

Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
 Data File : BM010702.D
 Acq On : 23 Jun 2017 22:26
 Operator : SJ/JU
 Sample : I3857-02MS
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 H2TR7MS

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.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	6.175	554	559	563	rVB3	16356	22353	1.17%	0.073%
2	6.469	604	609	616	rVB2	42790	58797	3.09%	0.191%
3	6.646	633	639	641	rBV	243222	378021	19.84%	1.226%
4	6.669	641	643	652	rVB	266667	369459	19.39%	1.199%
5	6.810	659	667	674	rBV	158251	236695	12.42%	0.768%
6	6.904	677	683	689	rBV3	13417	20128	1.06%	0.065%
7	6.999	693	699	702	rBV	249025	418376	21.95%	1.357%
8	7.028	702	704	711	rVB	242819	304833	16.00%	0.989%
9	7.463	771	778	780	rBV	306793	476724	25.02%	1.547%
10	7.493	780	783	790	rVB	291824	445942	23.40%	1.447%
11	7.734	818	824	830	rVB2	20684	31230	1.64%	0.101%
12	8.163	891	897	904	rVB	319230	500228	26.25%	1.623%
13	8.263	907	914	922	rBV	229597	336907	17.68%	1.093%
14	8.604	966	972	980	rBV	240795	382352	20.06%	1.241%
15	9.316	1086	1093	1100	rBB2	232197	366343	19.22%	1.189%
16	9.463	1111	1118	1125	rBB3	12601	21140	1.11%	0.069%
17	9.845	1177	1183	1191	rVB	376161	579751	30.42%	1.881%
18	10.087	1217	1224	1233	rBB	417007	685730	35.98%	2.225%
19	10.222	1239	1247	1254	rBV	478213	761394	39.95%	2.470%
20	10.363	1263	1271	1279	rBV	276172	433820	22.76%	1.408%
21	11.516	1460	1467	1475	rVB	447229	682262	35.80%	2.214%
22	12.245	1588	1591	1598	rBV2	34249	48037	2.52%	0.156%
23	13.533	1804	1810	1814	rBV	719948	974683	51.14%	3.162%
24	13.581	1814	1818	1824	rVB	317023	422598	22.18%	1.371%
25	13.798	1849	1855	1863	rVB	734918	1036794	54.40%	3.364%
26	14.110	1902	1908	1914	rBV2	758408	1153928	60.55%	3.744%
27	14.175	1914	1919	1924	rVV	796318	1148132	60.25%	3.725%
28	14.222	1924	1927	1935	rVB4	38719	69572	3.65%	0.226%
29	14.333	1938	1946	1956	rBV3	510103	977126	51.27%	3.170%
30	14.486	1966	1972	1978	rBV	496461	641072	33.64%	2.080%
31	14.998	2056	2059	2066	rVB3	19053	21907	1.15%	0.071%
32	15.110	2072	2078	2086	rBV	969651	1318377	69.18%	4.277%
33	15.233	2094	2099	2105	rBV	354466	477528	25.06%	1.549%
34	15.863	2202	2206	2209	rBV2	18094	24253	1.27%	0.079%

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35	15.898	2209	2212	2218	rVB3	20963	23755	1.25%	0.077%
36	16.516	2312	2317	2325	rBV	652871	880455	46.20%	2.857%
37	16.863	2370	2376	2383	rBV	1024695	1488889	78.13%	4.831%
38	16.963	2387	2393	2401	rBV	1087132	1485069	77.93%	4.818%
39	17.792	2527	2534	2540	rBV	208336	283307	14.87%	0.919%
40	19.086	2749	2754	2763	rBV	135814	190699	10.01%	0.619%
41	19.274	2780	2786	2789	rBV	1235703	1905725	100.00%	6.183%
42	19.304	2789	2791	2801	rVB	1390492	1523830	79.96%	4.944%
43	19.504	2820	2825	2830	rBV6	26035	44947	2.36%	0.146%
44	19.733	2861	2864	2868	rVB2	26712	29682	1.56%	0.096%
45	19.833	2875	2881	2886	rBV7	31350	49091	2.58%	0.159%
46	19.986	2903	2907	2913	rVB6	65196	86078	4.52%	0.279%
47	20.074	2917	2922	2927	rBV3	60261	72895	3.83%	0.237%
48	20.180	2936	2940	2945	rVB7	46584	59221	3.11%	0.192%
49	20.233	2945	2949	2951	rBV4	19109	25823	1.36%	0.084%
50	20.280	2951	2957	2962	rVV	52145	102268	5.37%	0.332%
51	20.327	2962	2965	2974	rVB9	37573	62174	3.26%	0.202%
52	20.480	2988	2991	2993	rBV3	19258	22143	1.16%	0.072%
53	20.651	3016	3020	3025	rBV8	74773	123649	6.49%	0.401%
54	20.780	3037	3042	3045	rBV	366404	474526	24.90%	1.540%
55	20.815	3045	3048	3061	rVB	264282	373246	19.59%	1.211%
56	20.998	3075	3079	3082	rBV3	69505	83078	4.36%	0.270%
57	21.027	3082	3084	3087	rVV3	44632	48750	2.56%	0.158%
58	21.080	3088	3093	3098	rVV	1344118	1607325	84.34%	5.215%
59	21.121	3098	3100	3104	rVB5	79322	94649	4.97%	0.307%
60	21.233	3117	3119	3122	rBV4	16925	22767	1.19%	0.074%
61	21.415	3147	3150	3153	rBV4	27384	26951	1.41%	0.087%
62	21.698	3194	3198	3205	rVB7	103582	152208	7.99%	0.494%
63	22.003	3246	3250	3255	rVB5	45517	72440	3.80%	0.235%
64	22.245	3288	3291	3298	rBV3	34637	48463	2.54%	0.157%
65	22.609	3349	3353	3356	rBV2	69032	83495	4.38%	0.271%
66	23.086	3428	3434	3441	rBV2	708341	1209046	63.44%	3.923%
67	23.145	3441	3444	3449	rVB4	49560	69125	3.63%	0.224%
68	23.221	3451	3457	3464	rVB	656593	1171720	61.48%	3.802%
69	23.756	3543	3548	3554	rVB3	96698	176852	9.28%	0.574%
70	23.827	3554	3560	3569	rVB3	124895	253514	13.30%	0.823%
71	26.091	3937	3945	3955	rVB7	208306	567403	29.77%	1.841%

