

Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
 Data File : BM010704.D
 Acq On : 23 Jun 2017 23:38
 Operator : SJ/JU
 Sample : I3857-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 H2TR8

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	6.646	633	639	648	rBV	282823	435772	23.62%	1.784%
2	6.810	657	667	674	rBV	182487	282208	15.30%	1.155%
3	6.998	693	699	705	rVB	281010	416079	22.56%	1.703%
4	7.457	771	777	785	rVB	334371	509993	27.65%	2.088%
5	8.163	891	897	904	rVB	363232	561955	30.46%	2.301%
6	8.604	965	972	980	rBB	284697	440779	23.89%	1.804%
7	9.316	1087	1093	1101	rVB	268077	417858	22.65%	1.711%
8	9.481	1112	1121	1126	rBV2	32719	59135	3.21%	0.242%
9	9.845	1177	1183	1191	rBB	425575	667430	36.18%	2.732%
10	10.086	1216	1224	1230	rBV3	32611	52994	2.87%	0.217%
11	10.222	1240	1247	1255	rBB	520301	814849	44.17%	3.336%
12	10.363	1264	1271	1278	rBV	223354	354977	19.24%	1.453%
13	13.374	1778	1783	1790	rBV2	56534	75129	4.07%	0.308%
14	13.533	1803	1810	1814	rBV	753209	1050271	56.93%	4.300%
15	13.580	1814	1818	1824	rVB	384374	506275	27.44%	2.073%
16	13.798	1849	1855	1863	rVB	817396	1171723	63.52%	4.797%
17	14.110	1902	1908	1916	rVB2	818589	1220796	66.18%	4.998%
18	14.321	1936	1944	1952	rBV	364589	497031	26.94%	2.035%
19	14.998	2054	2059	2065	rVB2	19238	23654	1.28%	0.097%
