

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
 Data File : BM013544.D
 Acq On : 26 Dec 2017 20:49
 Operator : SJ/JU
 Sample : I7046-15
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0FM5

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-BM113017.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	3.222	20	23	28	rBV2	46406	60897	1.49%	0.097%
2	4.834	294	297	303	rVB3	27237	45080	1.10%	0.072%
3	6.846	633	639	657	rVB2	810705	1562128	38.16%	2.479%
4	7.010	661	667	677	rVB	648652	997325	24.36%	1.582%
5	7.205	693	700	711	rBV	889023	1412846	34.51%	2.242%
6	7.669	772	779	786	rBV	814862	1322578	32.31%	2.099%
7	8.375	892	899	910	rBV	785213	1276729	31.19%	2.026%
8	8.822	968	975	985	rBV	932709	1499247	36.62%	2.379%
9	8.951	990	997	1002	rBV4	36664	66017	1.61%	0.105%
10	9.540	1090	1097	1106	rBV	746727	1257794	30.72%	1.996%
11	10.075	1181	1188	1201	rBV	1087442	1911408	46.69%	3.033%
12	10.446	1242	1251	1264	rVB	1164674	1938753	47.36%	3.076%
13	10.593	1268	1276	1295	rVV	317197	647073	15.81%	1.027%
14	13.034	1683	1691	1697	rBV5	43198	69741	1.70%	0.111%
15	13.134	1702	1708	1712	rBV3	43178	72764	1.78%	0.115%
16	13.728	1802	1809	1813	rVV	1941237	2702972	66.02%	4.289%
17	13.775	1813	1817	1824	rVB	683920	990100	24.18%	1.571%
18	14.004	1844	1856	1864	rBV	2164498	3286153	80.27%	5.214%
19	14.216	1884	1892	1896	rBV2	135743	188657	4.61%	0.299%
20	14.310	1900	1908	1916	rBV2	1653503	2540455	62.05%	4.031%
21	14.534	1940	1946	1960	rBV	484754	952503	23.27%	1.511%
22	14.833	1993	1997	2003	rVB3	35771	52161	1.27%	0.083%
23	15.139	2041	2049	2051	rBV2	75980	137745	3.36%	0.219%
24	15.169	2051	2054	2058	rVB	169284	201301	4.92%	0.319%
25	15.310	2071	2078	2085	rVB	2612894	3803757	92.91%	6.035%
26	15.439	2093	2100	2113	rBV	661565	989482	24.17%	1.570%
27	15.551	2113	2119	2120	rBV3	45378	58257	1.42%	0.092%
28	16.033	2197	2201	2208	rBV	150005	230371	5.63%	0.366%
29	16.827	2331	2336	2339	rBV	94094	122447	2.99%	0.194%
30	16.875	2341	2344	2349	rVB4	30613	41899	1.02%	0.066%
31	16.963	2354	2359	2367	rBV9	37740	58390	1.43%	0.093%
32	17.063	2367	2376	2384	rBV	1890792	2801634	68.43%	4.445%
33	17.157	2386	2392	2401	rVB2	2771627	3893670	95.11%	6.178%
34	17.257	2401	2409	2413	rBV2	21804	47485	1.16%	0.075%

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35	17.563	2456	2461	2467	rBV3	55419	83462	2.04%	0.132%
36	17.704	2481	2485	2488	rBV6	24661	43120	1.05%	0.068%
37	17.839	2503	2508	2515	rBV9	33217	65363	1.60%	0.104%
38	17.969	2522	2530	2538	rBV	905266	1377181	33.64%	2.185%
39	18.257	2575	2579	2584	rBV7	67127	107426	2.62%	0.170%
40	19.098	2718	2722	2724	rBV3	64475	85449	2.09%	0.136%
41	19.127	2725	2727	2730	rVV4	36873	43857	1.07%	0.070%
42	19.251	2743	2748	2758	rBV	499421	766284	18.72%	1.216%
43	19.457	2777	2783	2789	rBV	2988057	4094034	100.00%	6.496%
44	19.510	2790	2792	2797	rVB5	47191	58532	1.43%	0.093%
45	19.980	2870	2872	2875	rBV4	51693	55262	1.35%	0.088%
46	20.392	2939	2942	2949	rVB	244640	290976	7.11%	0.462%
47	20.968	3036	3040	3048	rBV	1154660	1430340	34.94%	2.270%
48	21.174	3072	3075	3079	rBV	198946	231804	5.66%	0.368%
49	21.251	3083	3088	3099	rBV	1933237	2550209	62.29%	4.046%
50	21.857	3184	3191	3201	rBV2	935756	2020928	49.36%	3.207%
51	21.992	3212	3214	3220	rVB2	154721	190940	4.66%	0.303%
52	22.421	3284	3287	3293	rVB2	208499	284767	6.96%	0.452%
53	22.798	3346	3351	3355	rBV	615118	913718	22.32%	1.450%
54	22.845	3355	3359	3369	rVB4	353418	640856	15.65%	1.017%
55	23.333	3435	3442	3452	rBV2	1782825	3539903	86.46%	5.617%
56	23.474	3460	3466	3476	rVB	1109133	2086441	50.96%	3.311%
57	23.992	3549	3554	3561	rVB2	391090	753943	18.42%	1.196%
58	24.080	3565	3569	3582	rVB6	336569	749169	18.30%	1.189%
59	24.733	3675	3680	3686	rVB5	186898	365088	8.92%	0.579%
60	26.462	3970	3974	3987	rVB9	264871	802843	19.61%	1.274%
61	27.733	4181	4190	4208	rBV10	580032	2151617	52.55%	3.414%

