

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM101317\
 Data File : BM012166.D
 Acq On : 14 Oct 2017 10:28
 Operator : SJ/JU
 Sample : I5548-16
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AF6

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-BM101217.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	6.993	657	664	679	rBV	466868	890507	11.49%	1.489%
2	7.151	684	691	705	rVB	360268	591534	7.63%	0.989%
3	7.351	718	725	741	rBV	543663	895154	11.55%	1.497%
4	7.822	798	805	818	rVB	760285	1267076	16.35%	2.119%
5	8.534	919	926	942	rBV	499450	907801	11.71%	1.518%
6	8.986	996	1003	1019	rBV	469052	856327	11.05%	1.432%
7	9.710	1120	1126	1142	rBV	419228	760996	9.82%	1.273%
8	10.251	1212	1218	1232	rBV	591635	1106191	14.27%	1.850%
9	10.622	1274	1281	1294	rVB	1028662	1757554	22.67%	2.939%
10	10.769	1299	1306	1320	rBV	340400	708782	9.14%	1.185%
11	13.333	1736	1742	1750	rVB3	82071	136561	1.76%	0.228%
12	13.780	1814	1818	1826	rVB3	95109	138354	1.78%	0.231%
13	13.874	1826	1834	1839	rBV	1115309	1688629	21.78%	2.824%
14	13.927	1839	1843	1849	rVB	532677	759100	9.79%	1.269%
15	14.169	1878	1884	1891	rBV	1458994	2169670	27.99%	3.628%
16	14.298	1900	1906	1911	rBV	98640	158741	2.05%	0.265%
17	14.421	1921	1927	1931	rBV	1131568	1605189	20.71%	2.684%
18	14.474	1931	1936	1942	rVV2	1358371	2116146	27.30%	3.539%
19	14.527	1942	1945	1958	rVB2	102652	201258	2.60%	0.337%
20	14.710	1969	1976	1984	rBV3	308610	614181	7.92%	1.027%
21	14.780	1984	1988	1996	rVB2	81853	160851	2.08%	0.269%
22	15.468	2098	2105	2112	rBV	1453598	2122297	27.38%	3.549%
23	15.610	2124	2129	2139	rBV	177912	291852	3.77%	0.488%
24	15.704	2139	2145	2151	rVB4	46813	84625	1.09%	0.142%
25	15.839	2164	2168	2172	rBV	86652	120557	1.56%	0.202%
26	15.933	2179	2184	2192	rVB4	86149	160785	2.07%	0.269%
27	16.033	2196	2201	2209	rVB6	49466	82812	1.07%	0.138%
28	17.221	2397	2403	2408	rBV2	1458331	2174924	28.06%	3.637%
29	17.262	2408	2410	2414	rVV	130638	157176	2.03%	0.263%
30	17.321	2414	2420	2430	rVB	1273179	1932718	24.93%	3.232%
31	18.098	2547	2552	2557	rBV	328075	496218	6.40%	0.830%
32	19.280	2749	2753	2759	rVB	271647	367076	4.74%	0.614%
33	19.374	2765	2769	2775	rBV2	245672	366434	4.73%	0.613%
34	19.615	2804	2810	2821	rBV2	1457488	2453913	31.66%	4.103%

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35	20.945	3031	3036	3045	rVB	6641995	7751591	100.00%	12.962%
36	21.086	3057	3060	3066	rBV	634852	677941	8.75%	1.134%
37	21.403	3108	3114	3118	rBV	1737559	2597396	33.51%	4.343%
38	21.986	3210	3213	3222	rVB	978550	1375162	17.74%	2.300%
39	22.956	3374	3378	3383	rVB	1798728	2576199	33.23%	4.308%
40	23.015	3384	3388	3394	rVB2	692525	1082323	13.96%	1.810%
41	23.550	3474	3479	3487	rVB3	1295378	3551037	45.81%	5.938%
42	23.715	3502	3507	3516	rVB2	1199057	2343670	30.23%	3.919%
43	24.215	3586	3592	3602	rVB	2547060	4965880	64.06%	8.304%
44	24.985	3719	3723	3734	rVB	1170129	2577422	33.25%	4.310%