20	15.110	2072	2078	2088	rVB	1054979	1468650	79.61%	6.012%
21	15.233	2093	2099	2106	rVV	366700	495127	26.84%	2.027%
22	15.863	2202	2206	2215	rBV2	18661	30580	1.66%	0.125%
23	16.021	2228	2233	2237	rVB5	16339	21159	1.15%	0.087%
24	16.868	2371	2377	2385	rVB2	1132490	1558713	84.50%	6.381%
25	16.962	2385	2393	2403	rBV2	1194047	1651080	89.50%	6.759%
26	17.662	2506	2512	2517	rBV5	10697	19743	1.07%	0.081%
27	17.792	2528	2534	2545	rBV	240700	331316	17.96%	1.356%
28	18.104	2581	2587	2597	rVB7	12235	30766	1.67%	0.126%
29	18.427	2639	2642	2645	rBV3	21454	25098	1.36%	0.103%
30	18.662	2677	2682	2686	rBV6	10914	19114	1.04%	0.078%
31	18.751	2693	2697	2705	rVB6	18944	26868	1.46%	0.110%
32	18.933	2725	2728	2730	rVV3	17777	21944	1.19%	0.090%
33	18.962	2730	2733	2742	rVB5	31862	59549	3.23%	0.244%
34	19.086	2749	2754	2763	rBV	175146	230259	12.48%	0.943%

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35	19.162	2763	2767	2773	rVB5	14535	25852	1.40%	0.106%
36	19.274	2780	2786	2792	rVB	1426096	1844703	100.00%	7.552%
37	19.733	2861	2864	2868	rBV6	16854	22973	1.25%	0.094%
38	19.833	2875	2881	2886	rBV10	49757	72209	3.91%	0.296%
39	19.986	2903	2907	2914	rBV4	63988	104221	5.65%	0.427%
40	20.174	2931	2939	2943	rBV2	182054	242892	13.17%	0.994%
41	20.292	2953	2959	2962	rBV	38714	86452	4.69%	0.354%