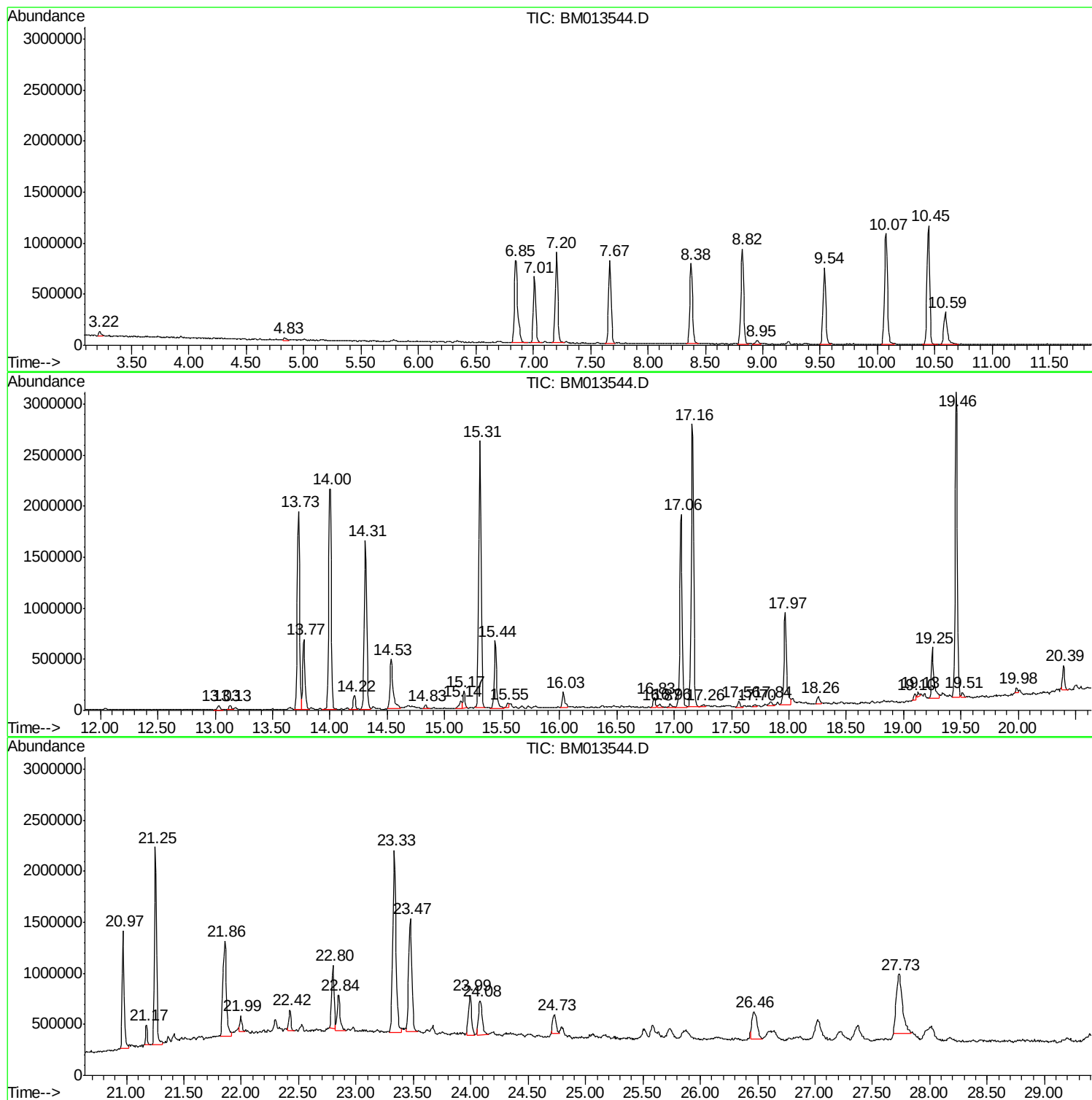
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TIC Library : C:\DATABASE\NIST11.L
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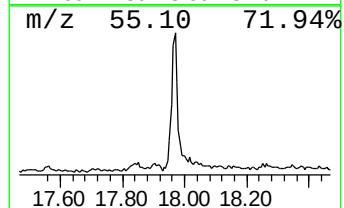
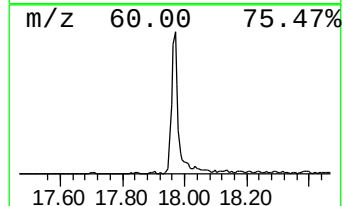
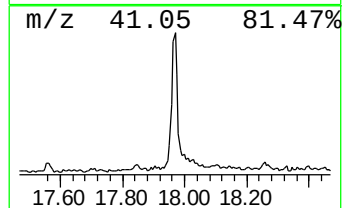
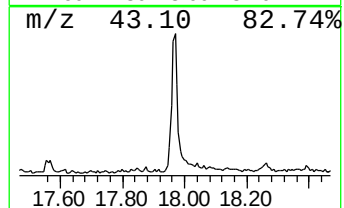
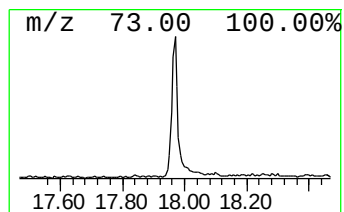
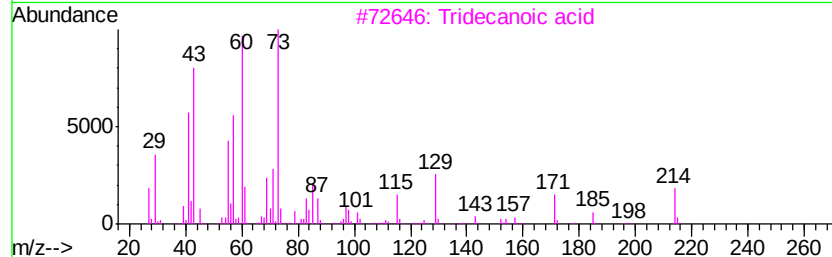
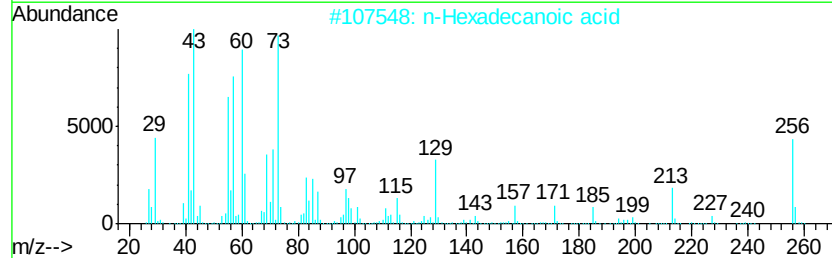
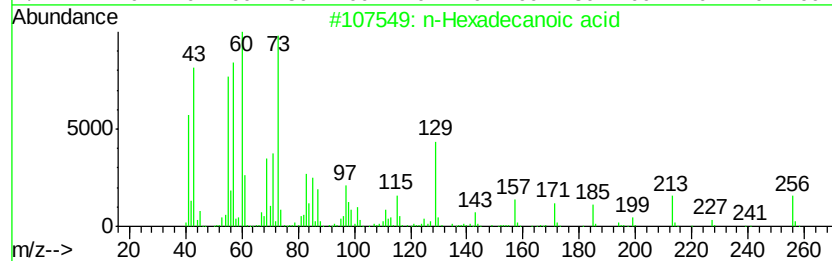
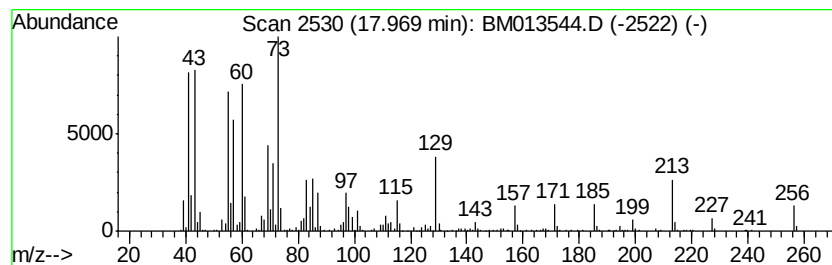
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	9.83 ng/ul	1377180	Phenanthrene-d10	17.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98	
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90	
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89	
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87	



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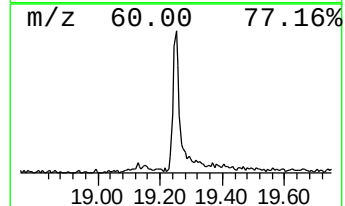
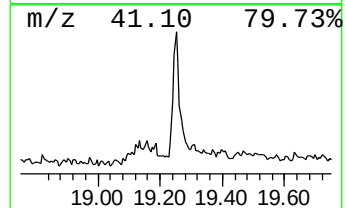
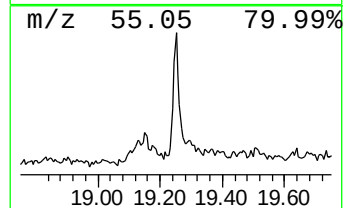
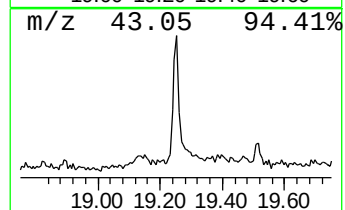
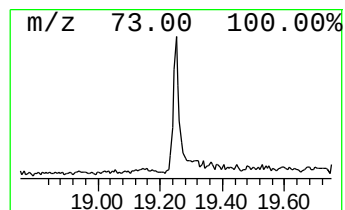
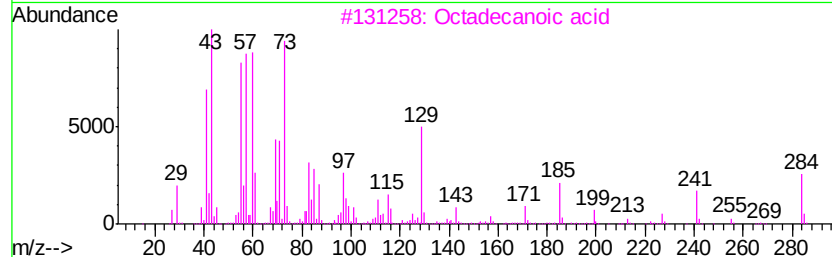
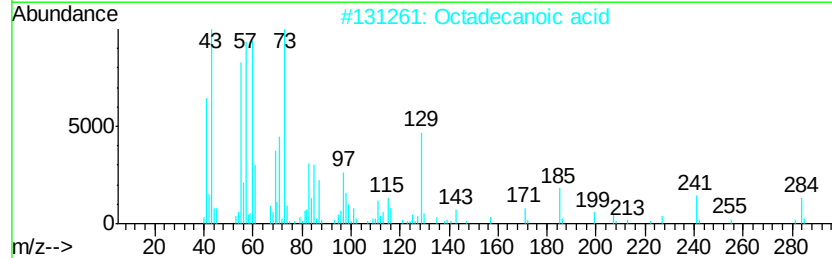
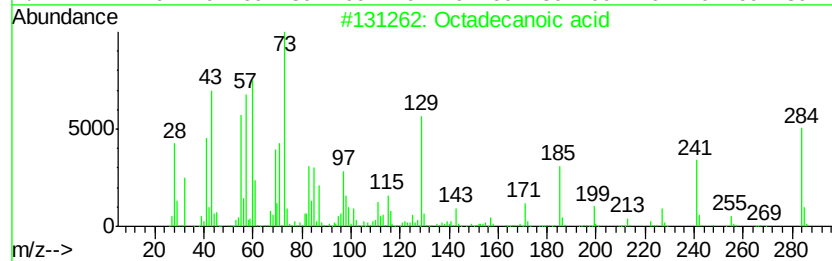
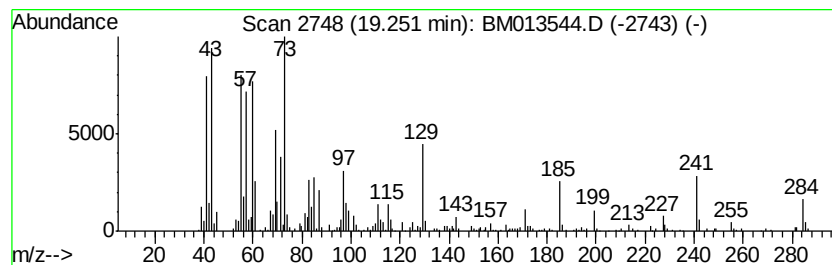
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.25	6.01 ng/ul	766284	Chrysene-d12	21.25		
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	99	
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99	
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98	
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94	