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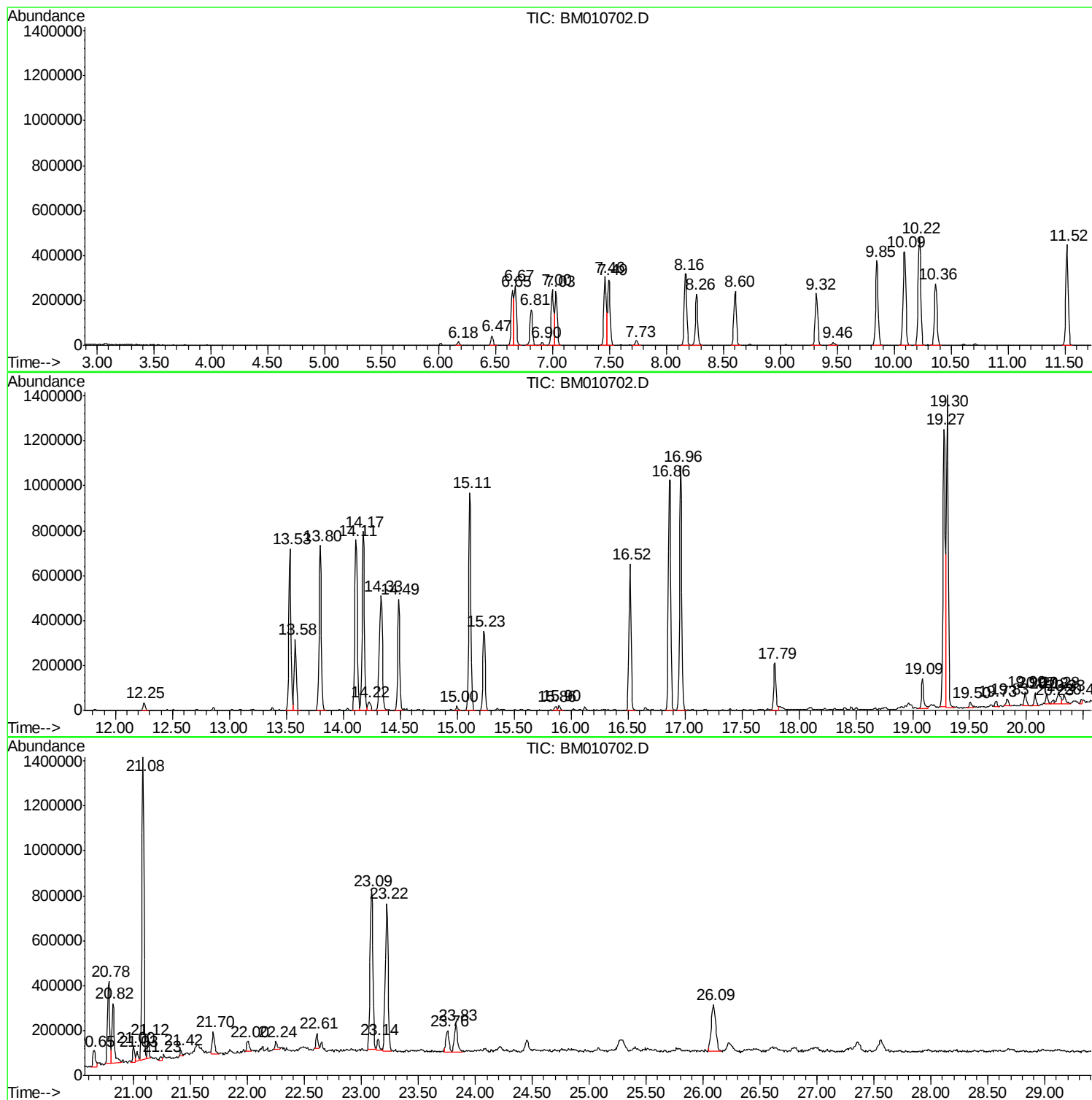
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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



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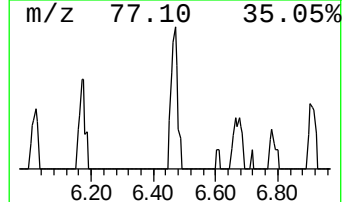
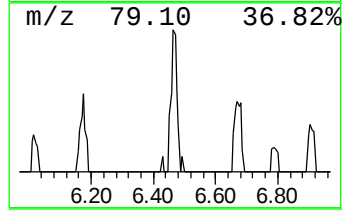
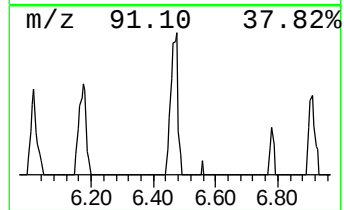
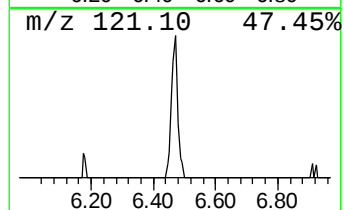
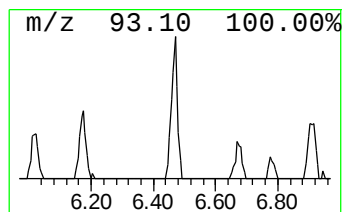
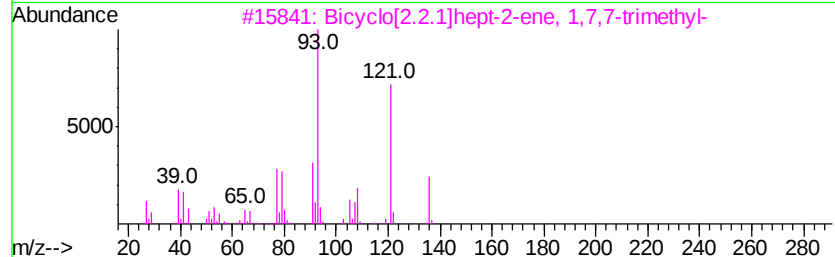
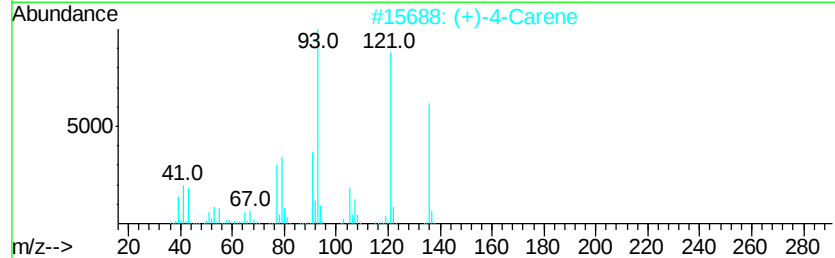
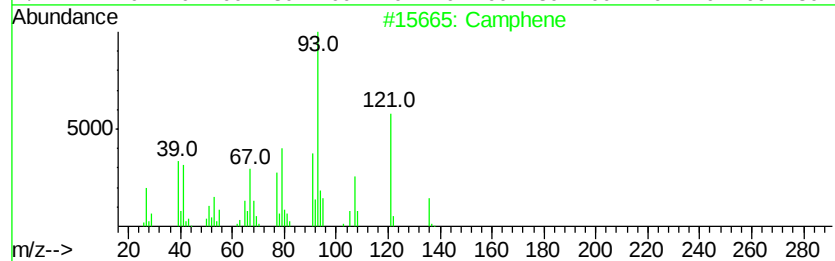
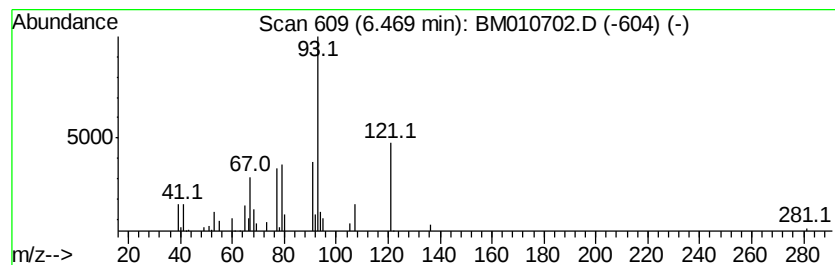
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Camphene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	2.47 ng/ul	58797	1,4-Dichlorobenzene-d4	7.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphene	136	C10H16	000079-92-5	90
2		(+)-4-Carene	136	C10H16	029050-33-7	86
3		Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	86
4		Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	86
5		2-Carene	136	C10H16	000554-61-0	86