42	20.650	3016	3020	3025	rBV6	65426	93233	5.05%	0.382%
43	20.774	3037	3041	3045	rBV	253788	330894	17.94%	1.355%
44	20.815	3045	3048	3058	rVV	301447	414165	22.45%	1.696%
45	21.027	3081	3084	3087	rBV4	28383	32581	1.77%	0.133%
46	21.080	3088	3093	3098	rBV	1397327	1671918	90.63%	6.845%
47	21.121	3098	3100	3105	rVB2	104187	115182	6.24%	0.472%
48	21.262	3121	3124	3129	rVB7	23226	25394	1.38%	0.104%
49	21.697	3194	3198	3201	rBV3	90421	105202	5.70%	0.431%
50	21.997	3246	3249	3255	rBV7	50393	64501	3.50%	0.264%
51	22.244	3288	3291	3298	rVB2	70753	92650	5.02%	0.379%
52	22.609	3350	3353	3356	rBV3	57486	67251	3.65%	0.275%
53	23.086	3428	3434	3441	rVB2	783533	1322834	71.71%	5.415%
54	23.144	3441	3444	3449	rVB7	29253	42429	2.30%	0.174%
55	23.221	3450	3457	3465	rVB	671701	1206022	65.38%	4.937%
56	23.750	3543	3547	3553	rVB3	59414	98995	5.37%	0.405%
57	23.827	3555	3560	3566	rBV5	99467	178795	9.69%	0.732%
58	24.080	3599	3603	3611	rVB10	38331	84414	4.58%	0.346%
59	26.085	3936	3944	3955	rVB7	194338	532508	28.87%	2.180%

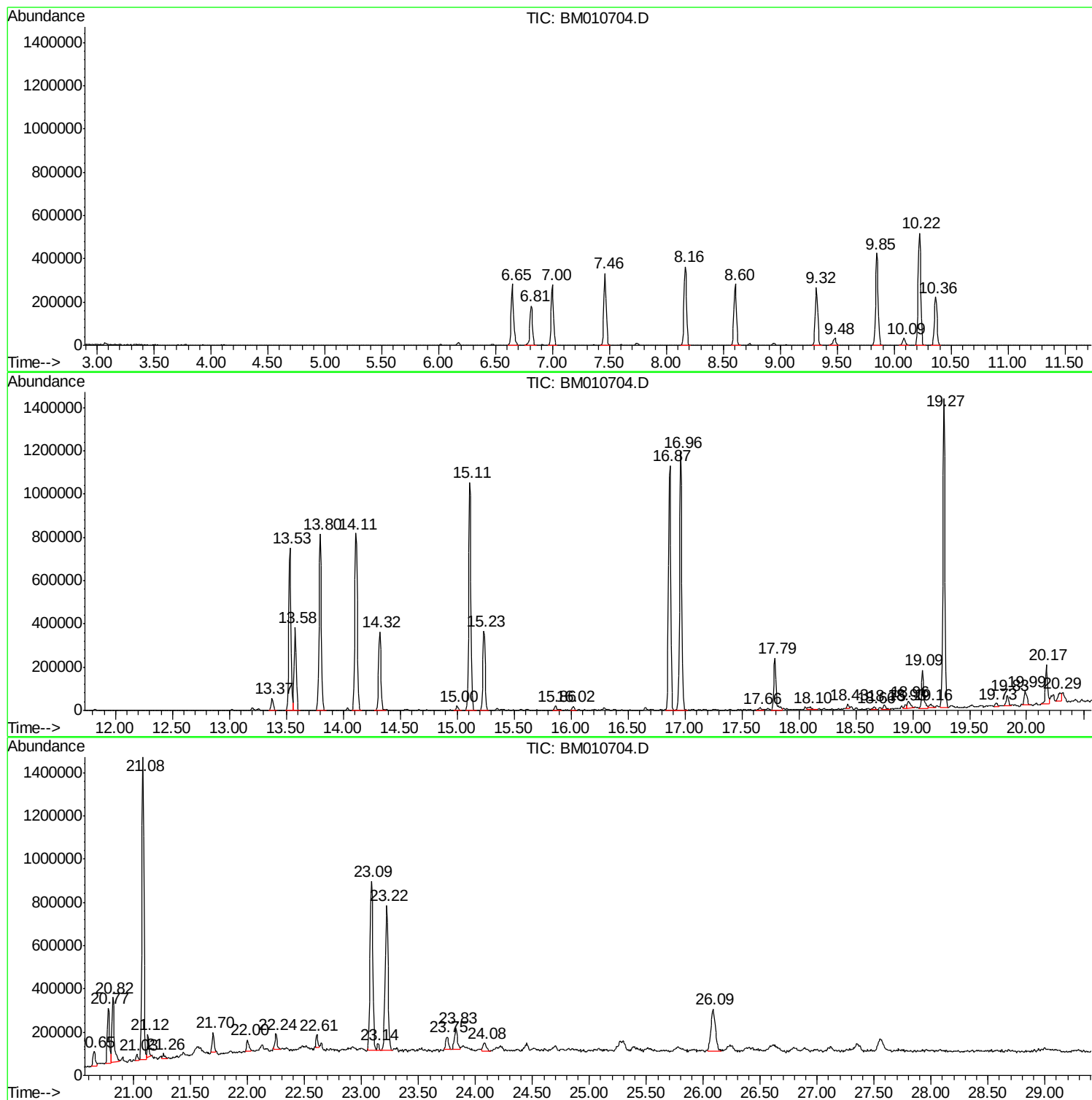
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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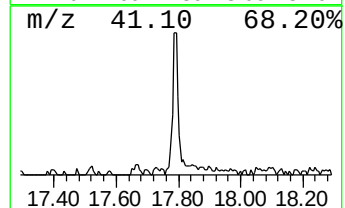
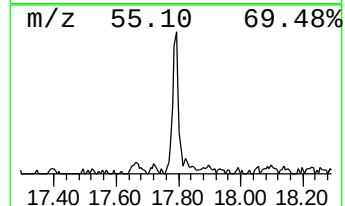
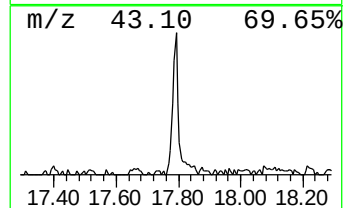
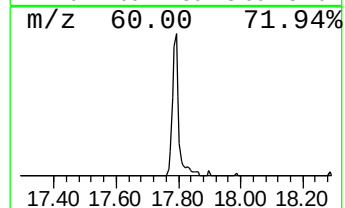