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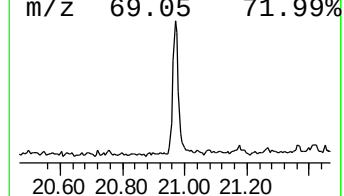
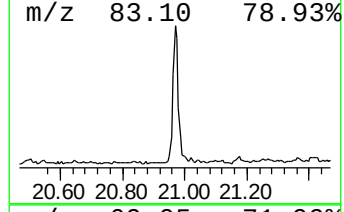
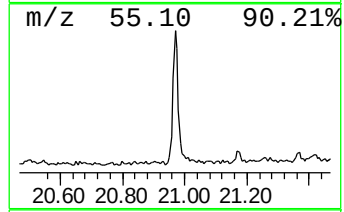
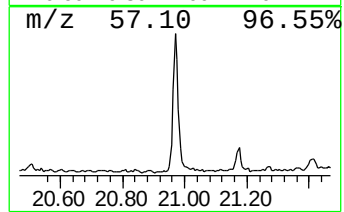
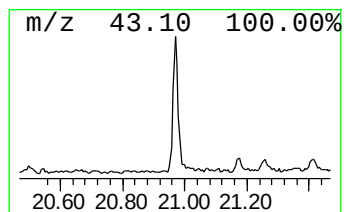
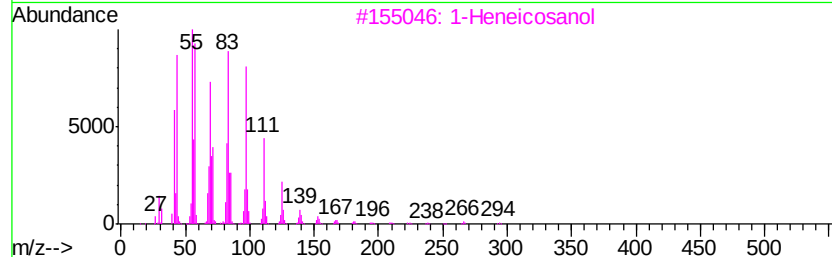
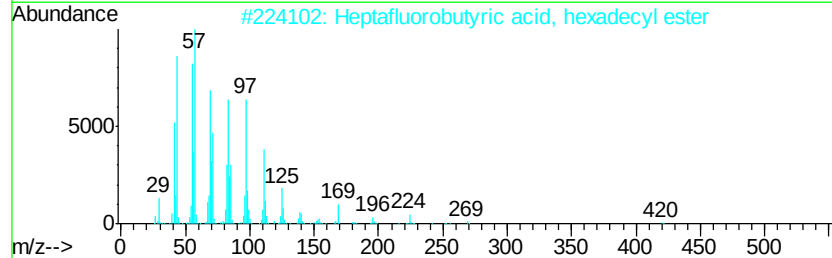
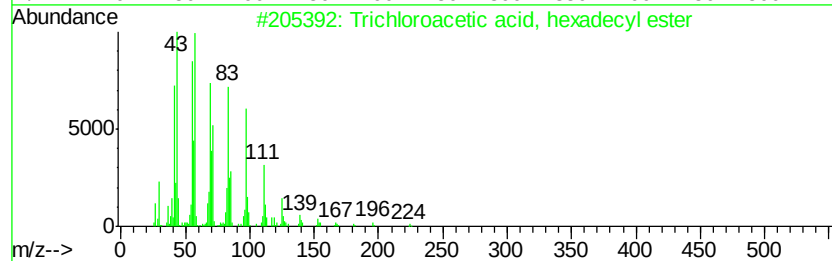
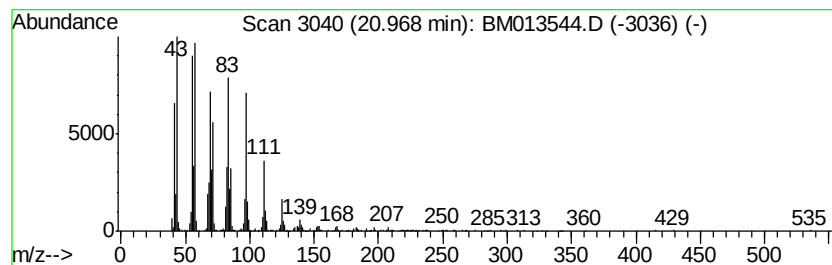
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	11.22 ng/ul	1430340	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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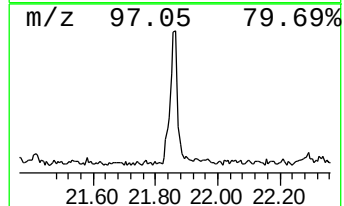
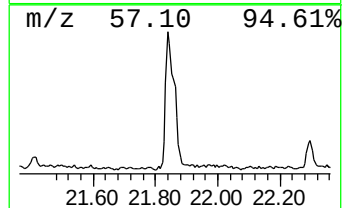
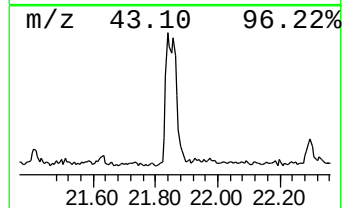
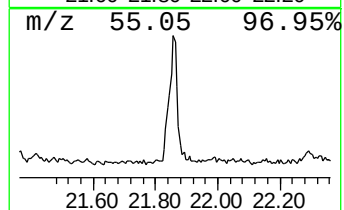
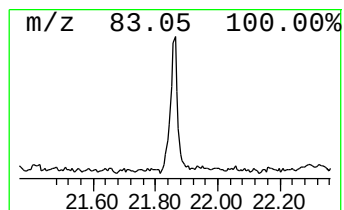
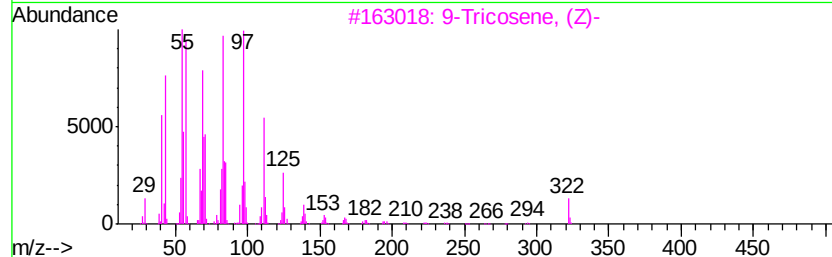
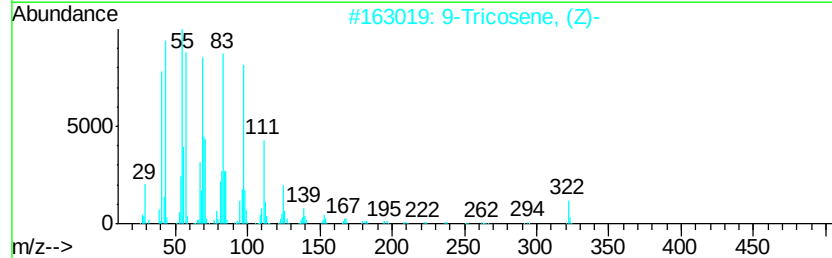
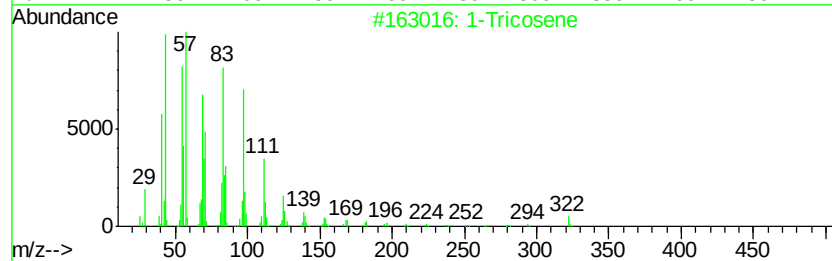
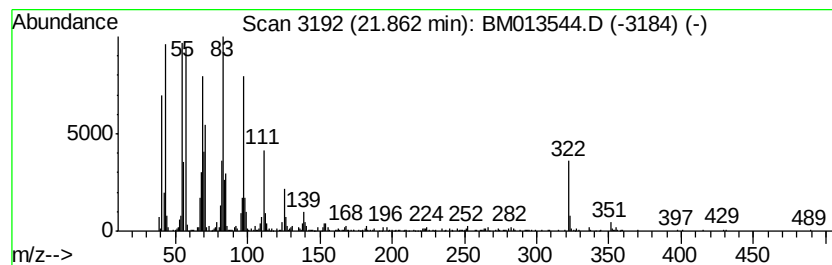
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Peak Number 4 (DEL) Alkane: Cyclic21.86 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	15.85 ng/ul	2020930	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tricosene	322	C23H46	018835-32-0	95
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3		9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		9-Nonadecene	266	C19H38	031035-07-1	93



