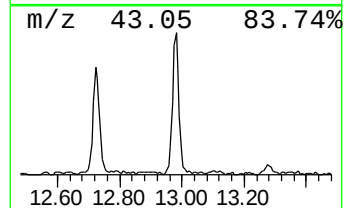
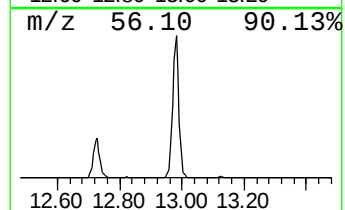
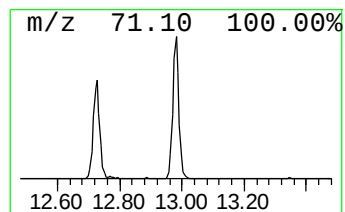
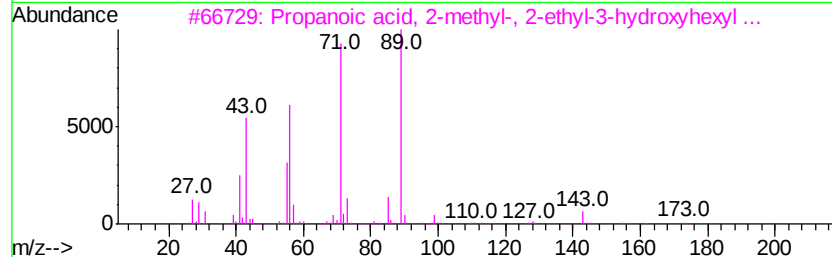
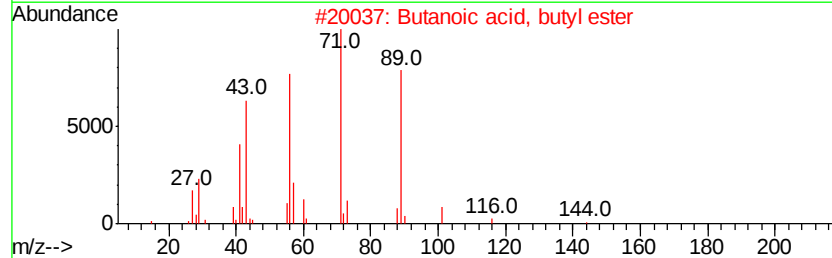
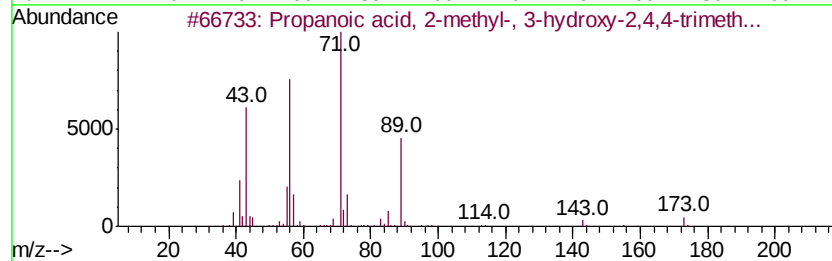
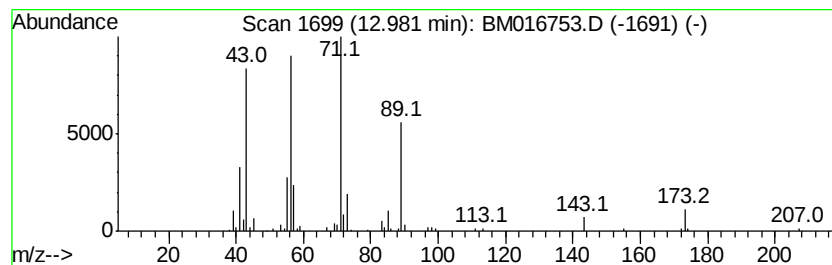
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	2.06 ng/ul	268010	Acenaphthene-d10	14.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	91
2		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
3		Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	47
4		trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	43
5		2,2,5,5,6-Pentamethyl-4,7,9-trio...	200	C11H20O3	062759-70-0	40



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Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
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Instrument :
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ClientSampleId :
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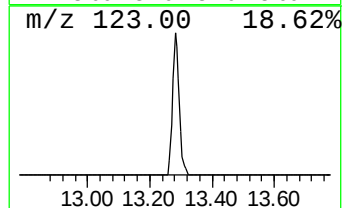
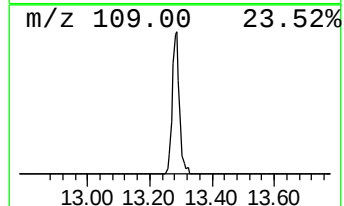
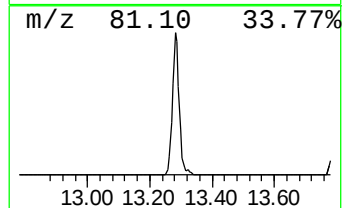
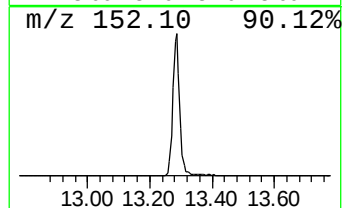
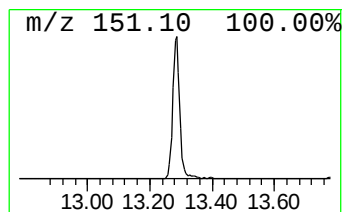
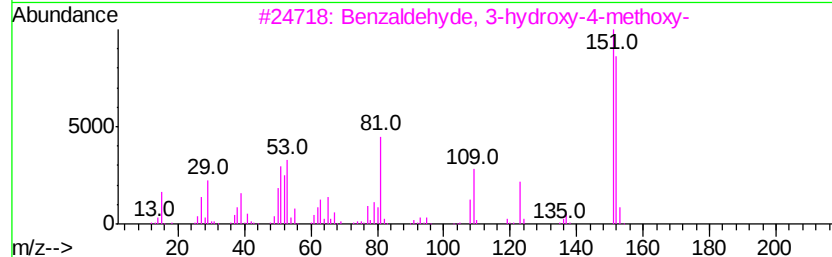
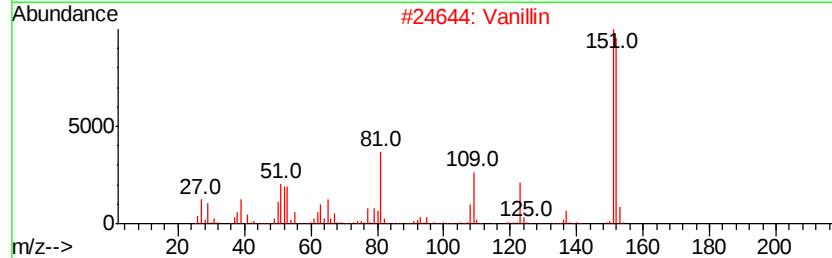
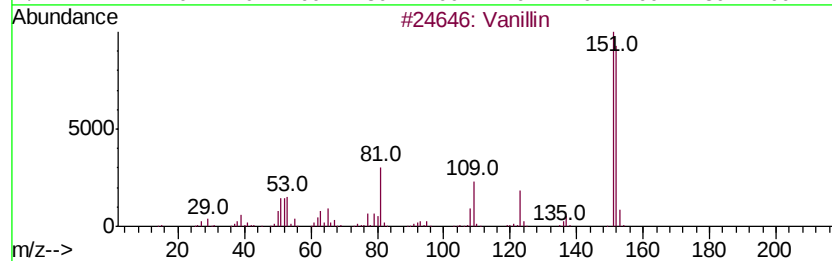
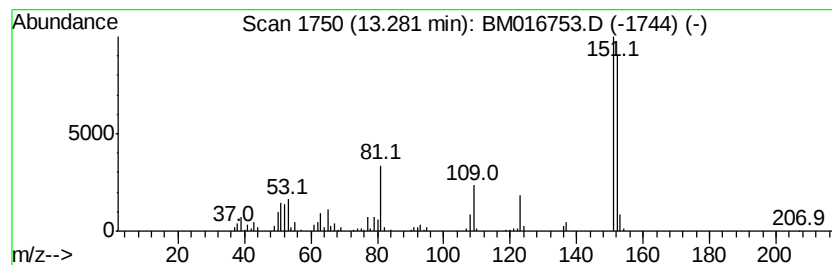
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Vanillin Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	2.51 ng/ul	326253	Acenaphthene-d10	14.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin		152	C8H8O3	000121-33-5	97
2	Vanillin		152	C8H8O3	000121-33-5	96
3	Benzaldehyde, 3-hydroxy-4-methoxy-		152	C8H8O3	000621-59-0	94
4	Benzaldehyde, 3-hydroxy-4-methoxy-		152	C8H8O3	000621-59-0	93
5	Vanillin		152	C8H8O3	000121-33-5	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
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Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
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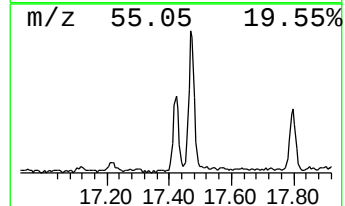