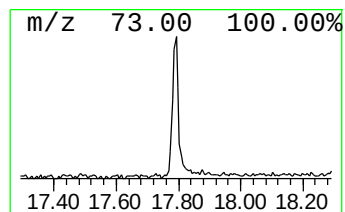
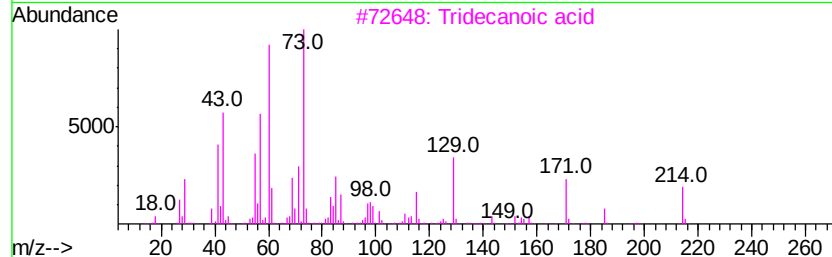
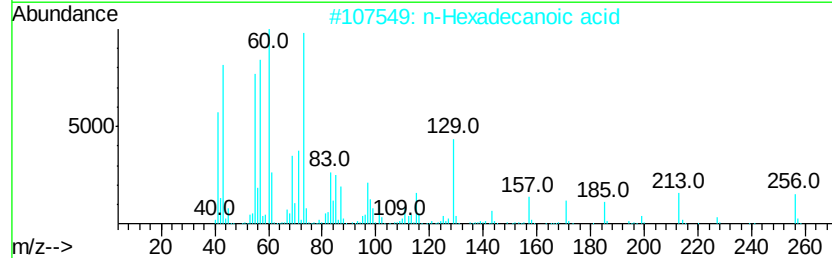
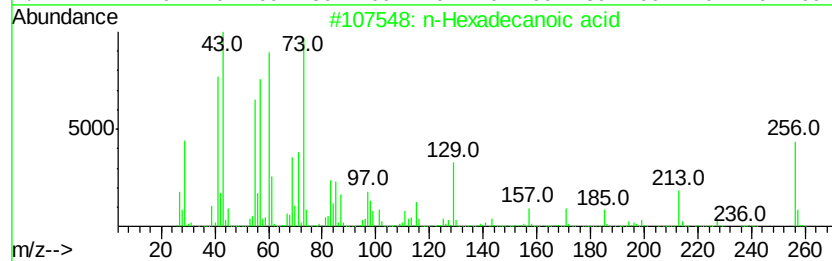
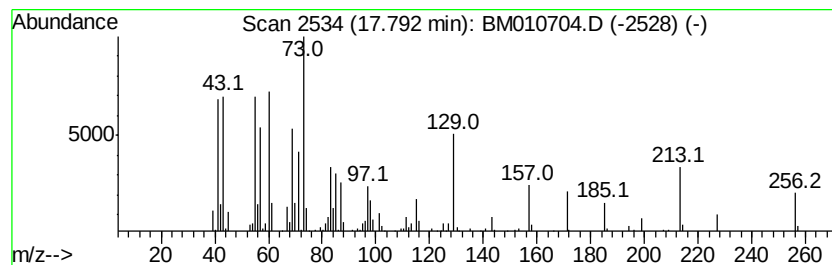
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.79	4.25 ng/ul	331316	Phenanthrene-d10	16.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78	
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52	
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50	
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47	



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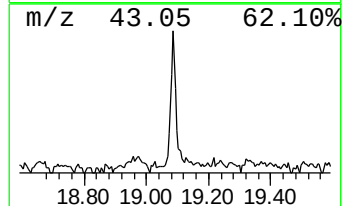
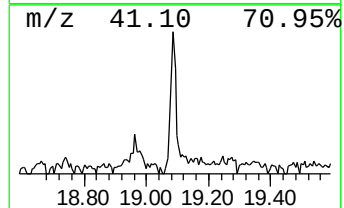
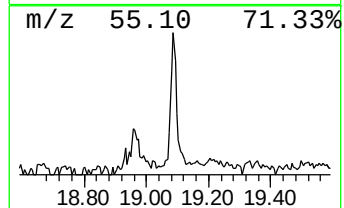
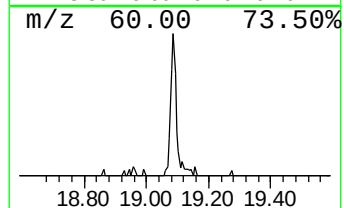
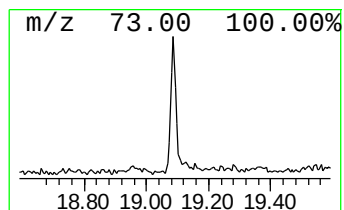
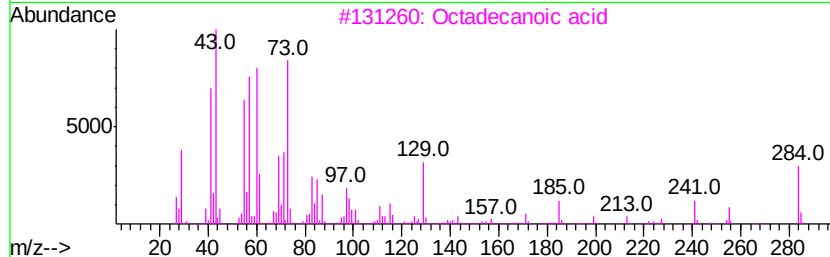
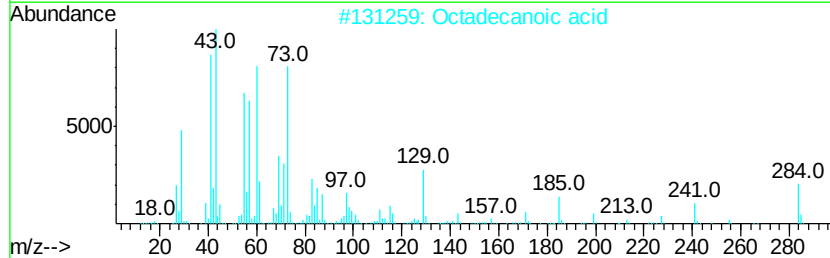
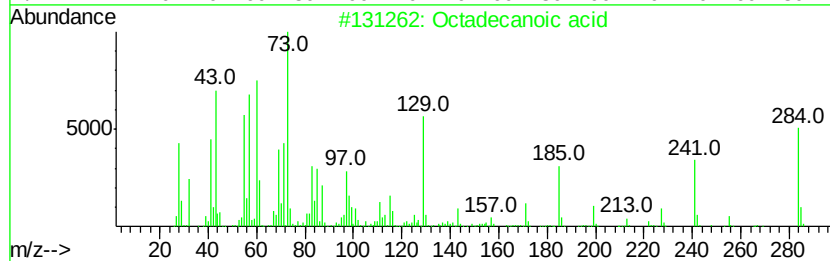
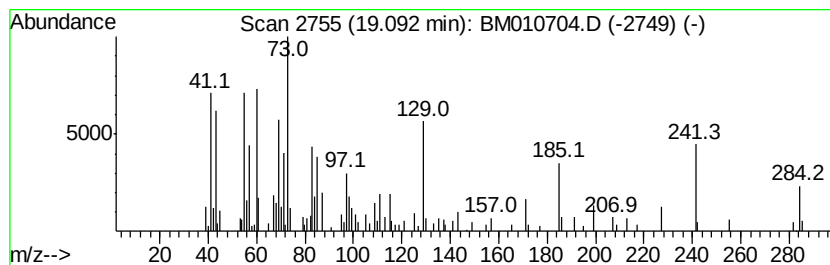
Instrument :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.09	2.75 ng/ul	230259	Chrysene-d12	21.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4 93
2	Octadecanoic acid	284	C18H36O2	000057-11-4 92
3	Octadecanoic acid	284	C18H36O2	000057-11-4 91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6 87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2 86