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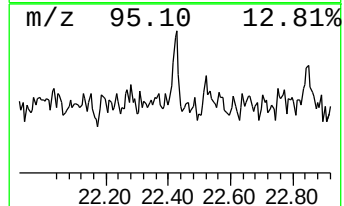
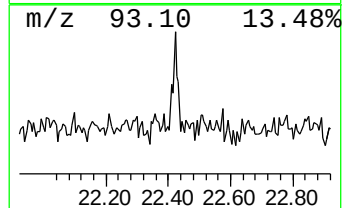
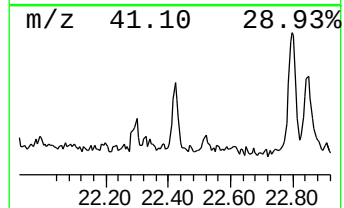
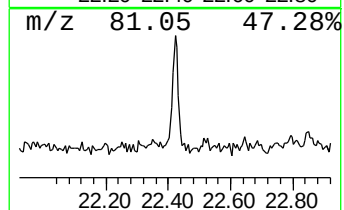
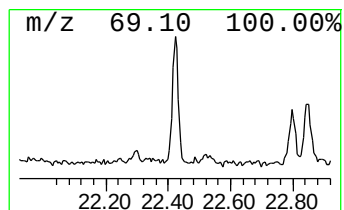
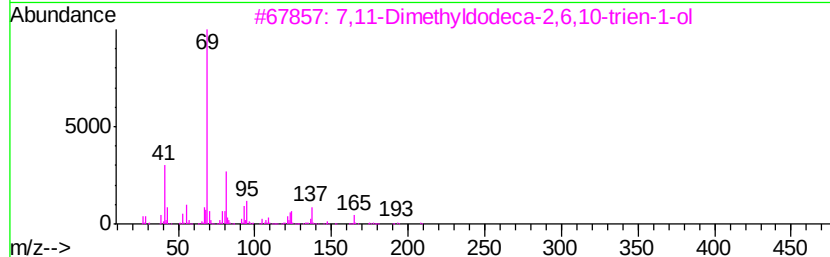
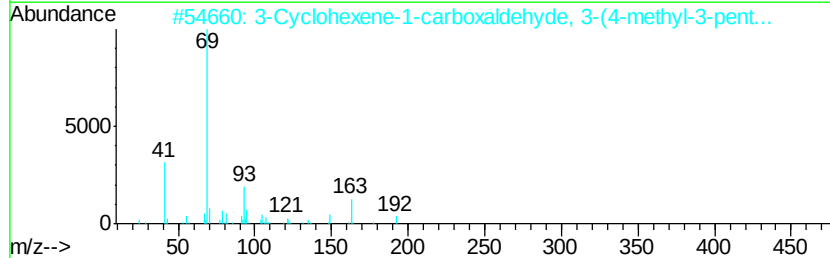
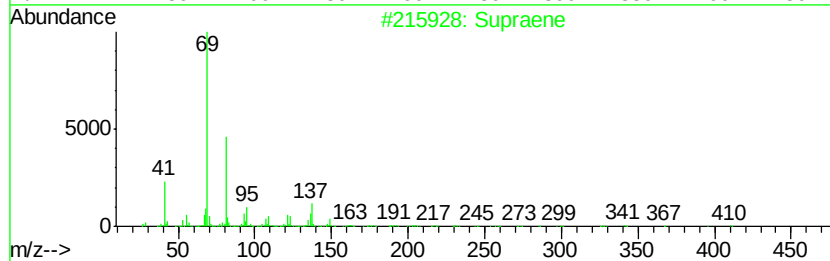
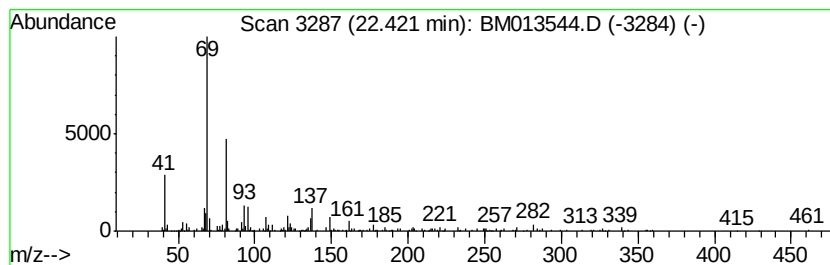
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	2.73 ng/ul	284767	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	64
2		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	53
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	50
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	50
5		1,5-Heptadiene, 3,6-dimethyl-	124	C9H16	034891-10-6	50



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
Operator : SJ/JU
Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0FM5