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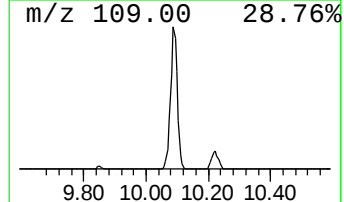
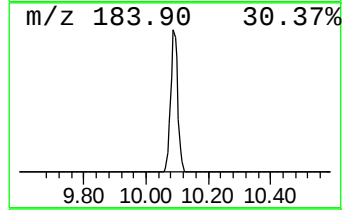
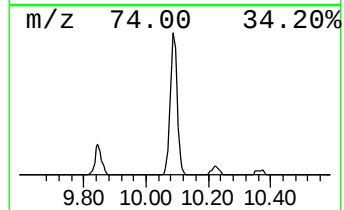
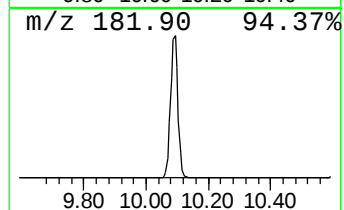
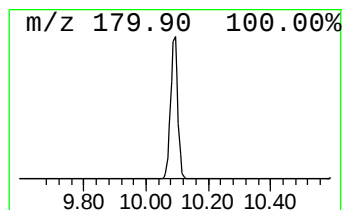
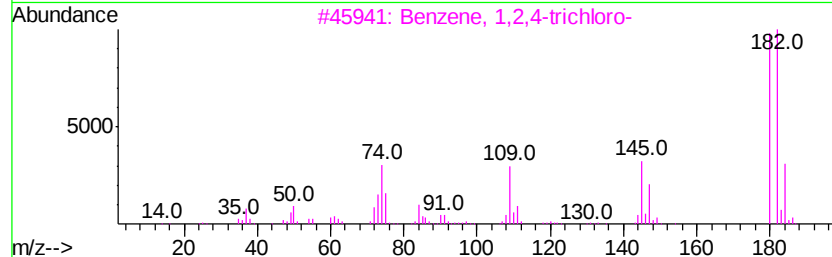
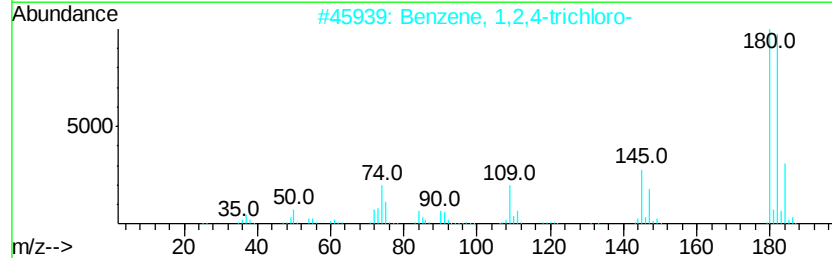
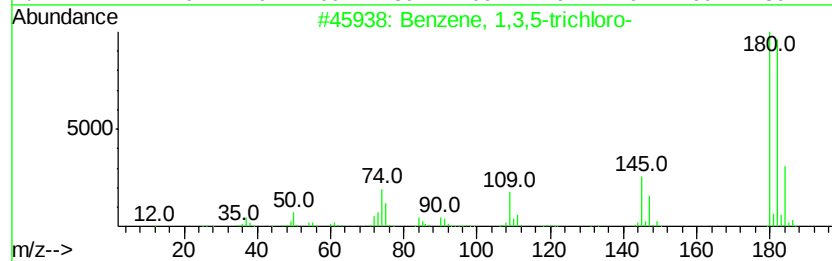
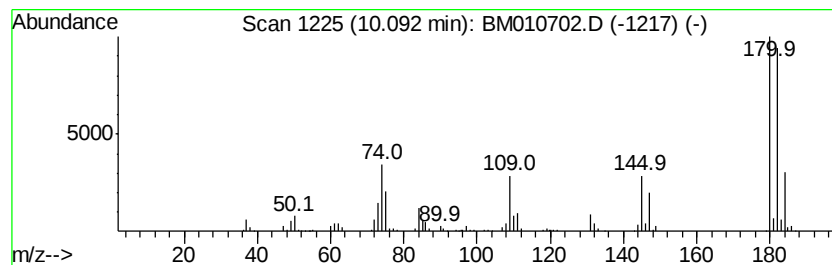
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.09	18.01 ng/ul	685730	Napthalene-d8	10.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	94
2		Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	94
3		Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	93
4		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	91
5		Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	91