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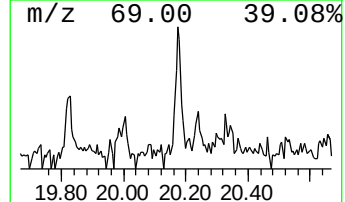
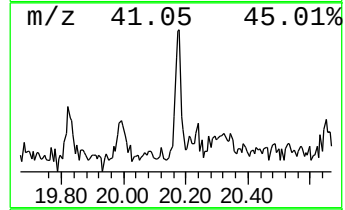
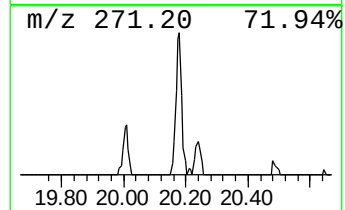
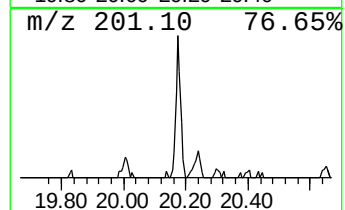
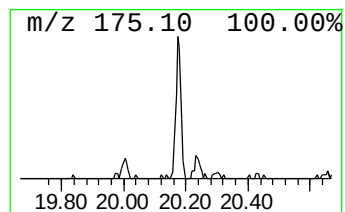
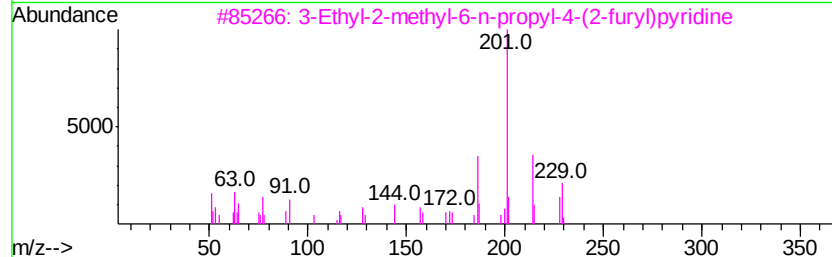
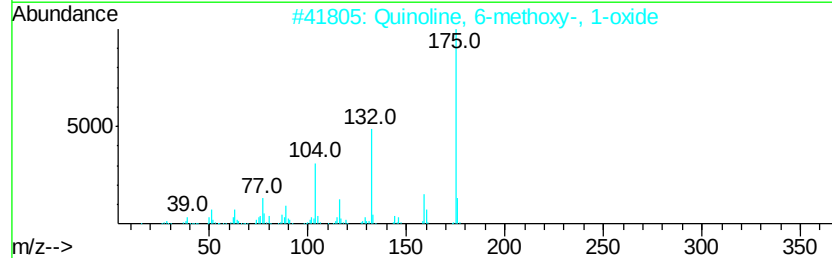
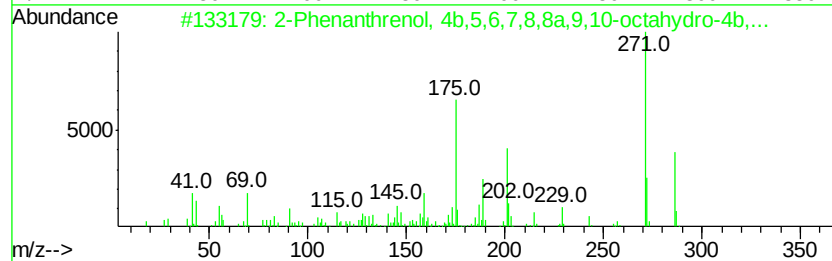
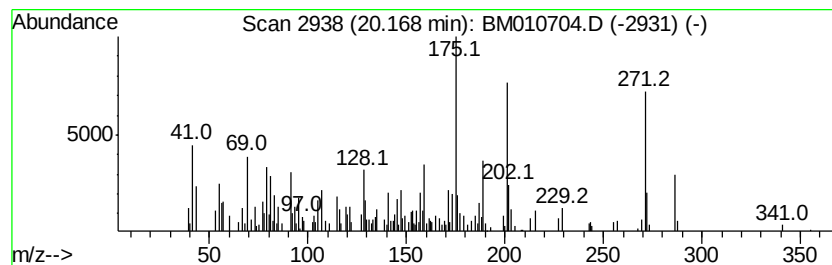
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.17	2.91 ng/ul	242892	Chrysene-d12	21.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286 C20H30O	000511-15-9	38
2	Quinoline, 6-methoxy-, 1-oxide	175 C10H9NO2	006563-13-9	15
3	3-Ethyl-2-methyl-6-n-propyl-4-(2...	229 C15H19NO	078563-70-9	11
4	Silane, dimethyl(2-chloro-5-meth...	286 C14H23ClO2Si	1000347-54-6	11
5	1H-Isoindole-1,3(2H)-dione, 4,5-...	175 C10H9NO2	066309-86-2	11



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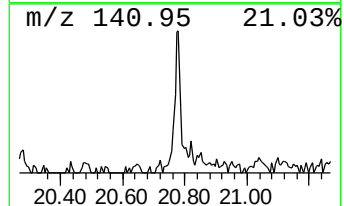
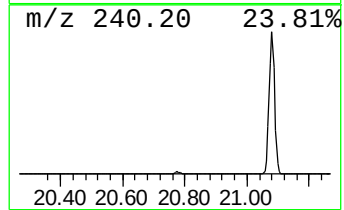
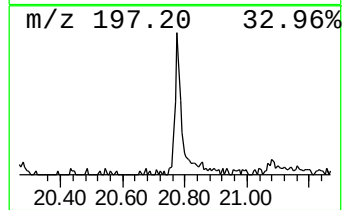
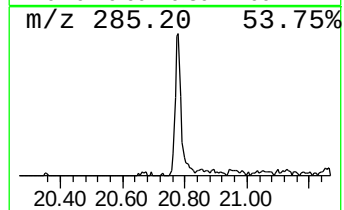
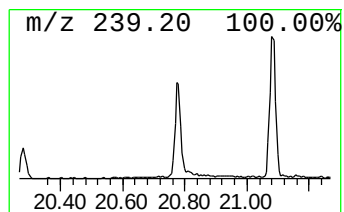
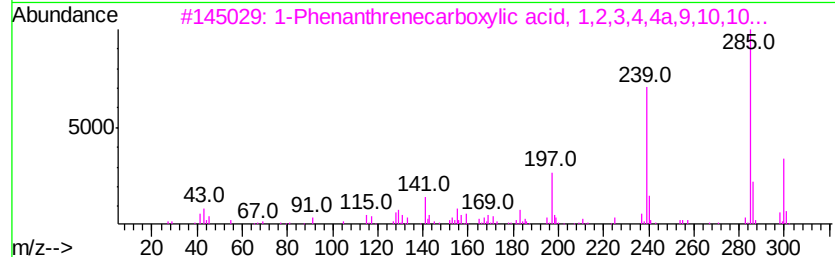
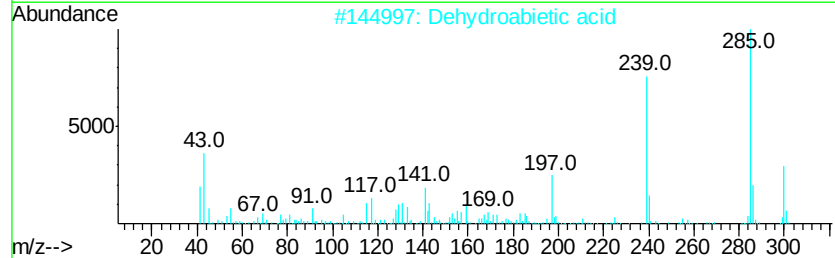
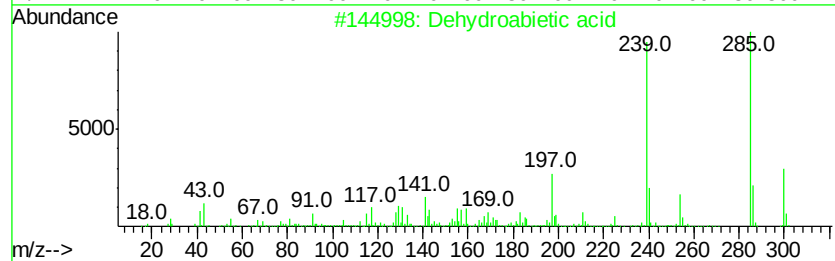
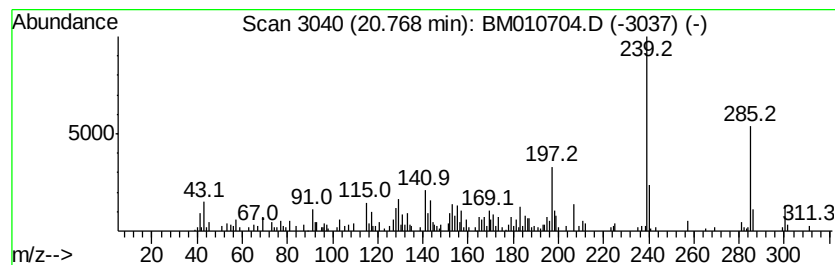