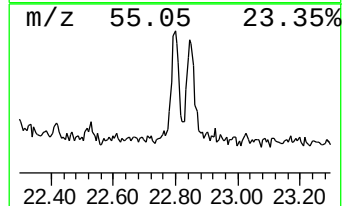
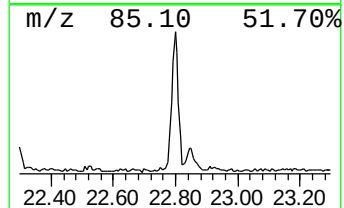
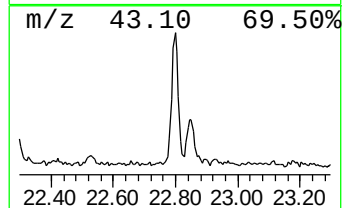
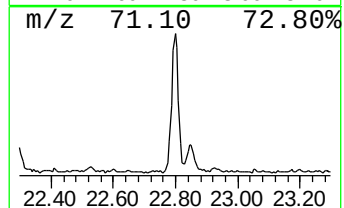
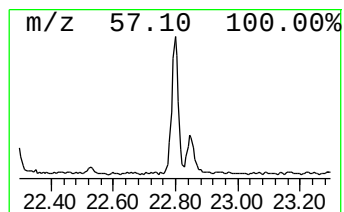
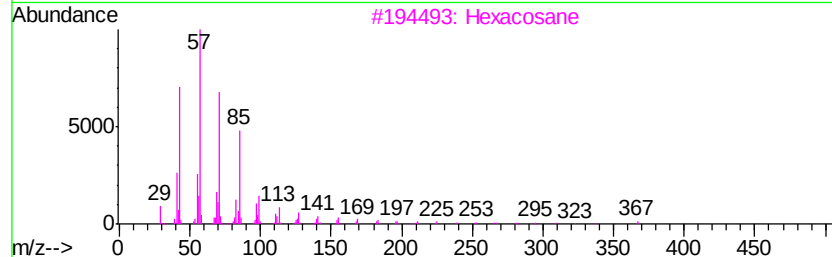
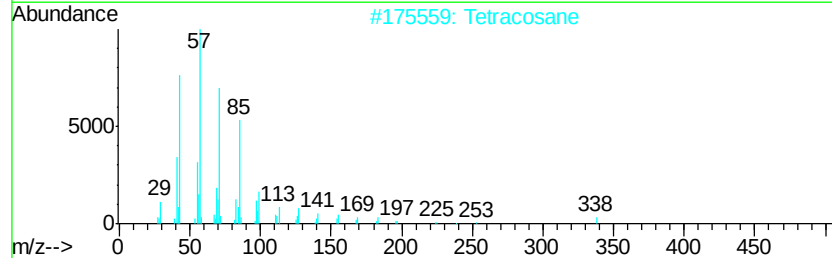
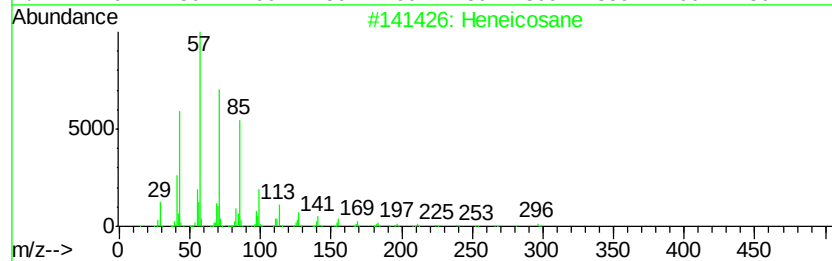
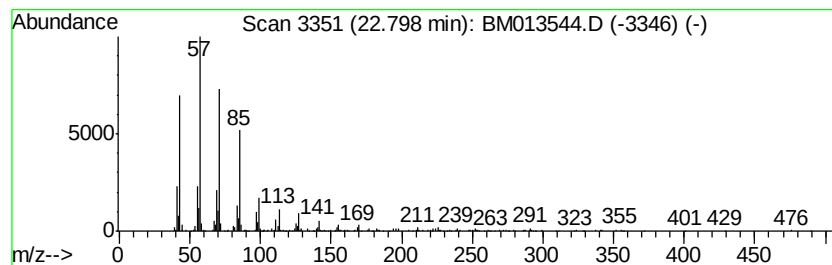
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	8.76 ng/ul	913718	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		triacontane	422	C30H62	000638-68-6	91
5		Heptadecane, 3-methyl-	254	C18H38	006418-44-6	91



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
Operator : SJ/JU
Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

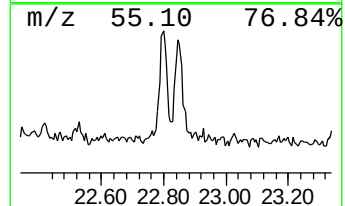
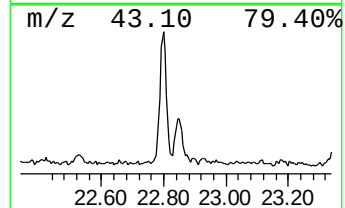
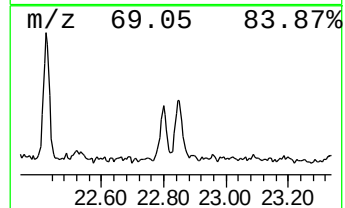
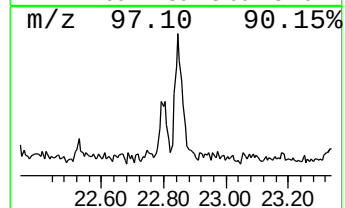
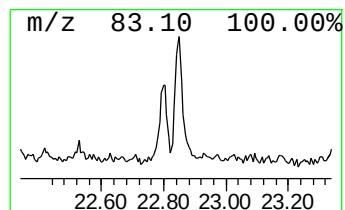
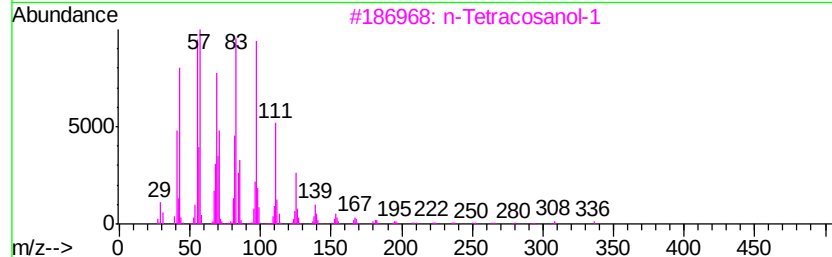
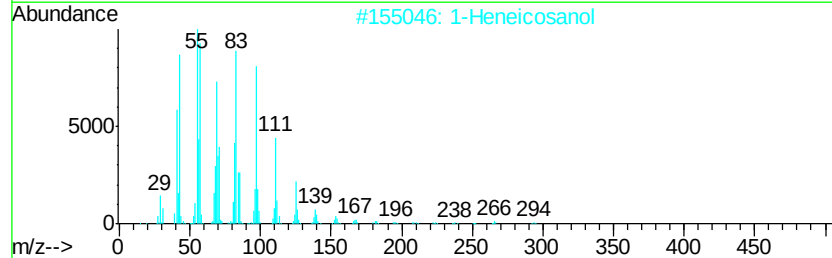
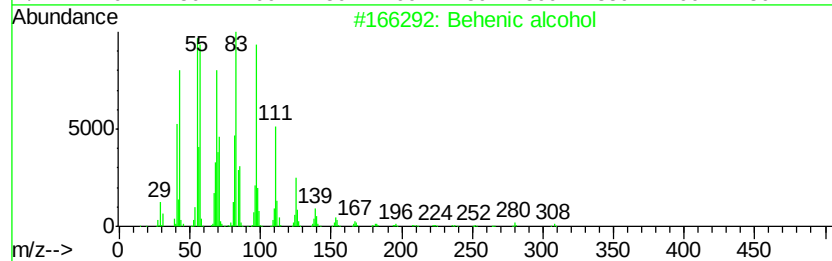
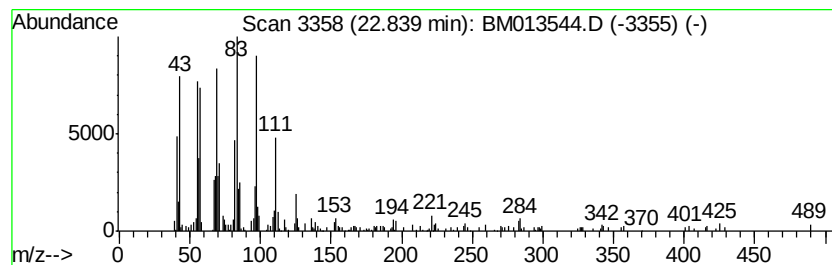
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.84	6.14 ng/ul	640856	Perylene-d12	23.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 91
2		1-Heneicosanol	312 C21H44O	015594-90-8 91
3		n-Tetracosanol-1	354 C24H50O	000506-51-4 87
4		1-Heneicosyl formate	340 C22H44O2	077899-03-7 83
5		Nonadecyl trifluoroacetate	380 C21H39F3O2	1000351-76-3 80