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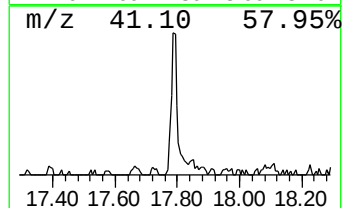
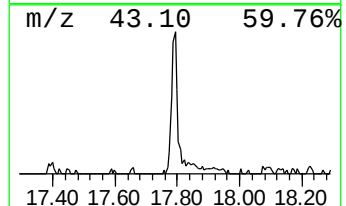
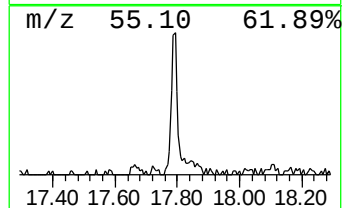
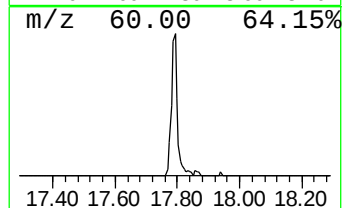
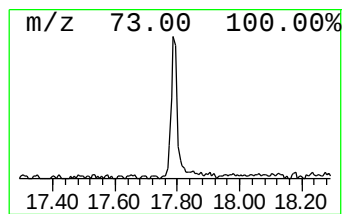
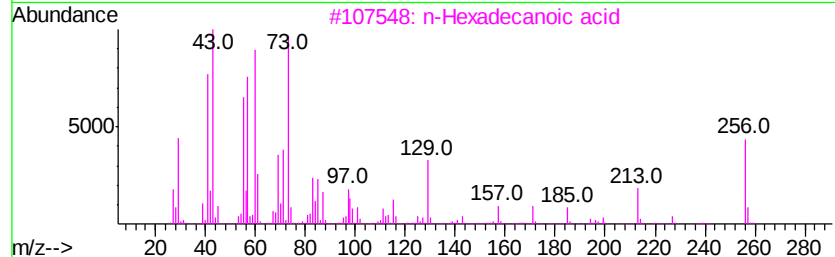
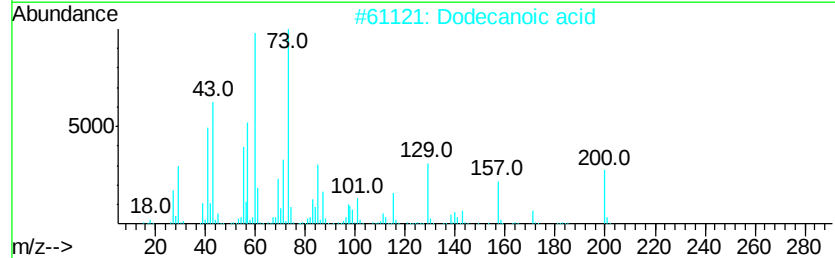
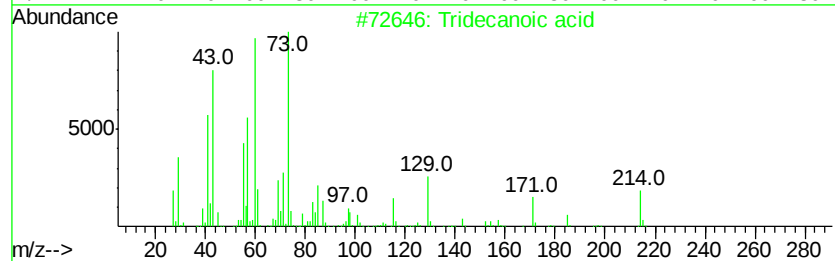
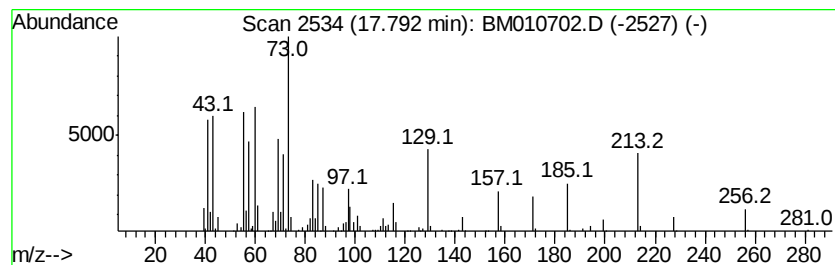
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.79	3.81 ng/ul	283307	Phenanthrene-d10		16.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	55
2	Dodecanoic acid	200	C12H24O2	000143-07-7	52
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



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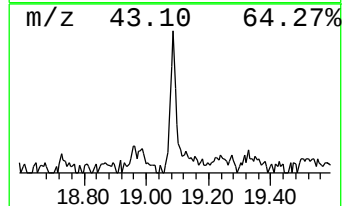
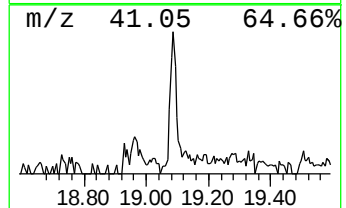
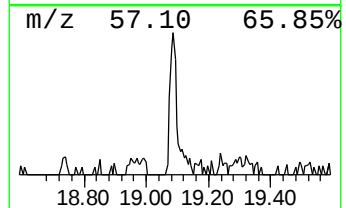
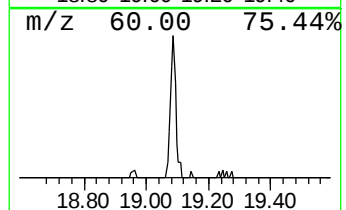
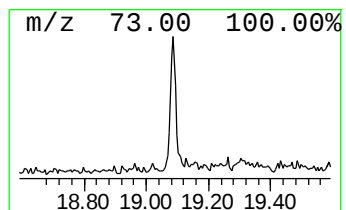
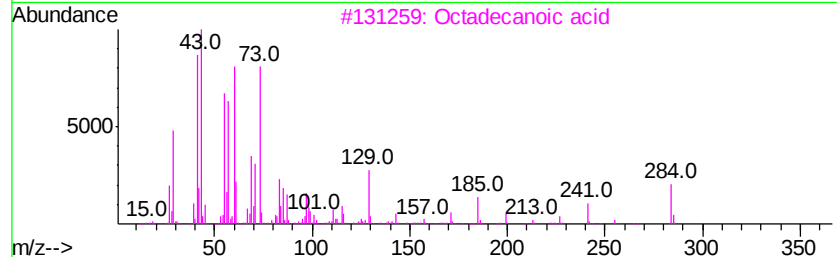
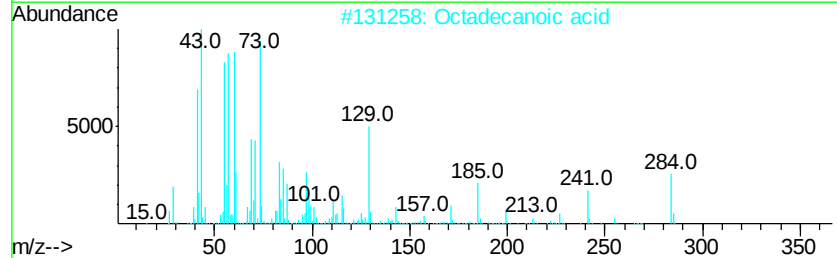
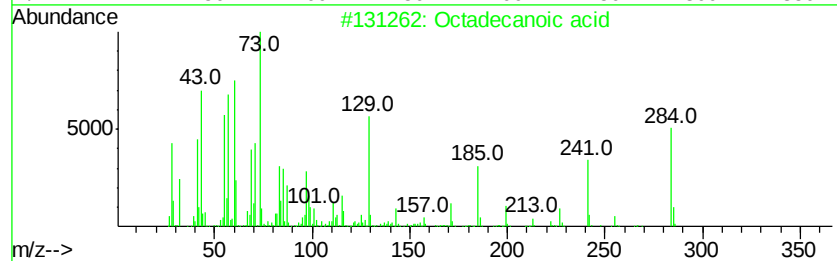
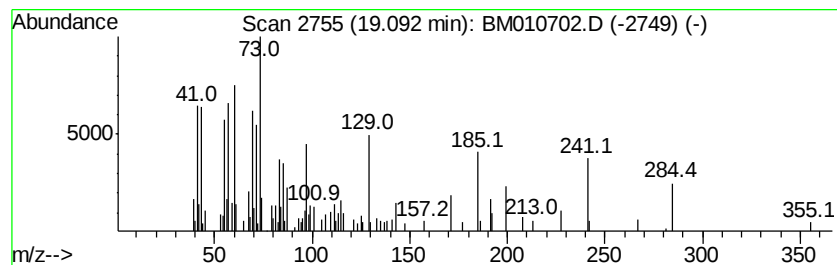
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
19.09	2.37 ng/ul	190699	Chrysene-d12		21.08		
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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	94
4			Octadecanoic acid	284	C18H36O2	000057-11-4	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	76



Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
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Acq On : 23 Jun 2017 22:26
Operator : SJ/JU
Sample : I3857-02MS
Misc :
ALS Vial : 19 Sample Multiplier: 1

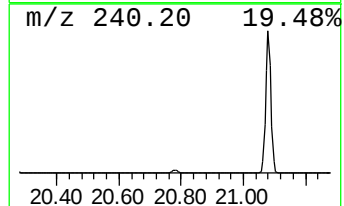
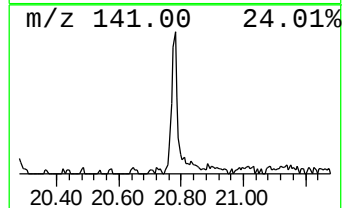
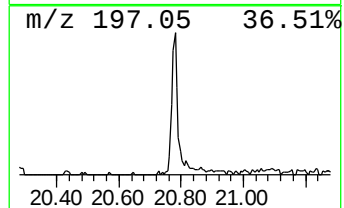
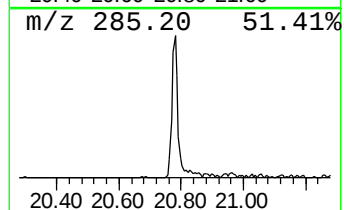
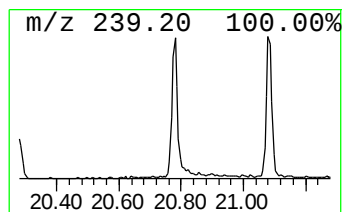
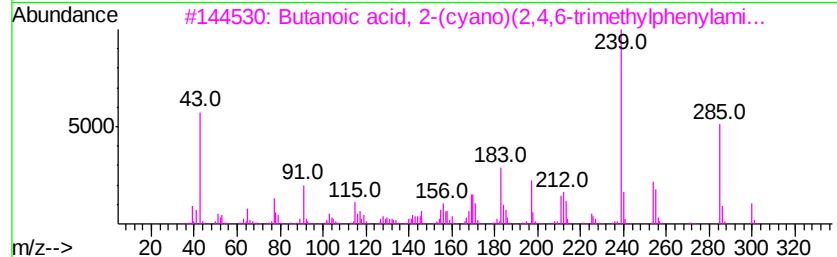
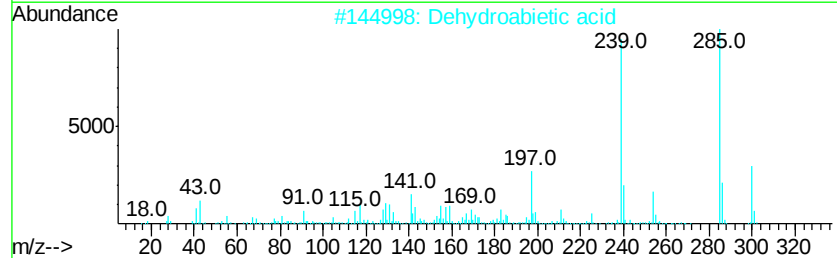
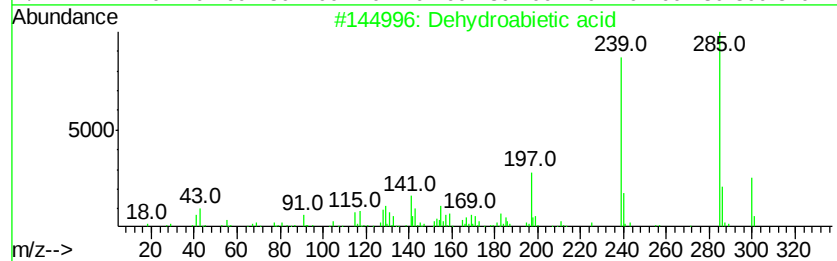
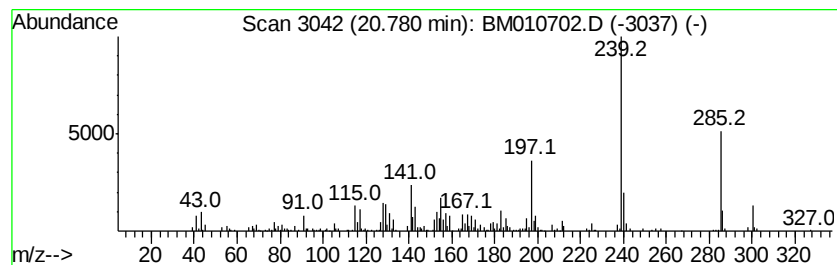
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Dehydroabietic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.78	5.90 ng/ul	474526	Chrysene-d12	21.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dehydroabietic acid	300	C20H28O2	001740-19-8	95
2		Dehydroabietic acid	300	C20H28O2	001740-19-8	91
3		Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	76
4		Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3NO3	000391-02-6	70
5		1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	59