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dehydroabietic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	3.96 ng/ul	330894	Chrysene-d12	21.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dehydroabietic acid	300	C20H28O2	001740-19-8	94
2		Dehydroabietic acid	300	C20H28O2	001740-19-8	91
3		1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	86
4		Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	81
5		Dehydroabietic acid	300	C20H28O2	001740-19-8	60



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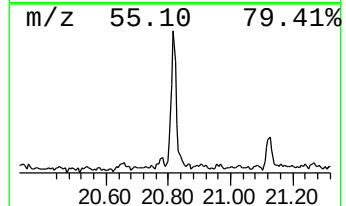
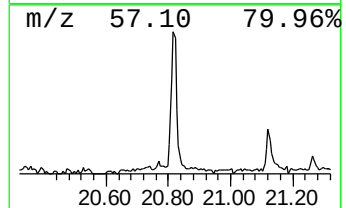
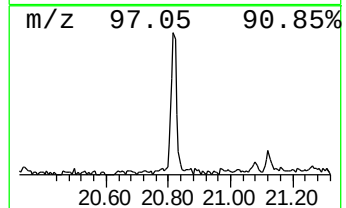
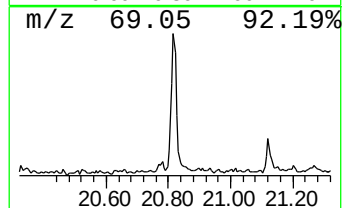
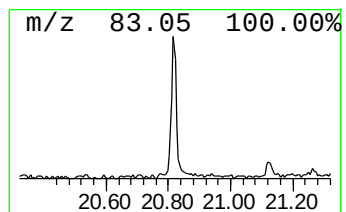
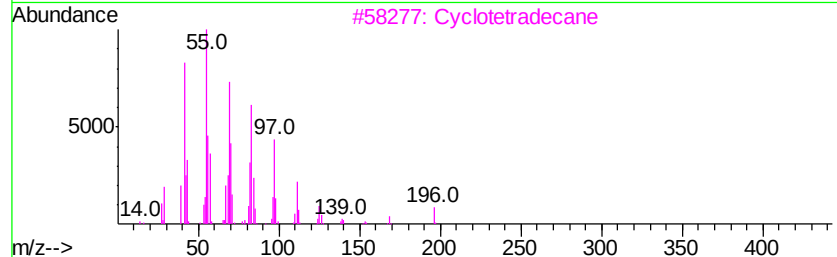
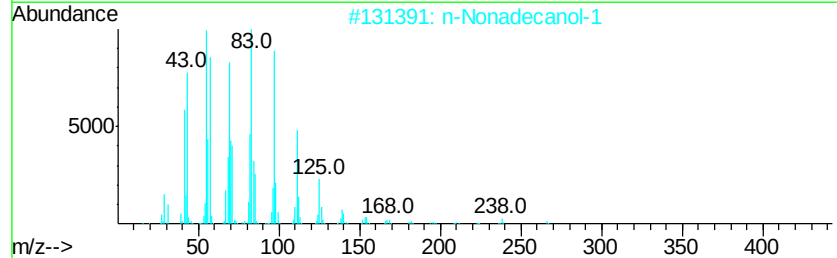
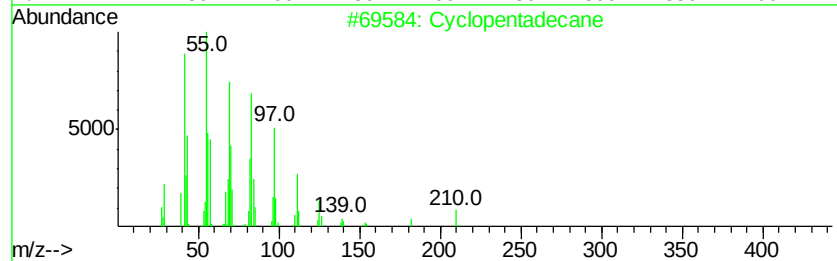
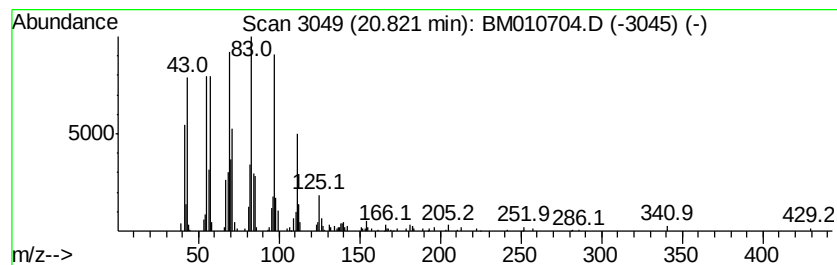
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Cyclic20.82 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	4.95 ng/ul	414165	Chrysene-d12	21.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	97
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3		Cyclotetradecane	196	C14H28	000295-17-0	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
Data File : BM010704.D