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
Operator : SJ/JU
Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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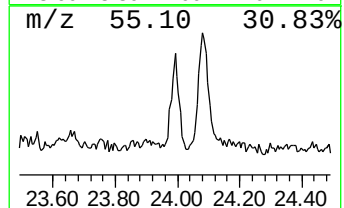
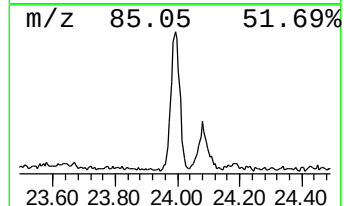
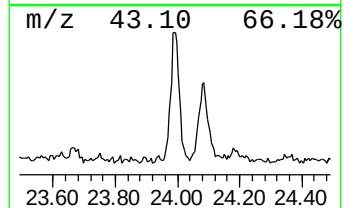
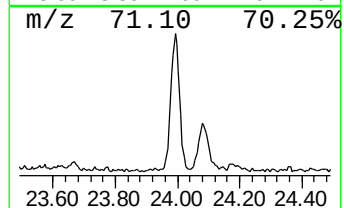
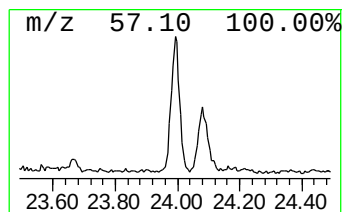
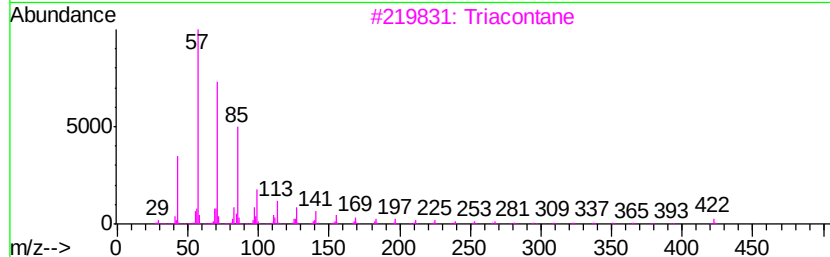
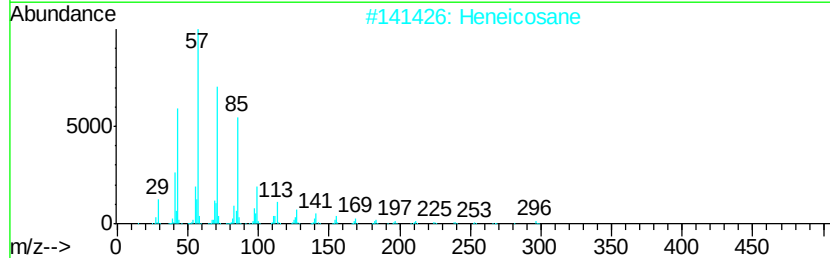
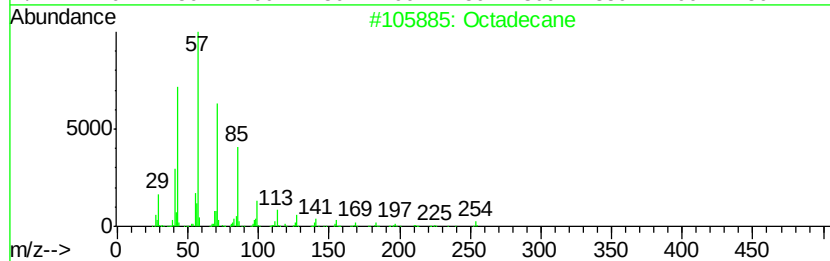
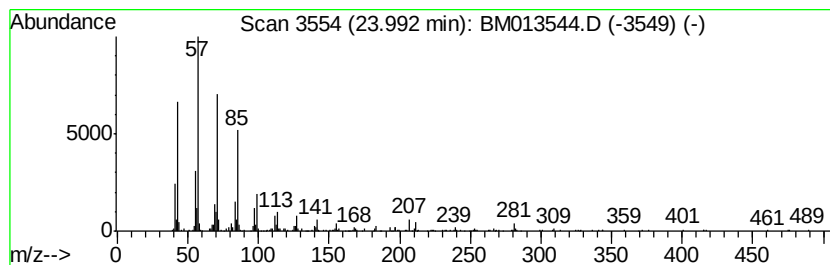
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	7.23 ng/ul	753943	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Triacotane	422	C30H62	000638-68-6	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
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Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
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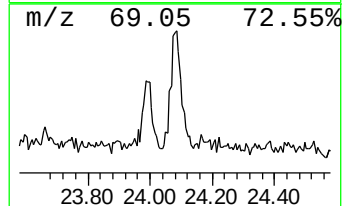
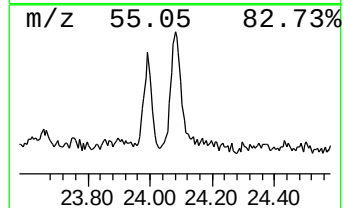
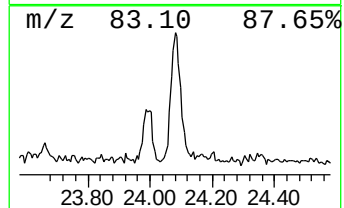
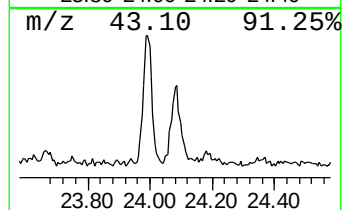
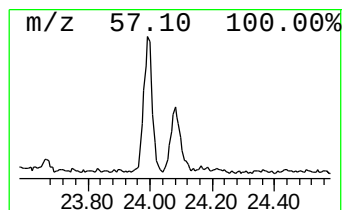
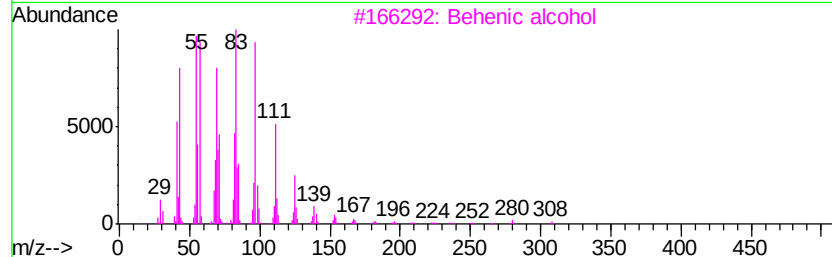
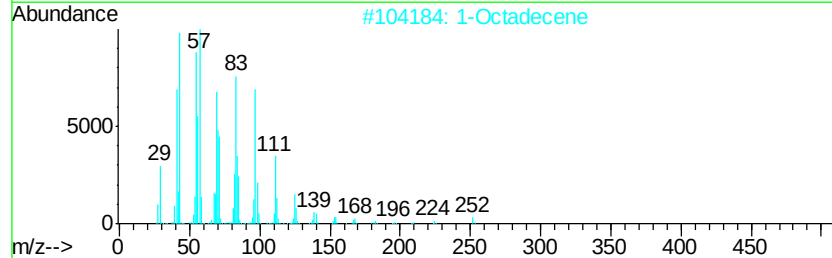
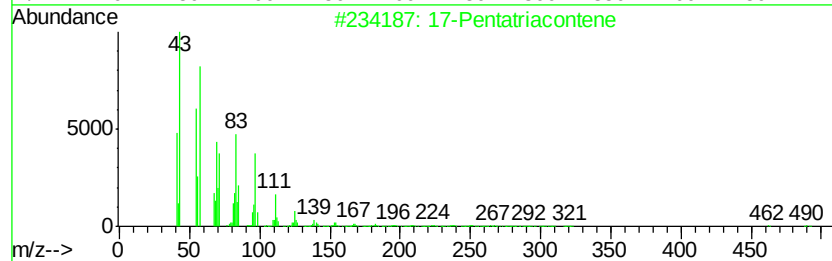
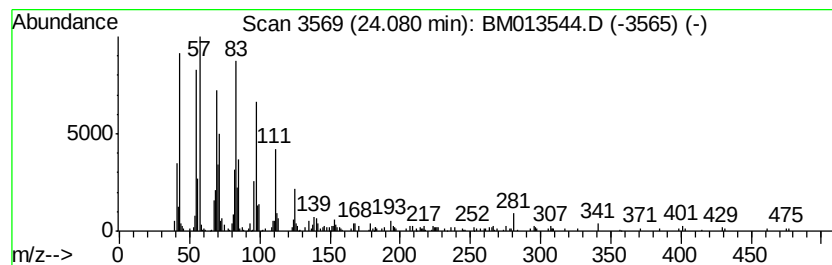
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Cyclic24.08 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	7.18 ng/ul	749169	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		1-Octadecene	252	C18H36	000112-88-9	91
3		Behenic alcohol	326	C22H46O	000661-19-8	87
4		1-Heptacosanol	396	C27H56O	002004-39-9	83
5		1-Triacontanol	438	C30H62O	000593-50-0	81