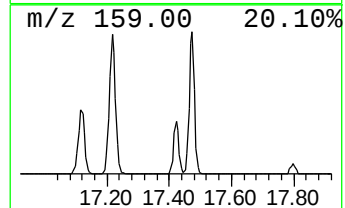
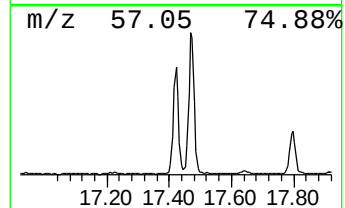
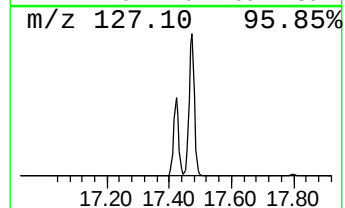
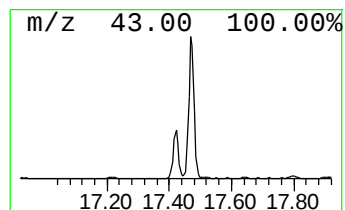
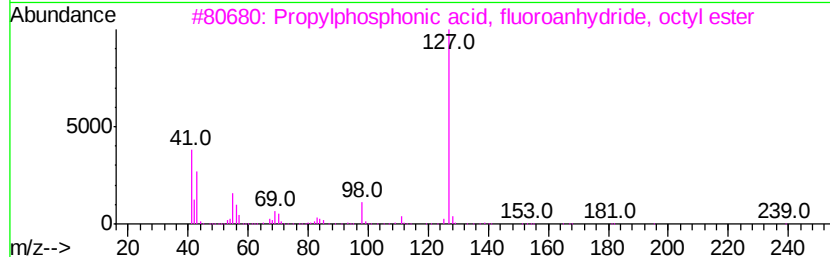
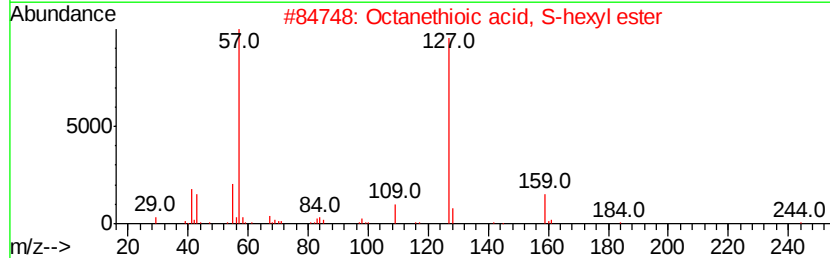
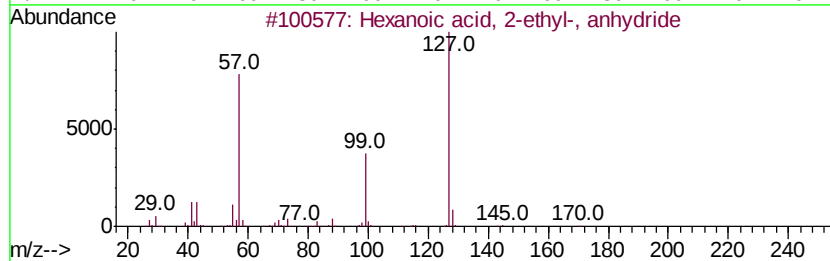
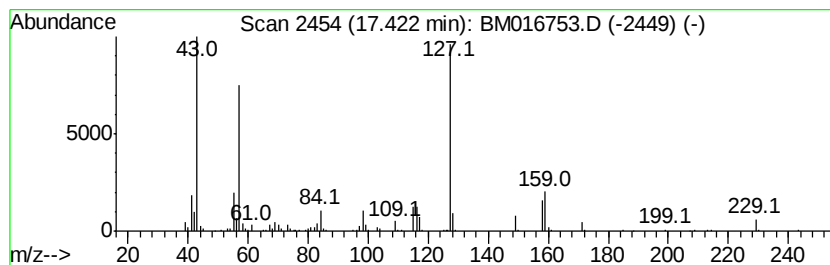
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.42	2.71 ng/ul	400391	Phenanthrene-d10	17.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	47
2	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	45
3	Propylphosphonic acid, fluoroanh...	238	C11H24F02P	333416-20-9	43
4	Octanoic acid, 2,6-dibromo-4-cva...	401	C15H17Br2NO2	001689-99-2	38
5	Octanoic acid, cyclobutyl ester	198	C12H22O2	1000282-86-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
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Sample : J4868-07
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ALS Vial : 10 Sample Multiplier: 1

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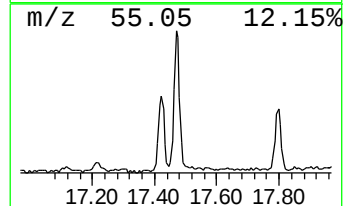
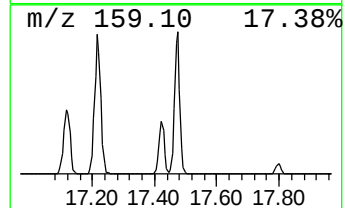
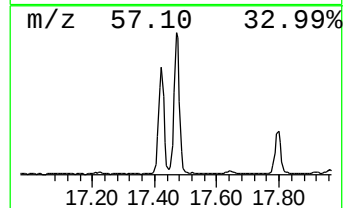
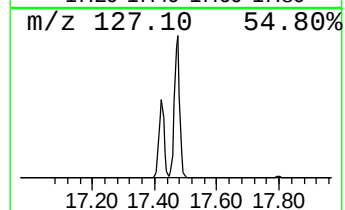
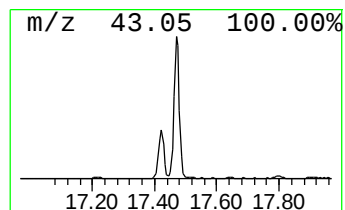
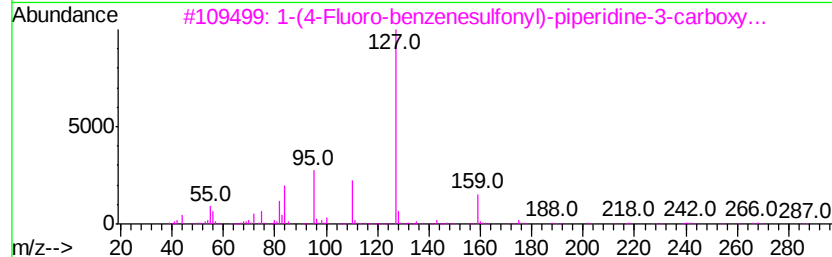
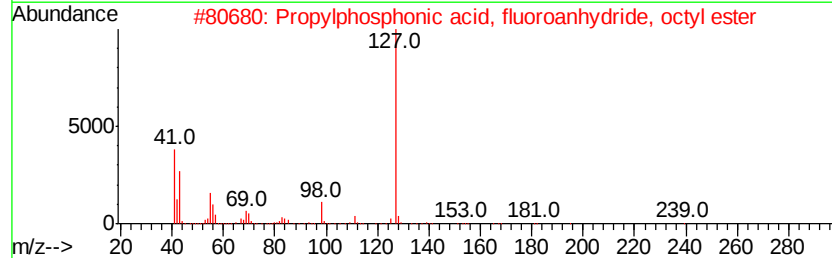
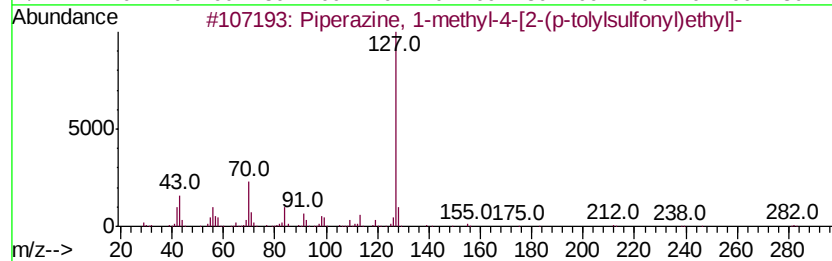
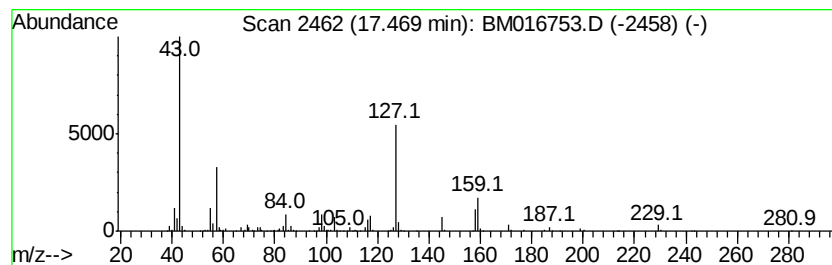
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	5.99 ng/ul	884656	Phenanthrene-d10	17.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Piperazine, 1-methyl-4-[2-(p-tol...	282	C14H22N2O2S	016191-68-7	38
2		Propylphosphonic acid, fluoroanh...	238	C11H24F02P	333416-20-9	32
3		1-(4-Fluoro-benzenesulfonyl)-pip...	286	C12H15FN2O3S	1000295-13-0	28
4		6-Azathymine	127	C4H5N3O2	000932-53-6	25
5		4-Amino-2,6-dihoxypyrimidine	127	C4H5N3O2	000873-83-6	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
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Sample : J4868-07
Misc :