Acq On : 23 Jun 2017 23:38
Operator : SJ/JU
Sample : I3857-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
H2TR8

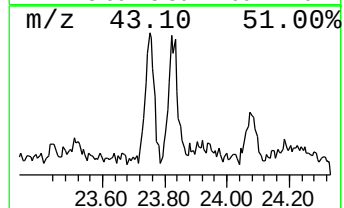
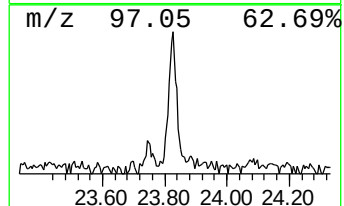
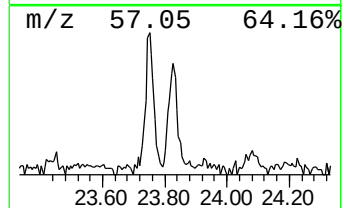
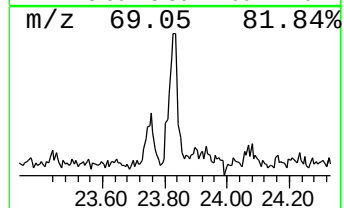
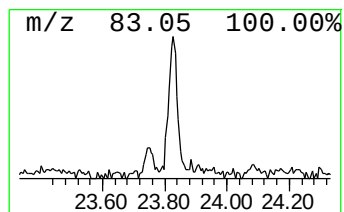
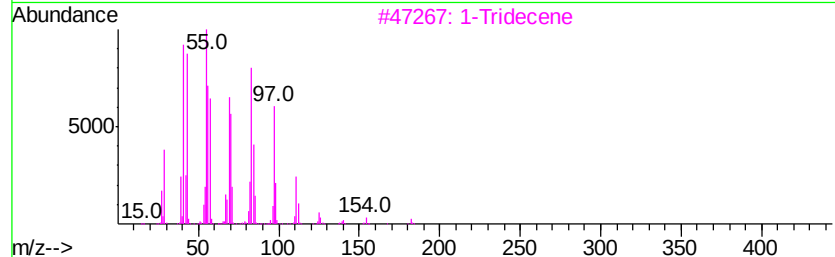
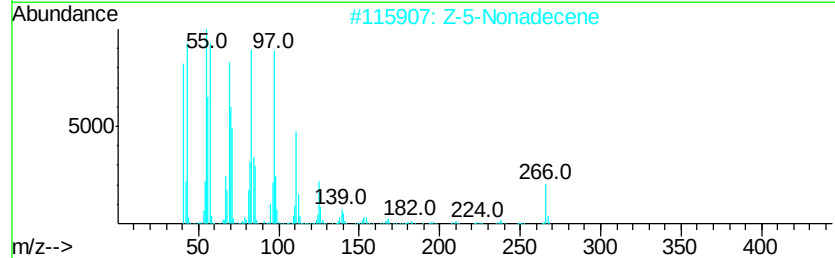
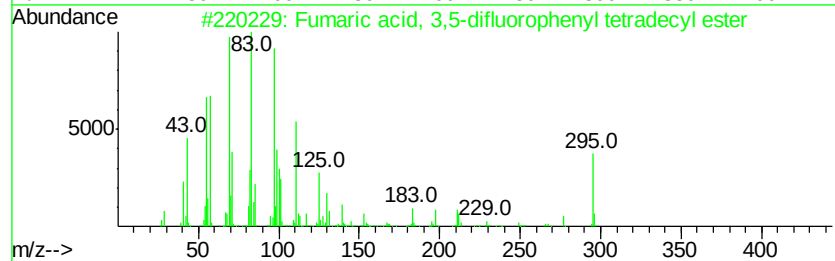
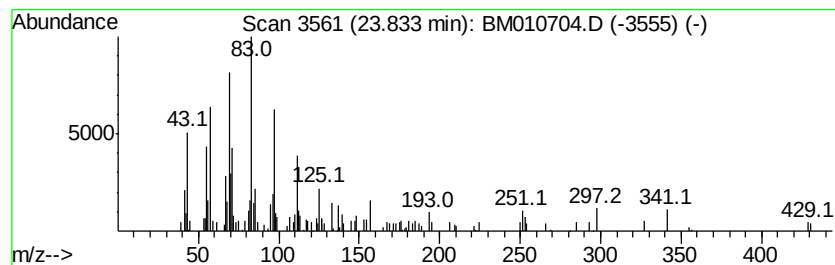
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Fumaric acid, 3,5-difluorop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.83	2.97 ng/ul	178795	Perylene-d12	23.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, 3,5-difluorophenyl...	424	C24H34F2O4	1000339-37-9	90
2		Z-5-Nonadecene	266	C19H38	1000131-11-8	83
3		1-Tridecene	182	C13H26	002437-56-1	74
4		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	64
5		1-Heptacosanol	396	C27H56O	002004-39-9	58



Data Path : Z:\HPCHEM1\BNA M\DATA\BM062317\
Data File : BM010704.D
Acq On : 23 Jun 2017 23:38
Operator : SJ/JU
Sample : I3857-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

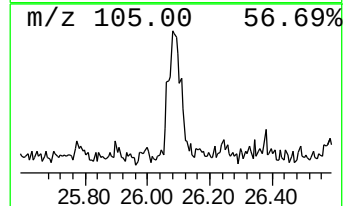
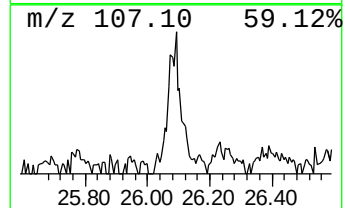
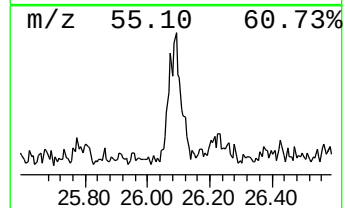
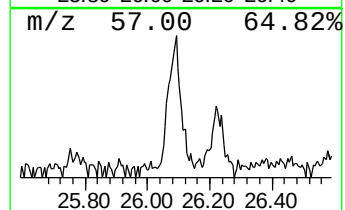