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
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Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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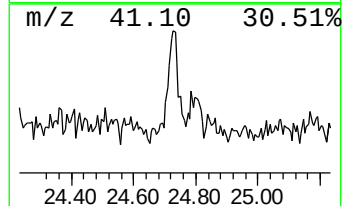
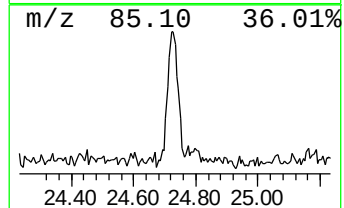
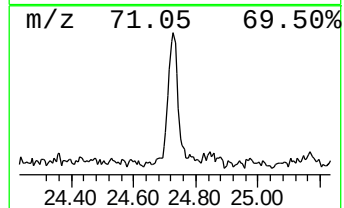
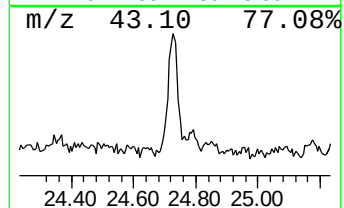
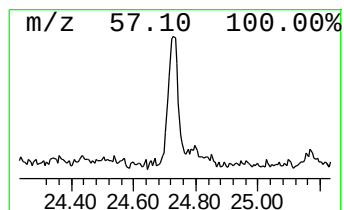
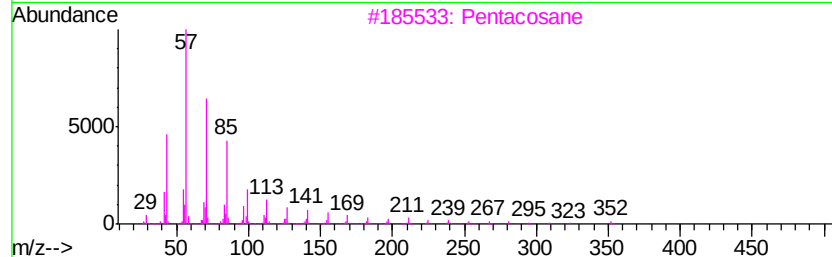
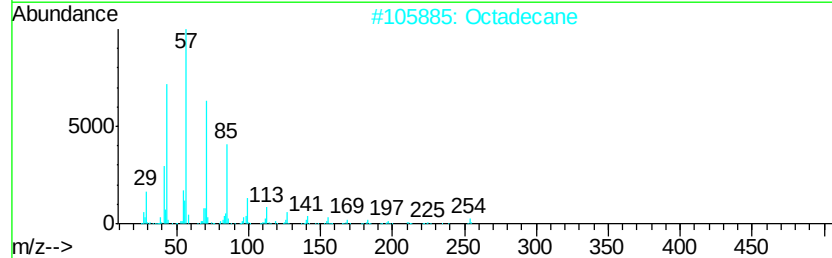
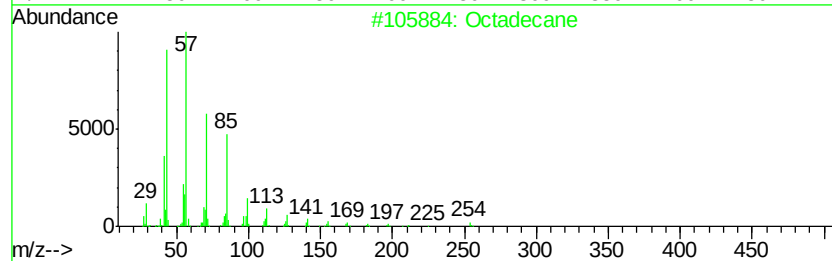
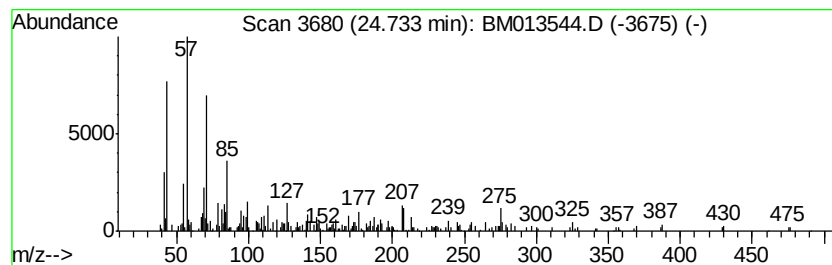
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.73	3.50 ng/ul	365088	Perylene-d12	23.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	60
2			Octadecane	254	C18H38	000593-45-3	60
3			Pentacosane	352	C25H52	000629-99-2	53
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	49
5			Hexacosane	366	C26H54	000630-01-3	49



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
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Sample : I7046-15
Misc :
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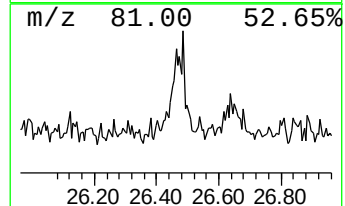
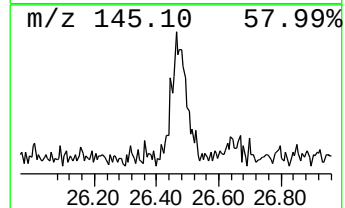
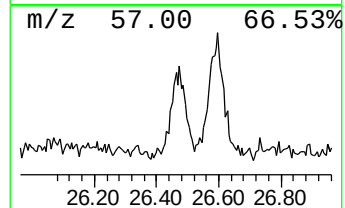
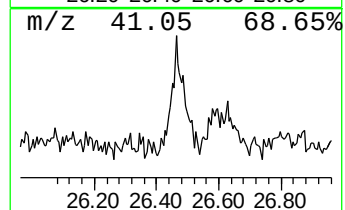
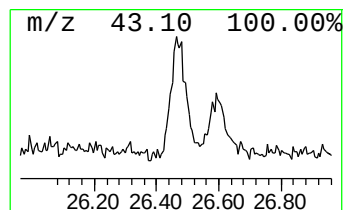
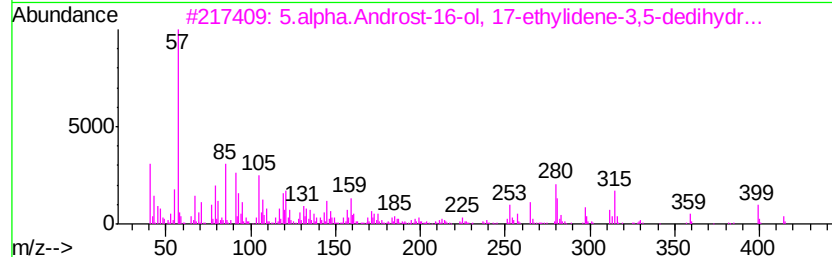
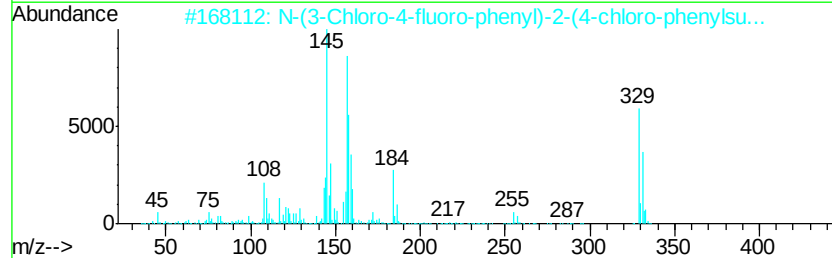
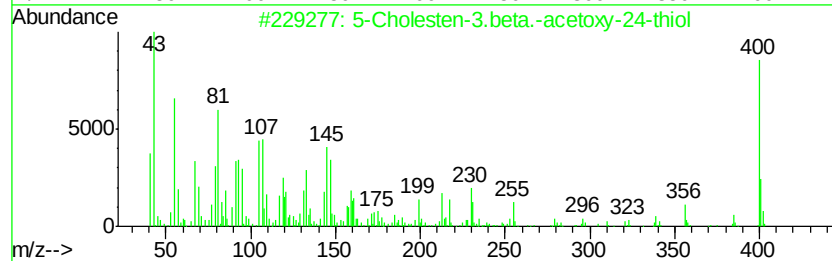
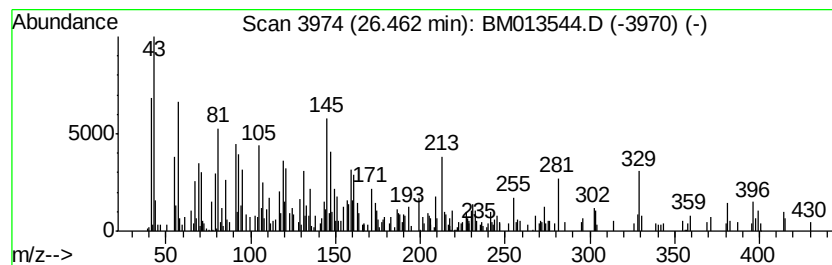
Instrument :
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ClientSampled :
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.46	7.70 ng/ul	802843	Perylene-d12	23.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Cholesten-3.beta.-acetoxy-24-t...	460	C29H48O2S	1000253-09-1	35
2	N-(3-Chloro-4-fluoro-phenyl)-2-(...	329	C14H10Cl2FNOS	1000295-12-7	25
3	5.alpha.Androst-16-ol, 17-ethyl...	414	C27H42O3	1000124-58-6	15
4	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	12
5	Imidazo[1,2-a]pyridine-2-methana...	255	C15H14FN3	1000319-95-6	11