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ClientSampleId :
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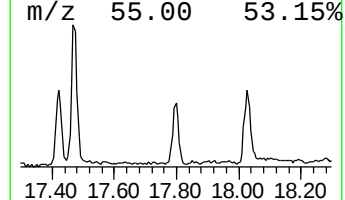
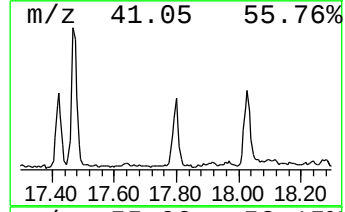
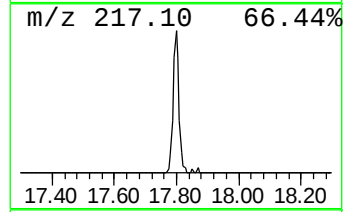
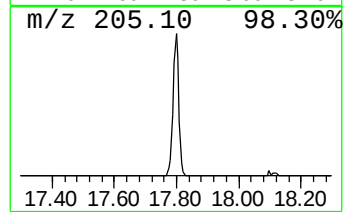
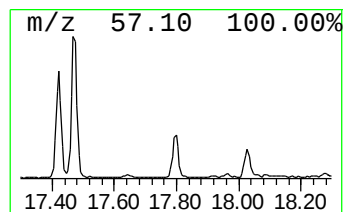
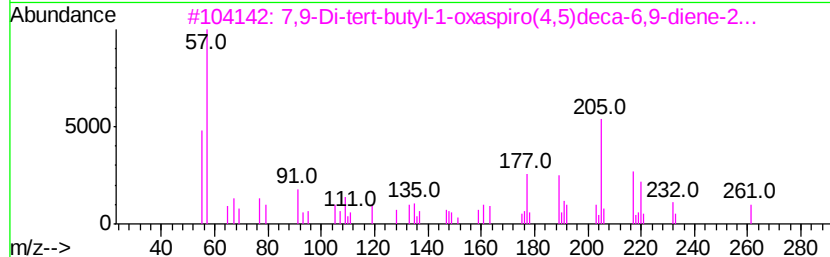
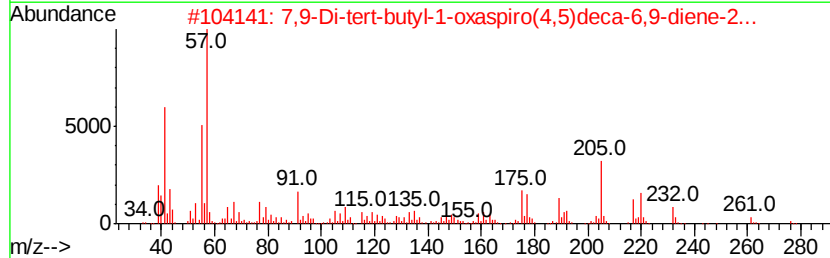
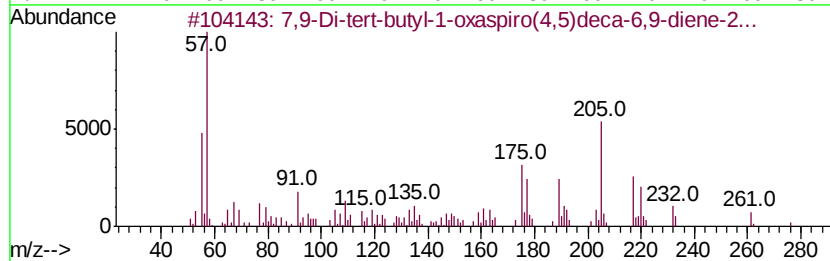
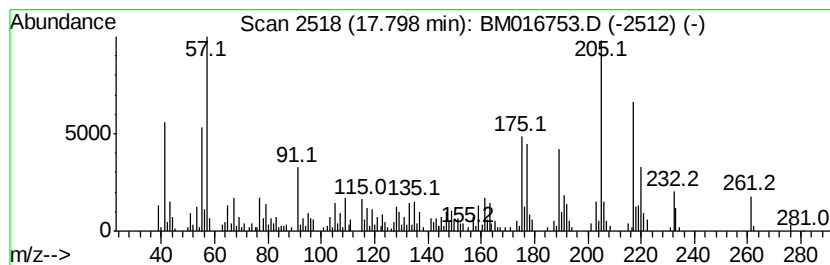
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.80	2.52 ng/ul	371938	Phenanthrene-d10	17.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	99
2			7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	96
3			7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	87
4			Ethanone, 1-(5,6,7,8-tetrahydro-2H-chromeno[2,1-b]pyridin-2-yl)-	220	C14H20O2	071596-88-8	83
5			2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	44



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
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Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

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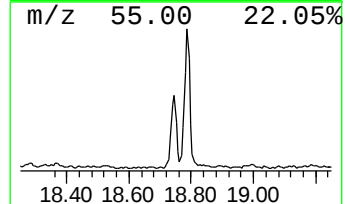
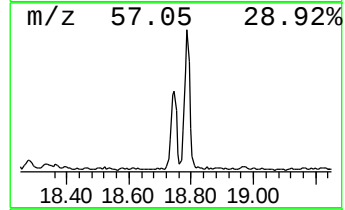
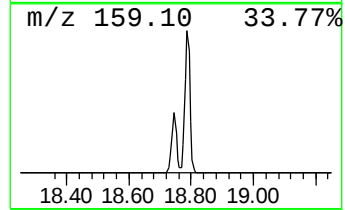
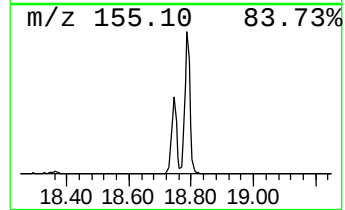
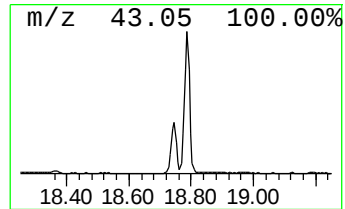
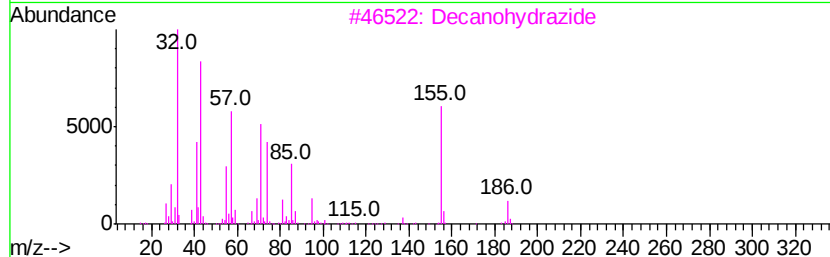
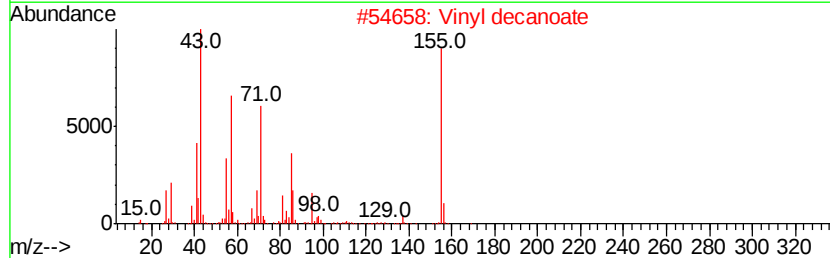
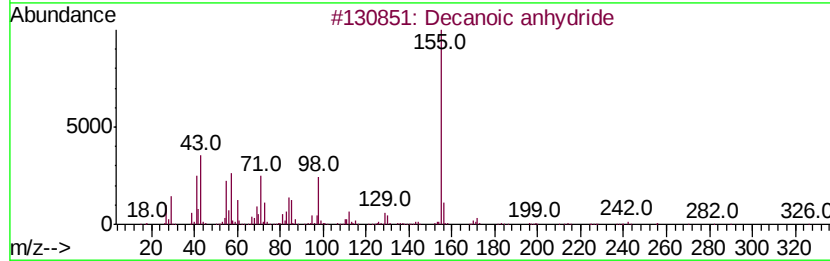
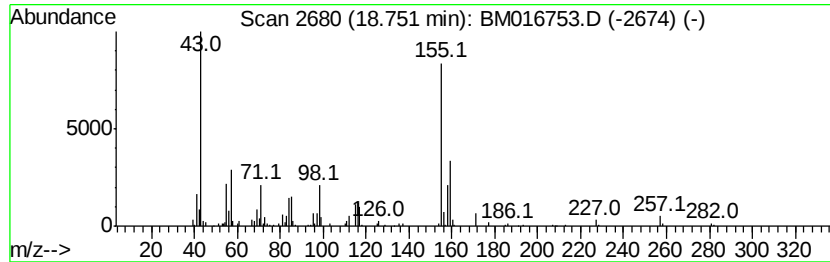
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown-03 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.75	2.80 ng/ul	413375	Phenanthrene-d10	17.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic anhydride	326	C20H38O3	002082-76-0	42
2			Vinyl decanoate	198	C12H22O2	004704-31-8	37
3			Decanohydrazide	186	C10H22N2O	020478-70-0	22
4			6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	22
5			4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