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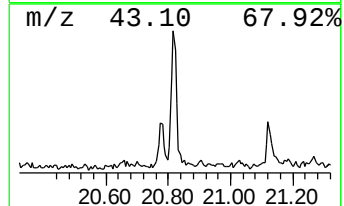
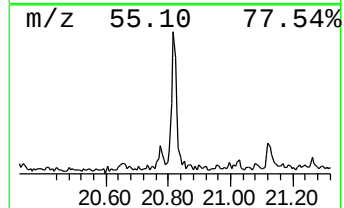
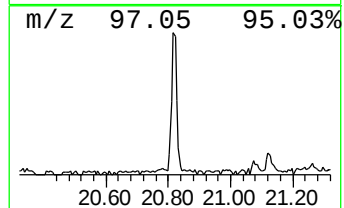
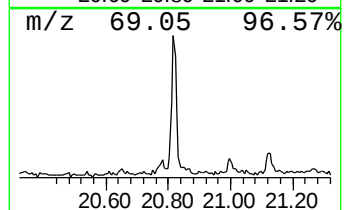
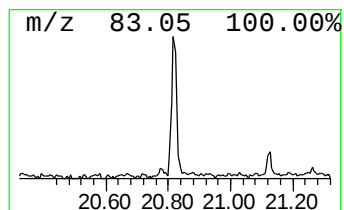
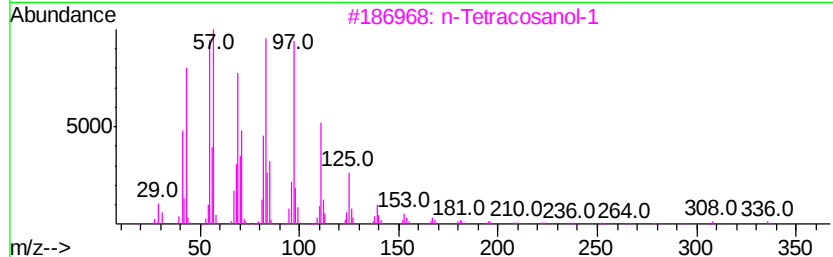
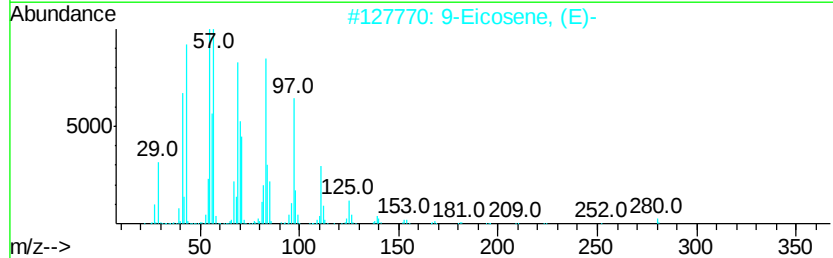
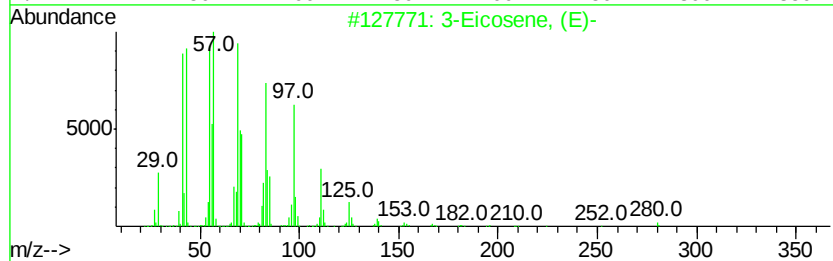
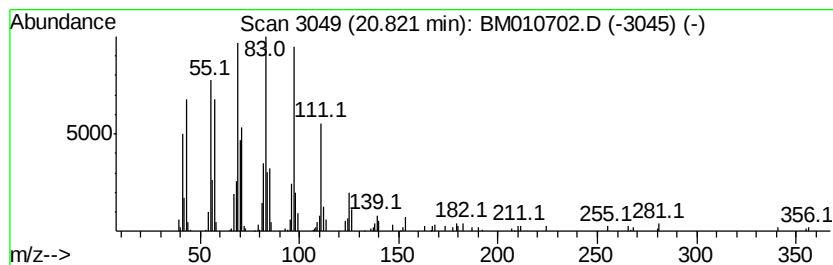
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	4.64 ng/ul	373246	Chrysene-d12	21.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	86
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	81
4		Behenic alcohol	326	C22H46O	000661-19-8	81
5		1-Heneicosanol	312	C21H44O	015594-90-8	76