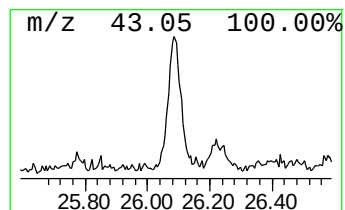
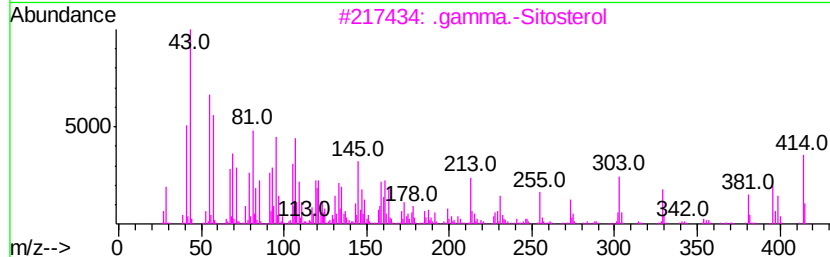
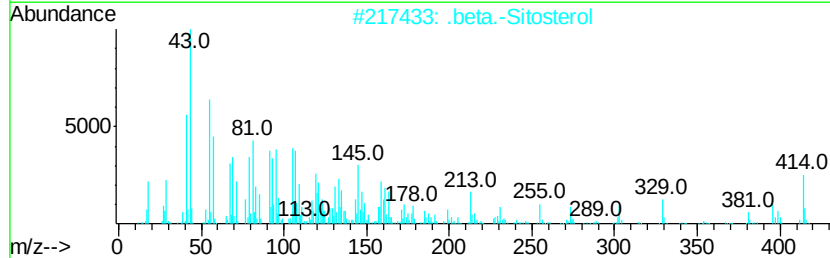
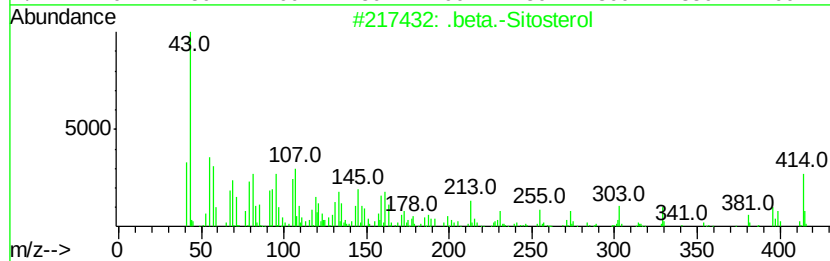
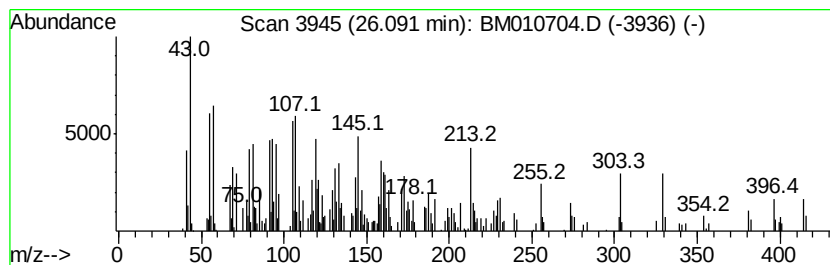
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.09	8.83 ng/ul	532508	Perylene-d12	23.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	98
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	96
3	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
4	.gamma.-Sitosterol	414	C29H50O	000083-47-6	50
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	46



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062317\
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Acq On : 23 Jun 2017 23:38
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Sample : I3857-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
H2TR8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	17.79	4.3	ng/ul	331316	4	16.87	1558710	20.0
Octadecanoic acid	19.09	2.8	ng/ul	230259	5	21.08	1671920	20.0
unknown-01	20.17	2.9	ng/ul	242892	5	21.08	1671920	20.0
Dehydroabietic acid	20.77	4.0	ng/ul	330894	5	21.08	1671920	20.0
(DEL) Alkane: Cyc...	20.82	5.0	ng/ul	414165	5	21.08	1671920	20.0
Fumaric acid, 3,5...	23.83	3.0	ng/ul	178795	6	23.22	1206020	20.0
.beta.-Sitosterol	26.09	8.8	ng/ul	532508	6	23.22	1206020	20.0