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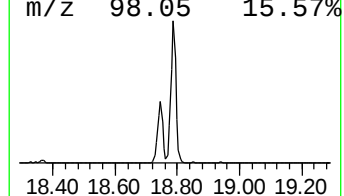
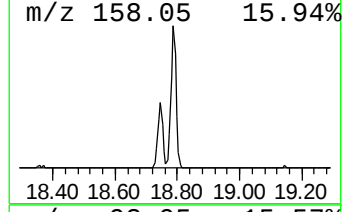
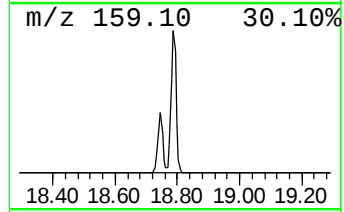
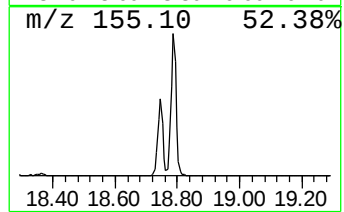
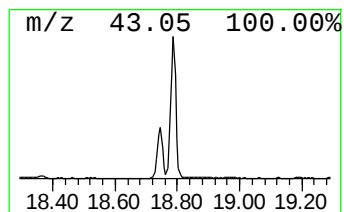
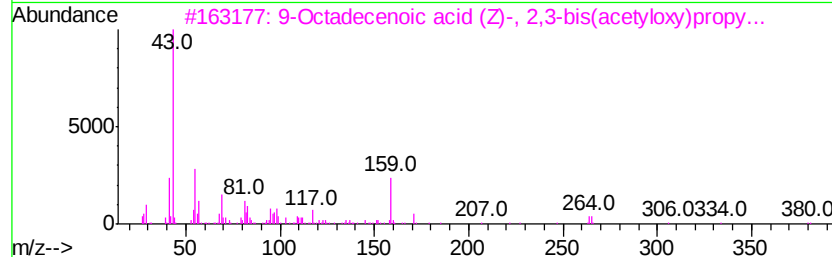
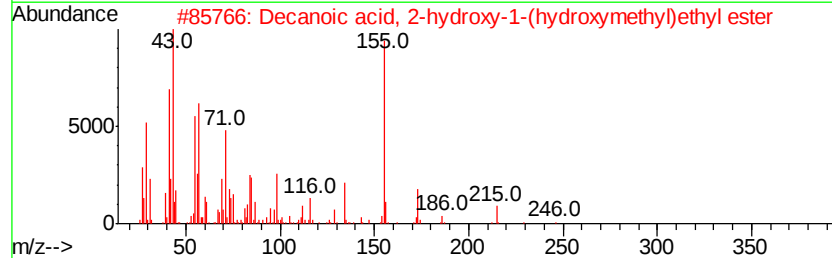
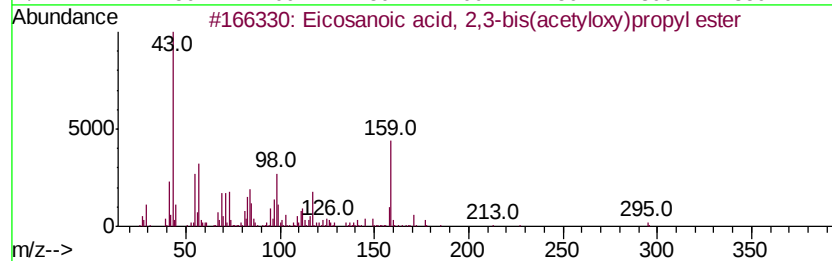
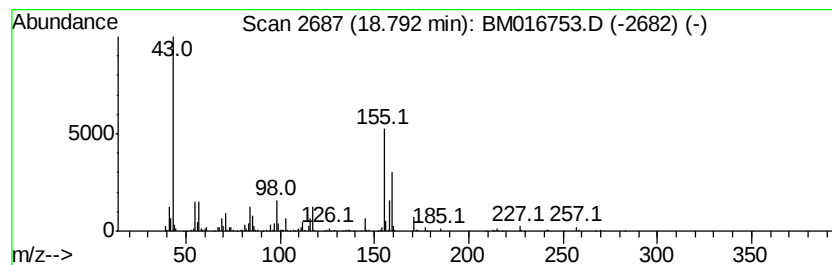
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-04 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.79	6.28 ng/ul	926425	Phenanthrene-d10	17.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	37
2			Decanoic acid, 2-hydroxy-1-(hydr...	246	C13H26O4	003376-48-5	25
3			9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	12
4			Oxiranecarbonitrile, 3-methyl-3-...	159	C10H9NO	028937-48-6	9
5			Acetamide, N-(2-methyl-3-oxo-4-i...	158	C6H10N2O3	014617-48-2	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DB3Q7

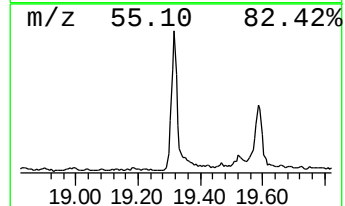
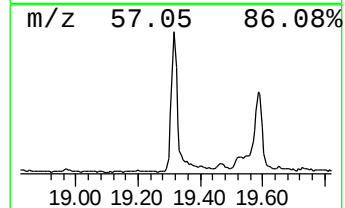
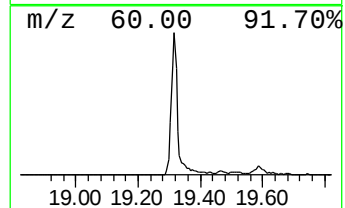
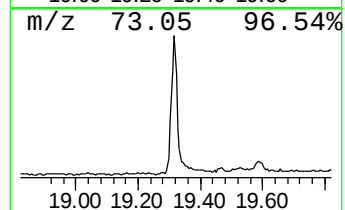
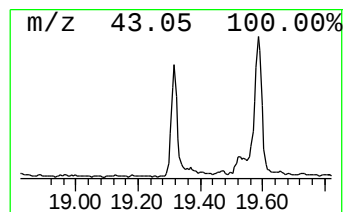
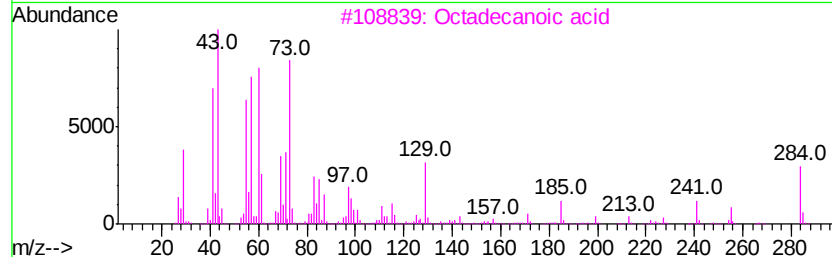
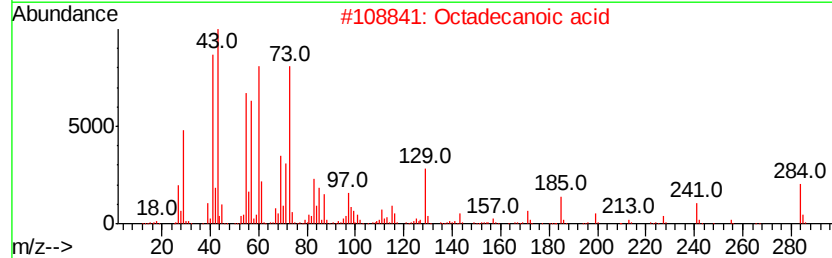
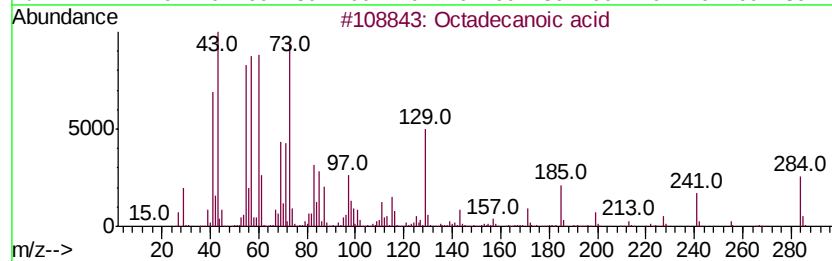
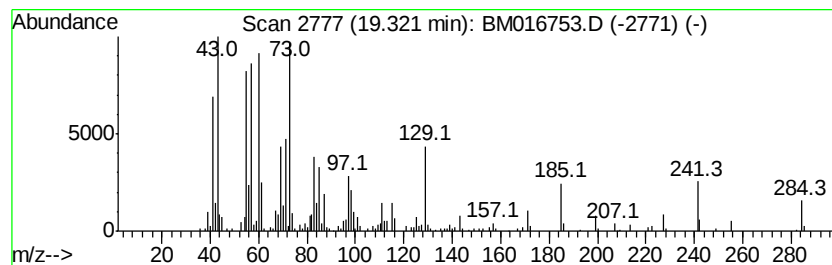
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	3.76 ng/ul	703508	Chrysene-d12	21.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	94
4			Octadecanoic acid	284	C18H36O2	000057-11-4	94
5			Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
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Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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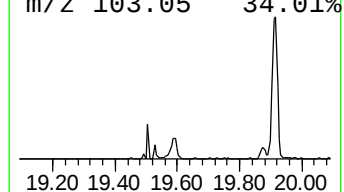
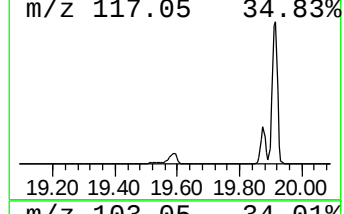
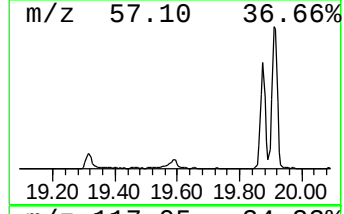
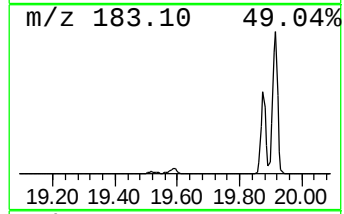
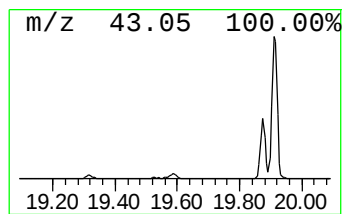
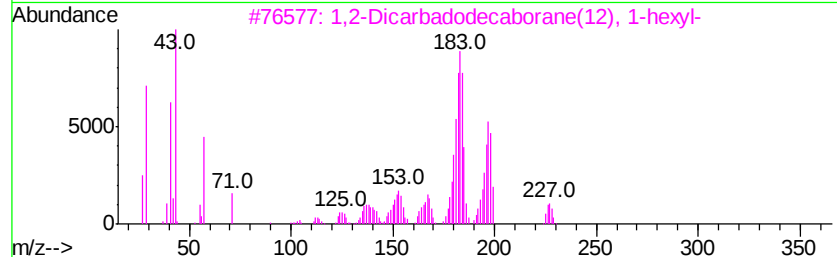
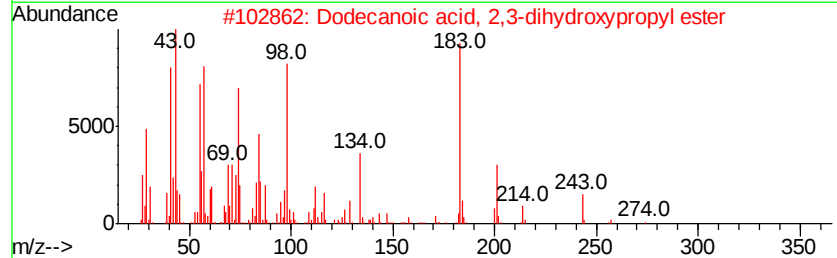
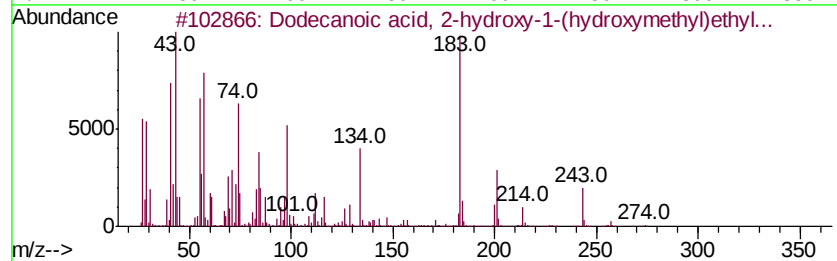