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Acq On : 23 Jun 2017 22:26
Operator : SJ/JU
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Misc :
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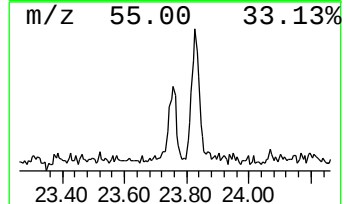
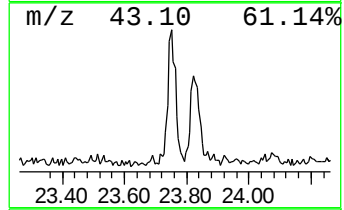
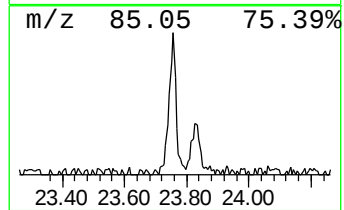
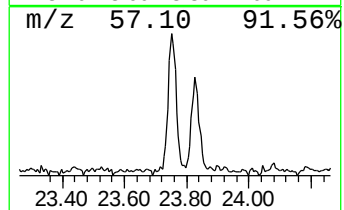
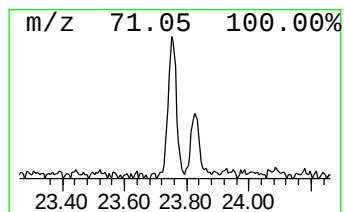
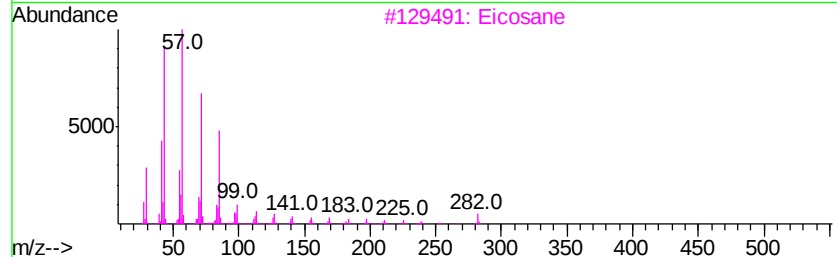
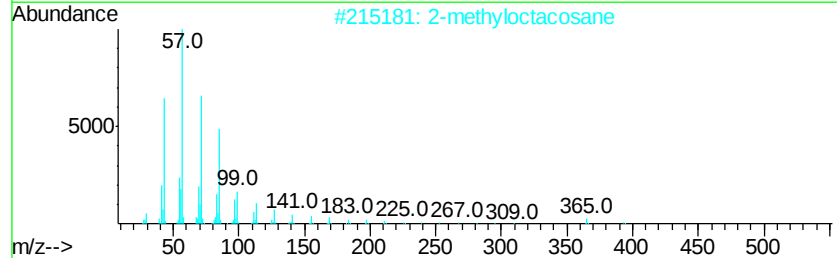
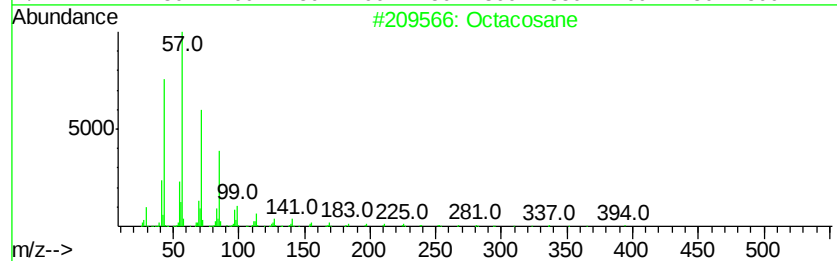
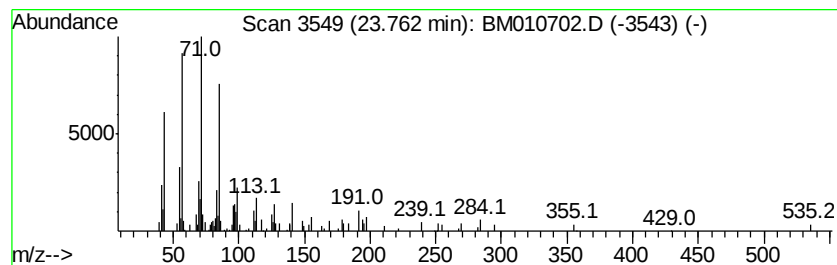
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	3.02 ng/ul	176852	Perylene-d12	23.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	62
2		2-methyloctacosane	408	C29H60	1000376-72-8	58
3		Eicosane	282	C20H42	000112-95-8	58
4		Hexacosane	366	C26H54	000630-01-3	53
5		triacontane	422	C30H62	000638-68-6	46



Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
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Acq On : 23 Jun 2017 22:26
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Sample : I3857-02MS
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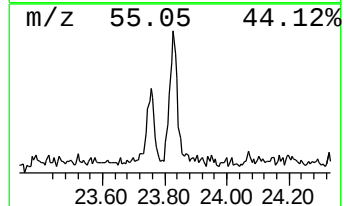
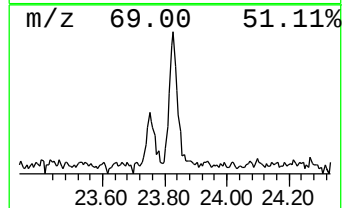
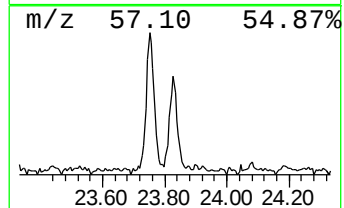
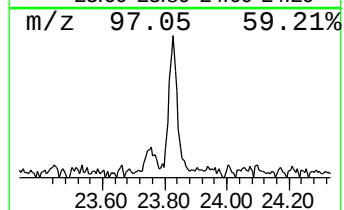
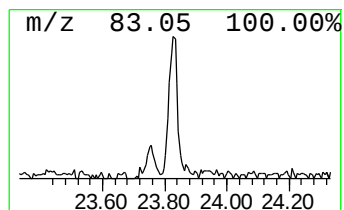
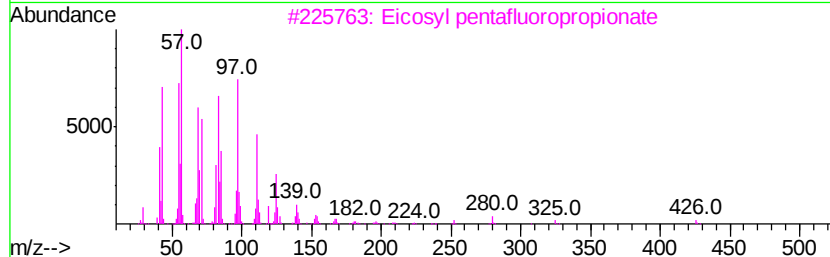
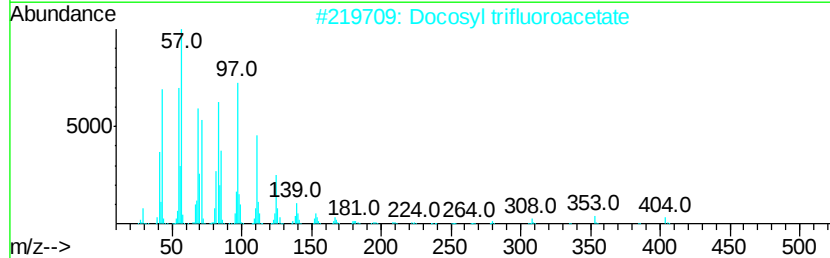
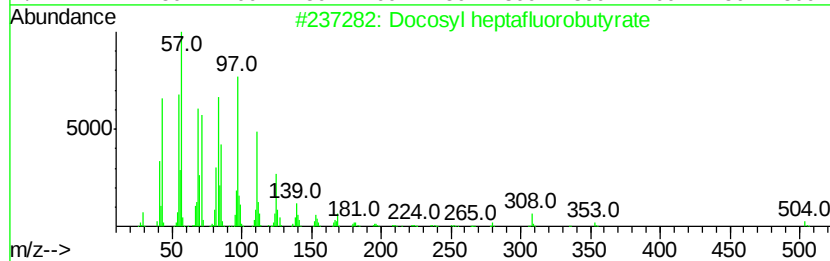
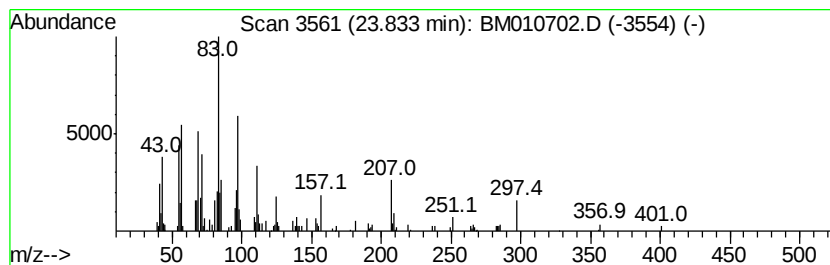
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Docosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
23.83	4.33 ng/ul	253514	Perylene-d12		23.22		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	55
2			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	55
3			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	55
4			Heptacosyl trifluoroacetate	492	C29H55F3O2	1000351-75-8	50
5			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	50