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
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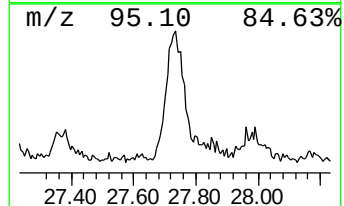
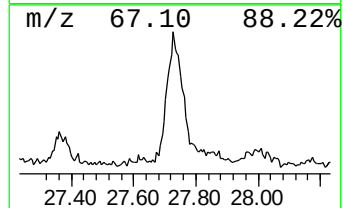
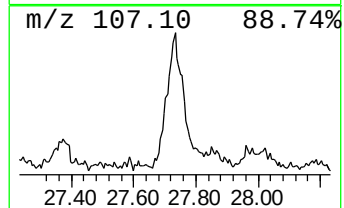
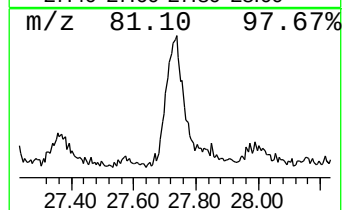
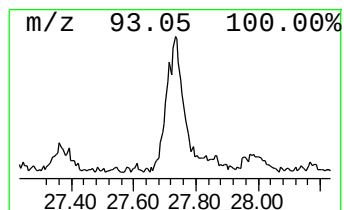
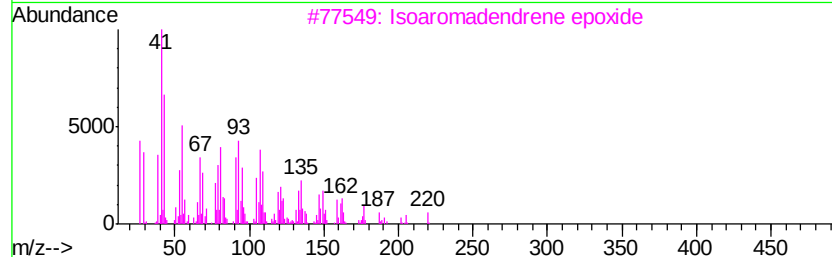
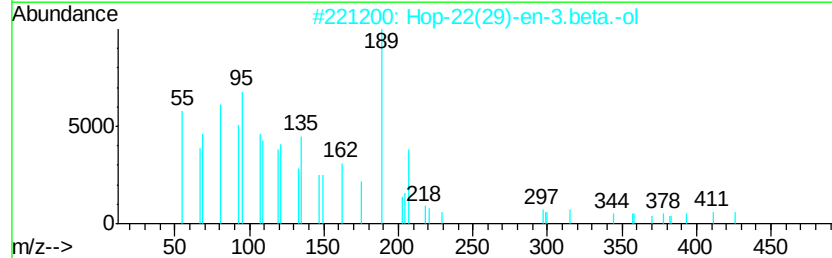
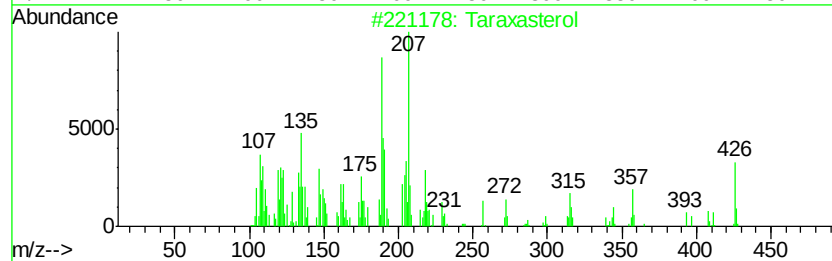
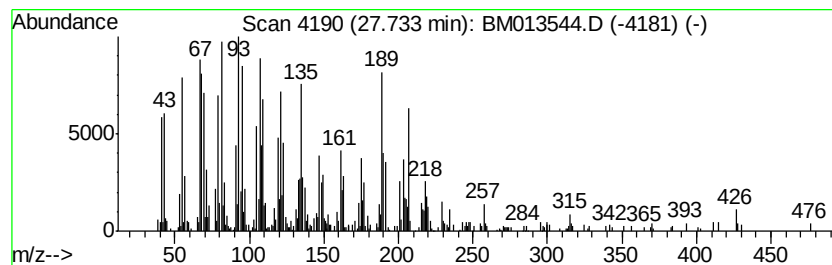
Instrument :
BNA_M
ClientSampleId :
C0FM5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 12 Taraxasterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.73	20.62 ng/ul	2151620	Perylene-d12	23.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Taraxasterol	426 C30H50O	001059-14-9 90
2		Hop-22(29)-en-3.beta.-ol	426 C30H50O	058801-23-3 55
3		Isoaromadendrene epoxide	220 C15H24O	1000159-36-6 50
4		4-(2', 4', 4'-trimethyl-yciclo[4...	204 C14H20O	1000373-94-4 48
5		2,6,10,10-Tetramethylbicyclo[7.2...	204 C15H24	136296-37-2 45



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013544.D
Acq On : 26 Dec 2017 20:49
Operator : SJ/JU
Sample : I7046-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0FM5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.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	17.97	9.8	ng/ul	1377180	4	17.06	2801630	20.0
Octadecanoic acid	19.25	6.0	ng/ul	766284	5	21.25	2550210	20.0
Trichloroacetic a...	20.97	11.2	ng/ul	1430340	5	21.25	2550210	20.0
(DEL) Alkane: Cyc...	21.86	15.9	ng/ul	2020930	5	21.25	2550210	20.0
Supraene	22.42	2.7	ng/ul	284767	6	23.47	2086440	20.0
(DEL) Alkane: Str...	22.80	8.8	ng/ul	913718	6	23.47	2086440	20.0
Behenic alcohol	22.84	6.1	ng/ul	640856	6	23.47	2086440	20.0
(DEL) Alkane: Str...	23.99	7.2	ng/ul	753943	6	23.47	2086440	20.0
(DEL) Alkane: Cyc...	24.08	7.2	ng/ul	749169	6	23.47	2086440	20.0
(DEL) Alkane: Str...	24.73	3.5	ng/ul	365088	6	23.47	2086440	20.0
unknown-01	26.46	7.7	ng/ul	802843	6	23.47	2086440	20.0
Taraxasterol	27.73	20.6	ng/ul	2151620	6	23.47	2086440	20.0