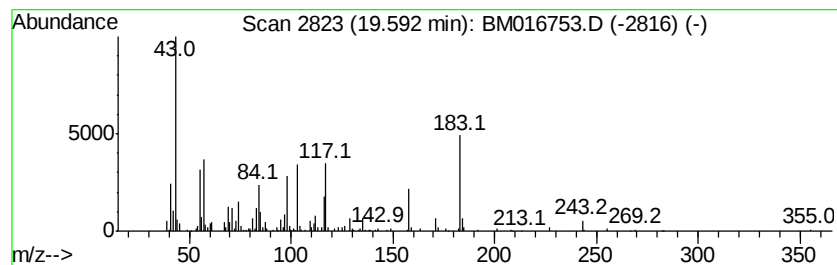
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-05 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.76 ng/ul	516118	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	28
2		Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	27
3		1,2-Dicarbadodecaborane(12), 1-h...	230	C8H24B10	020740-05-0	10
4		Heptane, 4-ethyl-	128	C9H20	002216-32-2	10
5		2,7-Octanedione	142	C8H14O2	001626-09-1	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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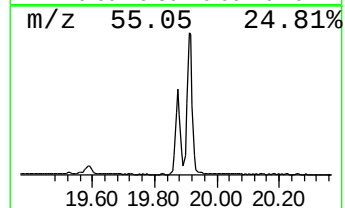
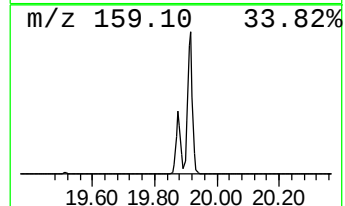
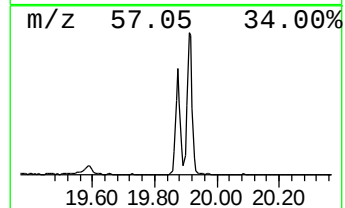
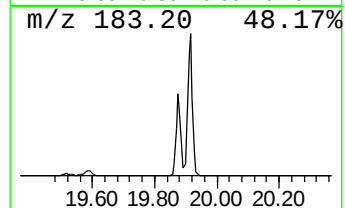
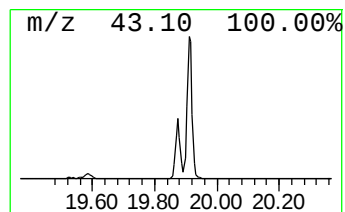
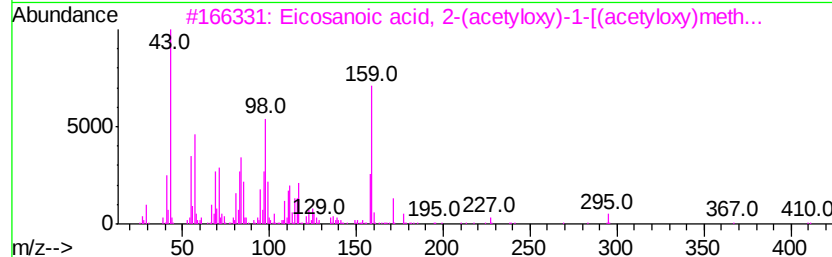
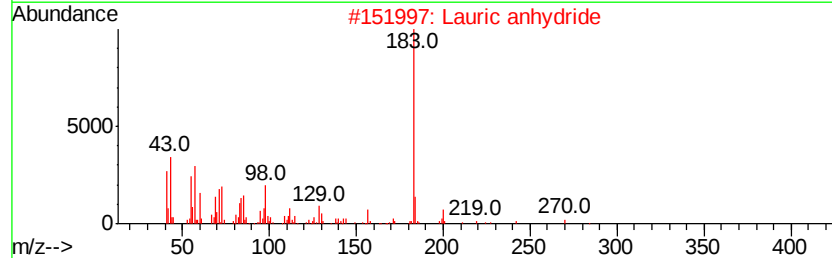
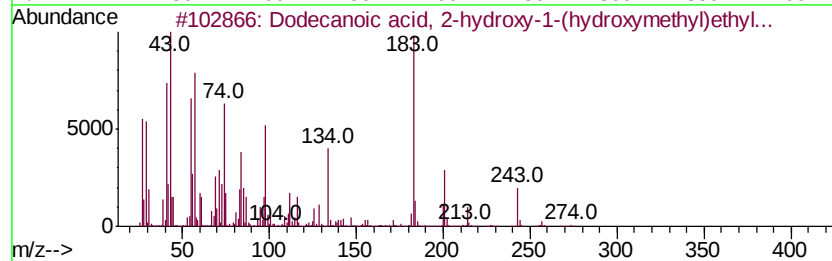
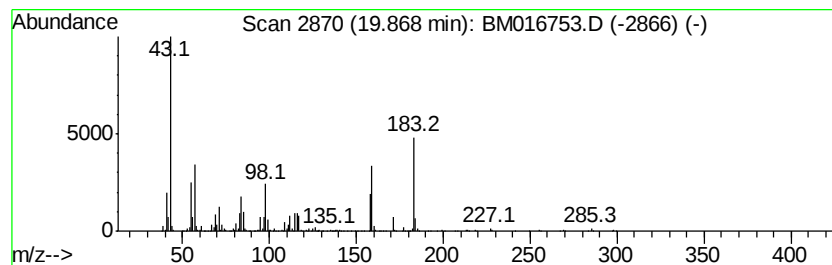
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 unknown-06 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	21.11 ng/ul	3946720	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	37
2		Lauric anhydride	382	C24H46O3	000645-66-9	27
3		Eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]...	470	C27H50O6	055429-68-0	25
4		5,8-Methano-4H-3,1-benzoxazine-2-one	183	C9H13NOS	1000142-76-7	16
5		Eicosanoic acid, 2,3-bis(acetyloxy)-1-[(acetyloxy)methyl]...	470	C27H50O6	055429-67-9	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
 Data File : BM016753.D
 Acq On : 14 Sep 2018 14:58
 Operator : SJ/JU
 Sample : J4868-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
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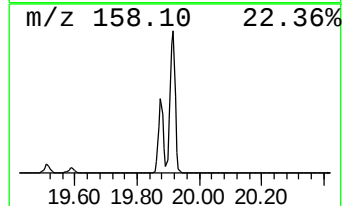
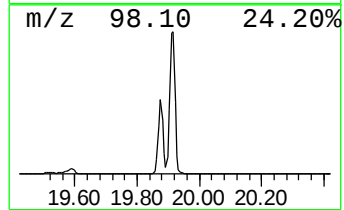
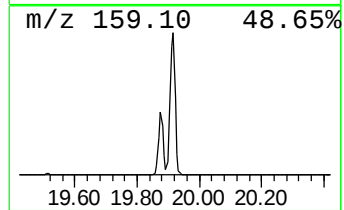
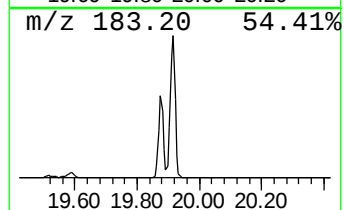
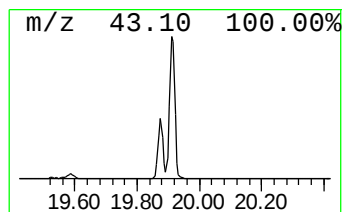
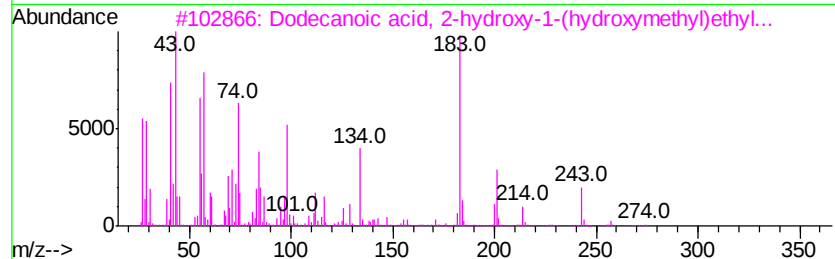
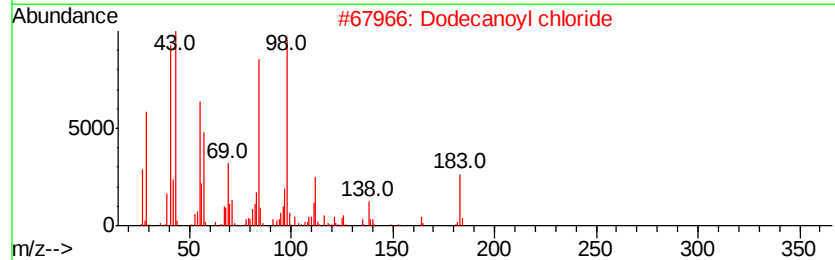
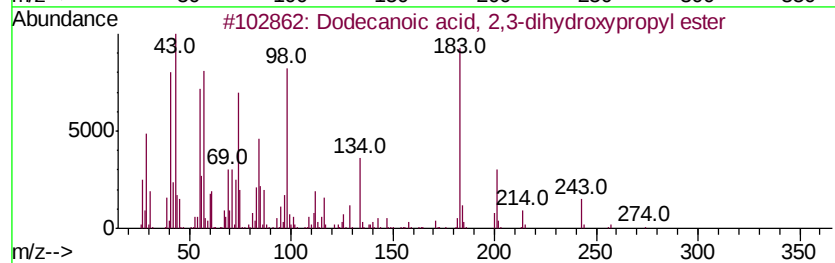