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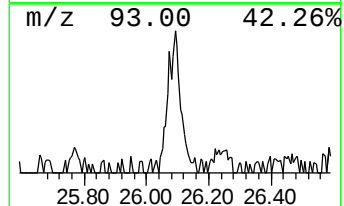
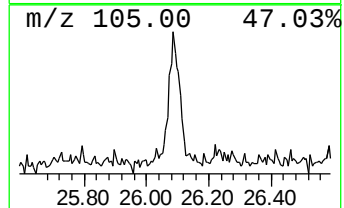
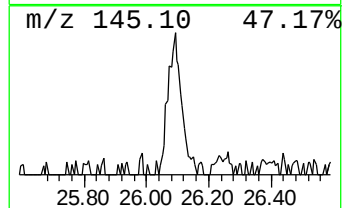
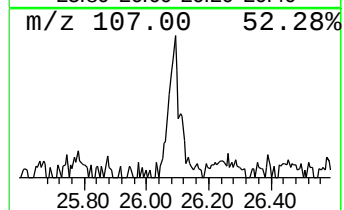
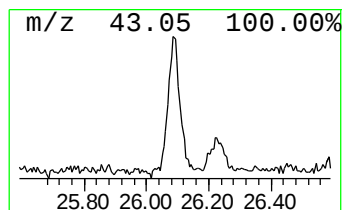
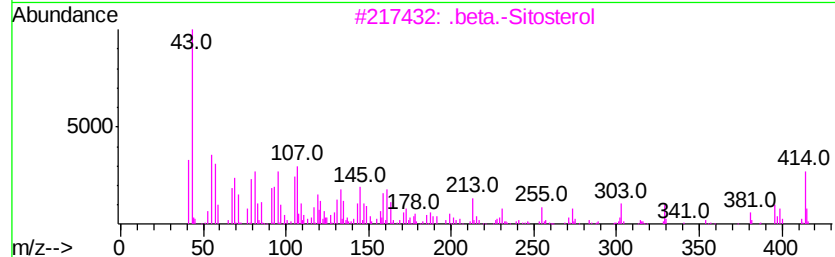
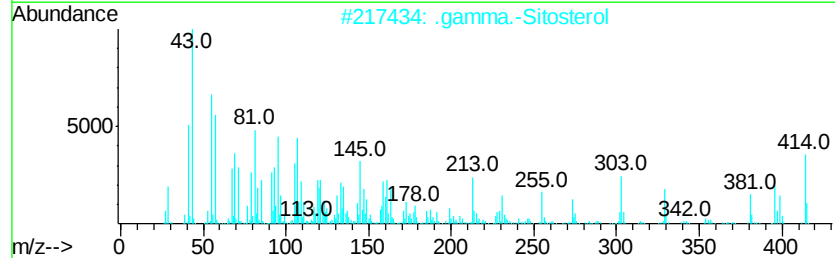
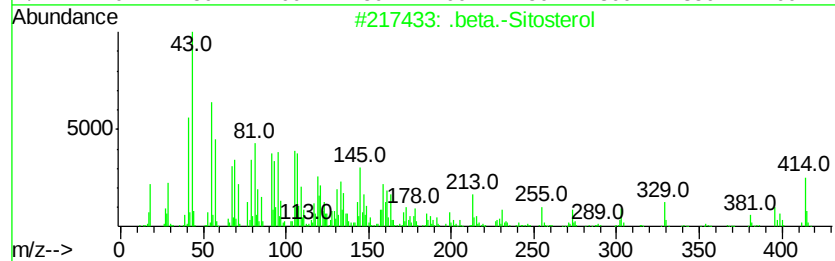
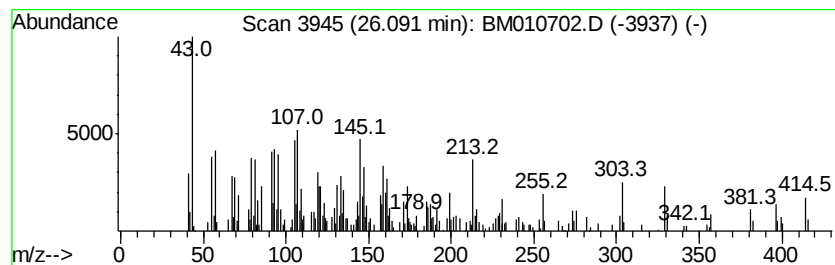
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.09	9.68 ng/ul	567403	Perylene-d12	23.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
3		.beta.-Sitosterol	414	C29H50O	000083-46-5	87
4		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	86
5		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	60



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Instrument :
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Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1,3,5-tr...	10.09	18.0	ng/ul	685730	2	10.22	761394	20.0
Tridecanoic acid	17.79	3.8	ng/ul	283307	4	16.86	1488890	20.0
Octadecanoic acid	19.09	2.4	ng/ul	190699	5	21.08	1607330	20.0
Dehydroabietic acid	20.78	5.9	ng/ul	474526	5	21.08	1607330	20.0
3-Eicosene, (E)-	20.82	4.6	ng/ul	373246	5	21.08	1607330	20.0
Octacosane	23.76	3.0	ng/ul	176852	6	23.22	1171720	20.0
Docosyl heptaflu...	23.83	4.3	ng/ul	253514	6	23.22	1171720	20.0
.beta.-Sitosterol	26.09	9.7	ng/ul	567403	6	23.22	1171720	20.0