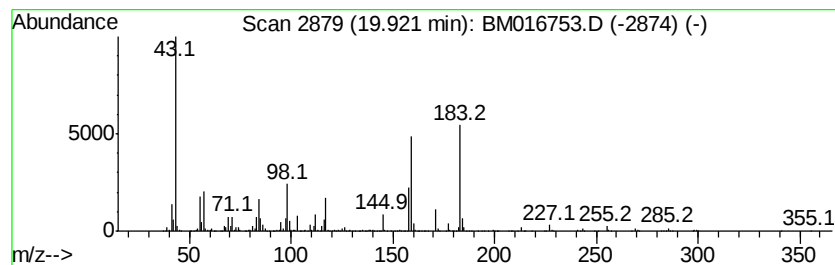
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 14 unknown-07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	44.16 ng/ul	8254730	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2,3-dihydroxypropyl...	274	C15H30O4	000142-18-7	22
2		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	16
3		Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	12
4		1,2-Dicarbadodecaborane(12), 1-hydroxy-1,2-dihydroxypropyl...	230	C8H24B10	020740-05-0	10
5		Eicosanoic acid, 2,3-bis(acetyloxy)propyl...	470	C27H50O6	055429-67-9	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
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Misc :
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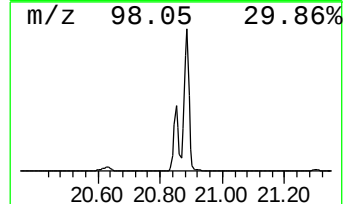
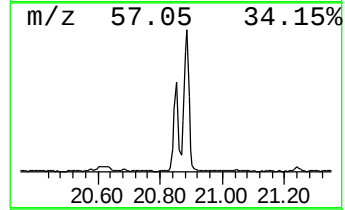
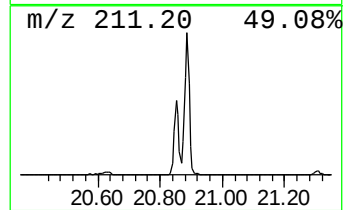
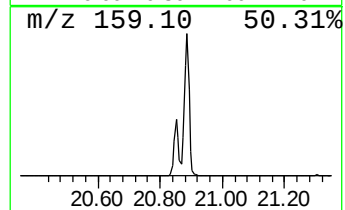
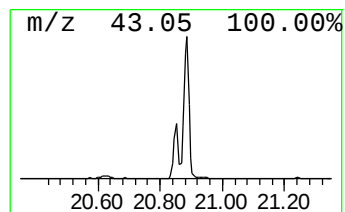
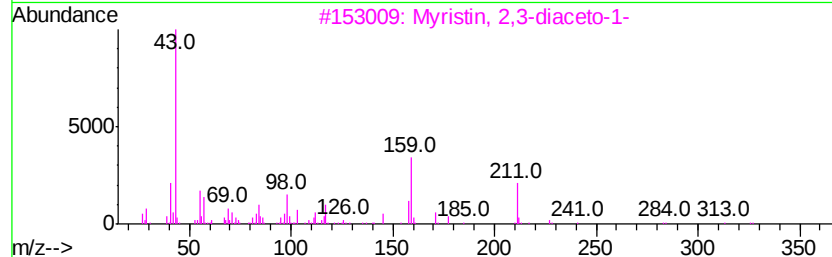
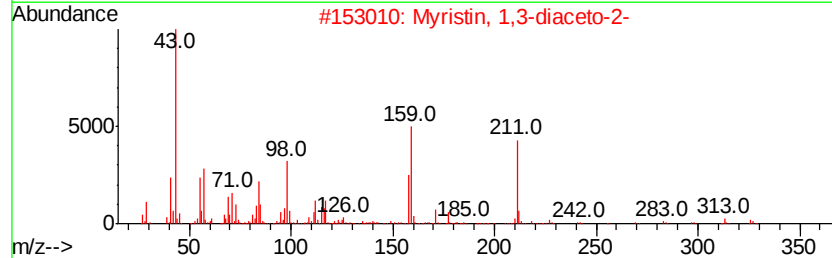
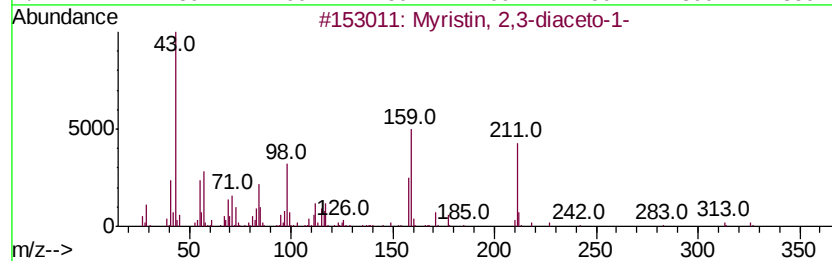
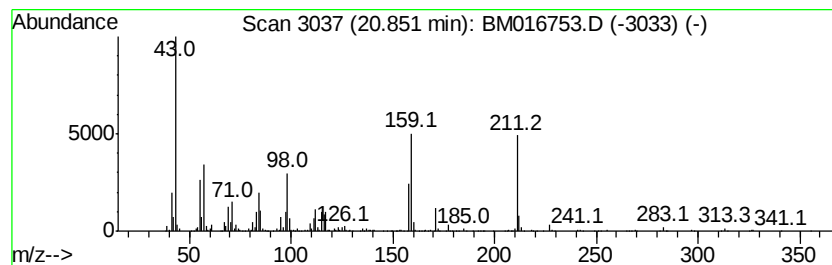
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Quant Title : SVOA CALIBRATION

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

Peak Number 15 Myristin, 2,3-diaceto-1- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	10.19 ng/ul	1903970	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	91
2		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
3		Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	72
4		Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	52
5		2-Ethoxymethyl-3-methyl-4-nitro-...	211	C10H13NO4	1000191-44-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
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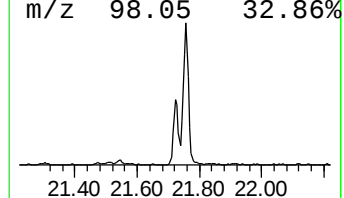
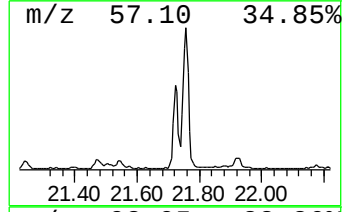
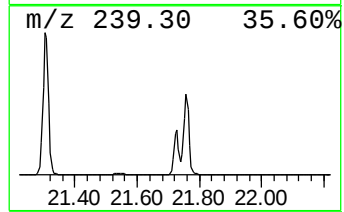
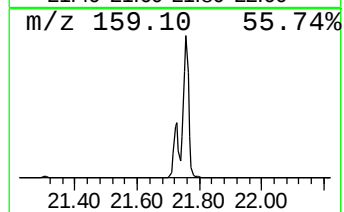
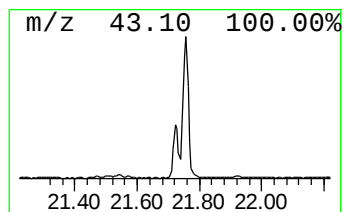
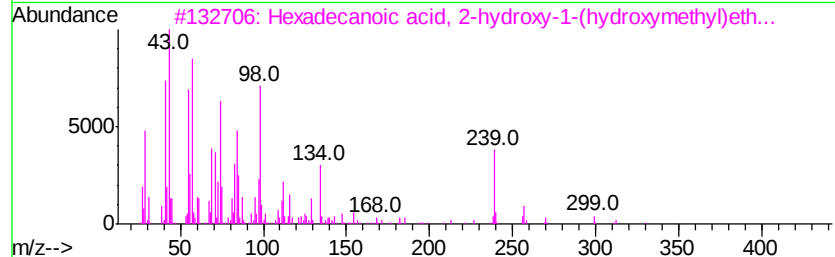
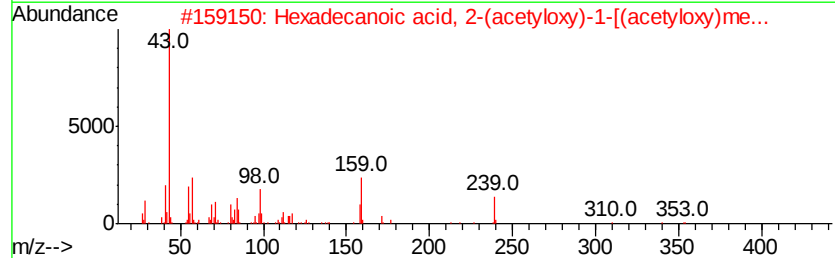
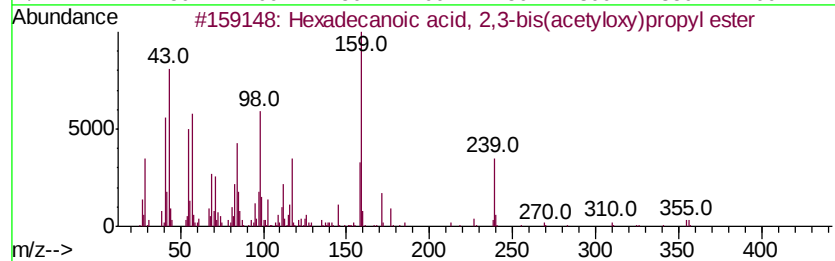
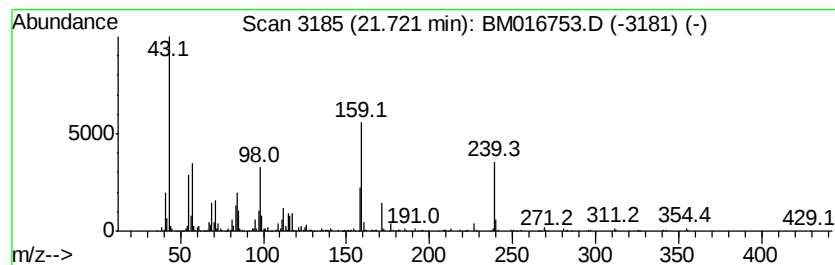
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	5.36 ng/ul	1000970	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	87
2		Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	68
3		Hexadecanoic acid, 2-hydroxy-1-(...	330	C19H38O4	023470-00-0	27
4		9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	25
5		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DB3Q7

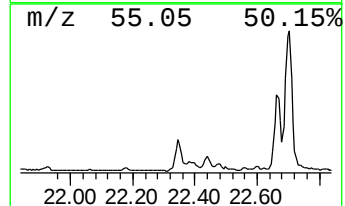
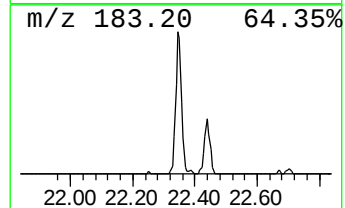
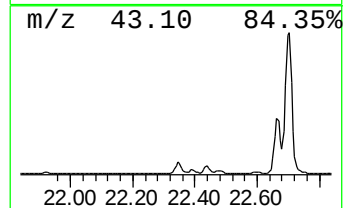
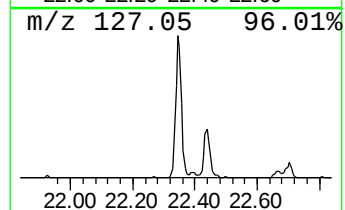
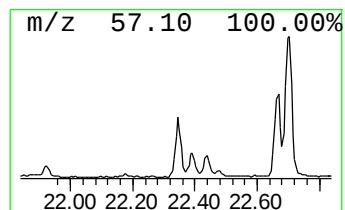
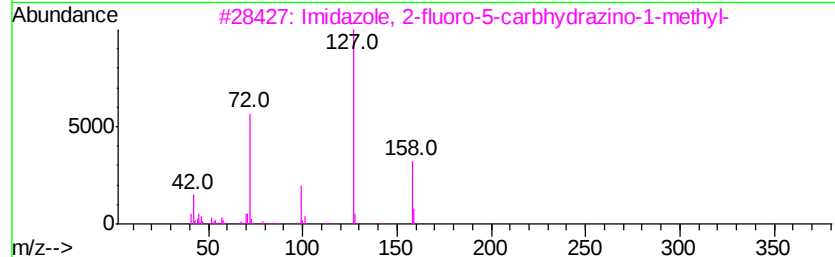
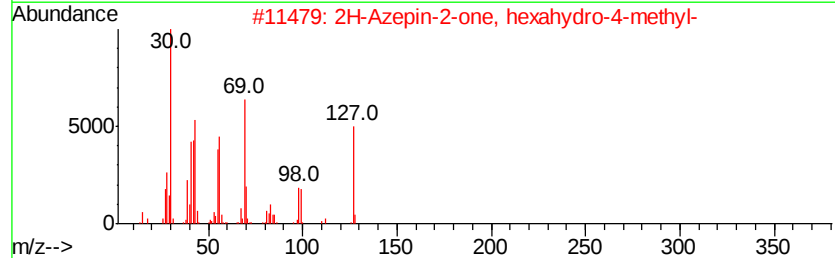
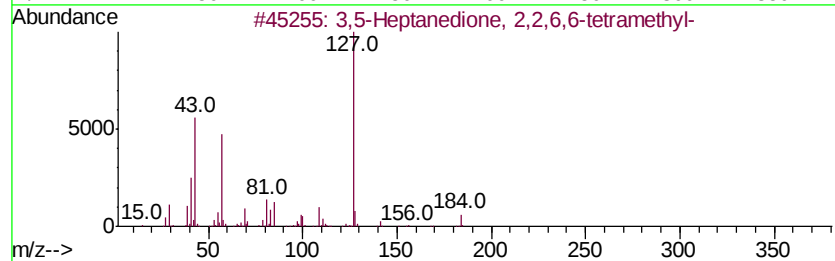
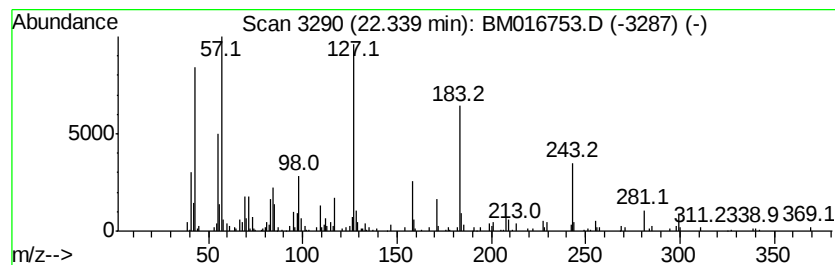
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Quant Title : SVOA CALIBRATION

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

Peak Number 19 unknown-08 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	2.08 ng/ul	388178	Chrysene-d12	21.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	30
2			2H-Azepin-2-one, hexahydro-4-met...	127	C7H13NO	003623-05-0	27
3			Imidazole, 2-fluoro-5-carbhvdraz...	158	C5H7FN4O	1000129-58-0	27
4			4-Amino-2,6-dihydroxypvrimidine	127	C4H5N3O2	000873-83-6	27
5			3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM091418\
Data File : BM016753.D
Acq On : 14 Sep 2018 14:58
Operator : SJ/JU
Sample : J4868-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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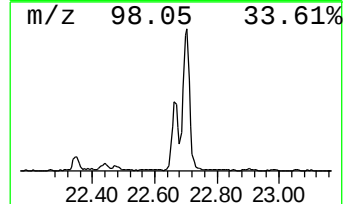
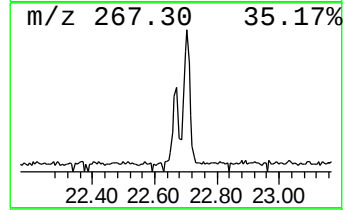
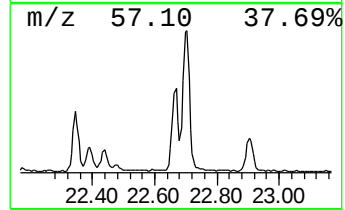
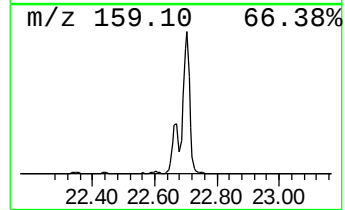
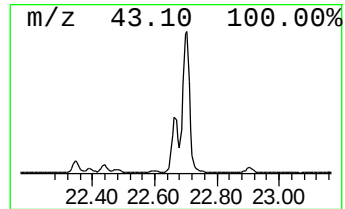
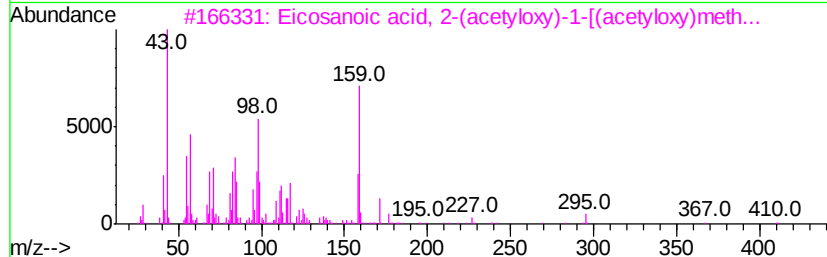
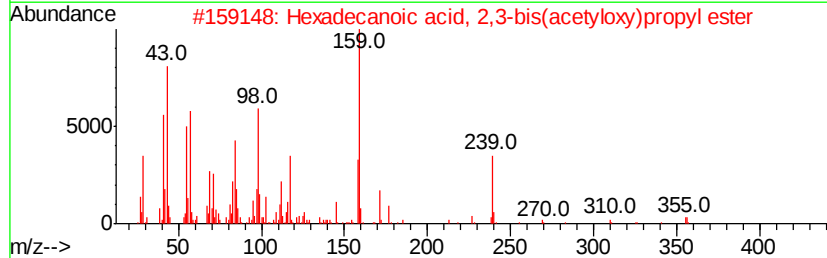
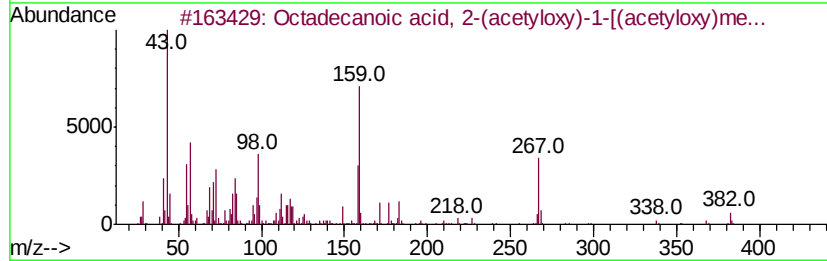
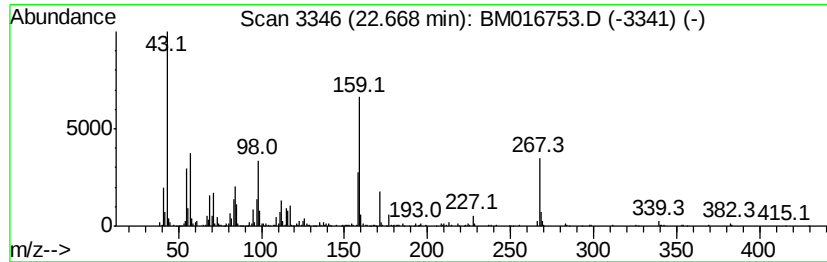
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Quant Title : SVOA CALIBRATION

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

Peak Number 20 Octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.67	5.48 ng/ul	1099450	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester	442	C25H46O6	055401-62-2	91
2		Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	58
3		Eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester	470	C27H50O6	055429-68-0	46
4		Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	25
5		2,3,4-Trifluorobenzoic acid, 2-pyridyl ester	386	C22H33F3O2	1000280-62-1	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM091418\
 Data File : BM016753.D
 Acq On : 14 Sep 2018 14:58
 Operator : SJ/JU
 Sample : J4868-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DB3Q7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM091018MA.M
 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
Butane, 2-methoxy...	3.02	39.6	ng/ul	2896030	1	7.73	1463830	20.0
1-Hexanol, 2-ethyl-	7.80	5.7	ng/ul	417722	1	7.73	1463830	20.0
Phenol, 2-methoxy-	8.82	3.5	ng/ul	255153	1	7.73	1463830	20.0
Propanoic acid, 2...	12.98	2.1	ng/ul	268010	3	14.37	2604760	20.0
Vanillin	13.28	2.5	ng/ul	326253	3	14.37	2604760	20.0
unknown-01	17.42	2.7	ng/ul	400391	4	17.12	2951600	20.0
unknown-02	17.47	6.0	ng/ul	884656	4	17.12	2951600	20.0
7,9-Di-tert-butyl...	17.80	2.5	ng/ul	371938	4	17.12	2951600	20.0
unknown-03	18.75	2.8	ng/ul	413375	4	17.12	2951600	20.0
unknown-04	18.79	6.3	ng/ul	926425	4	17.12	2951600	20.0
Octadecanoic acid	19.32	3.8	ng/ul	703508	5	21.30	3738360	20.0
unknown-05	19.59	2.8	ng/ul	516118	5	21.30	3738360	20.0
unknown-06	19.87	21.1	ng/ul	3946720	5	21.30	3738360	20.0
unknown-07	19.92	44.2	ng/ul	8254730	5	21.30	3738360	20.0
Myristin, 2,3-dia...	20.85	10.2	ng/ul	1903970	5	21.30	3738360	20.0
Hexadecanoic acid...	21.72	5.4	ng/ul	1000970	5	21.30	3738360	20.0
unknown-08	22.34	2.1	ng/ul	388178	5	21.30	3738360	20.0
Octadecanoic acid...	22.67	5.5	ng/ul	1099450	6	23.54	4009850	20.0