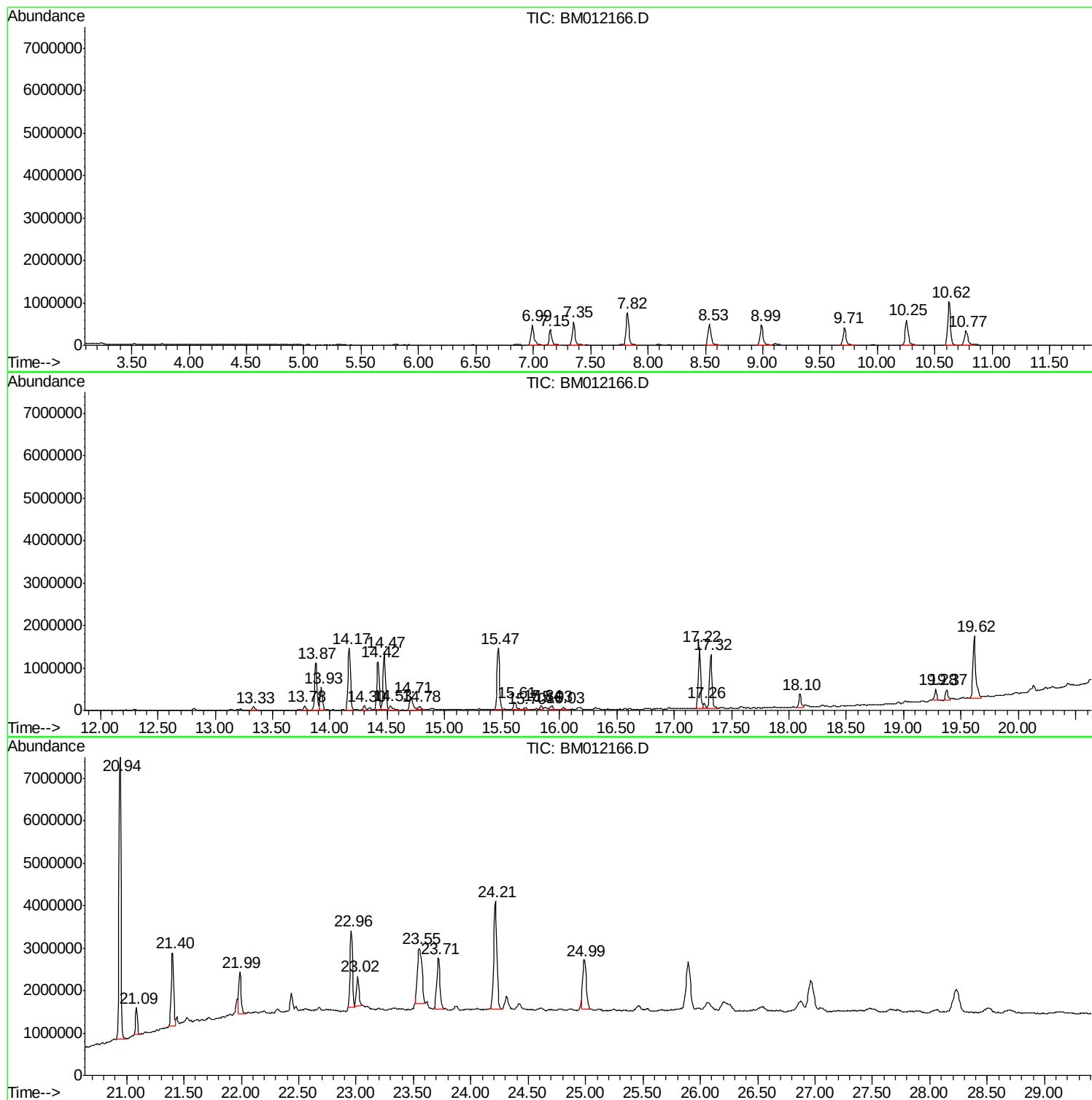
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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



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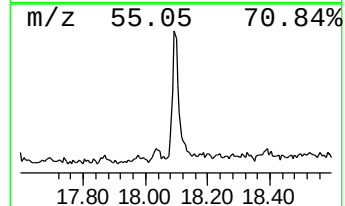
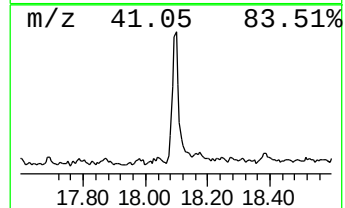
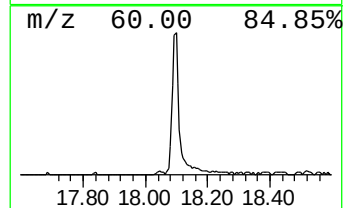
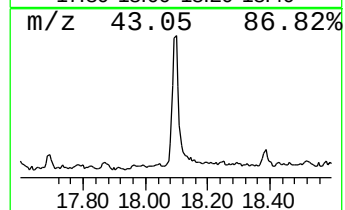
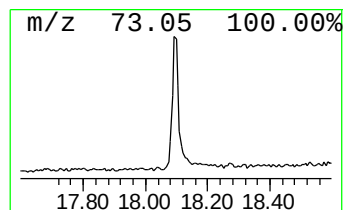
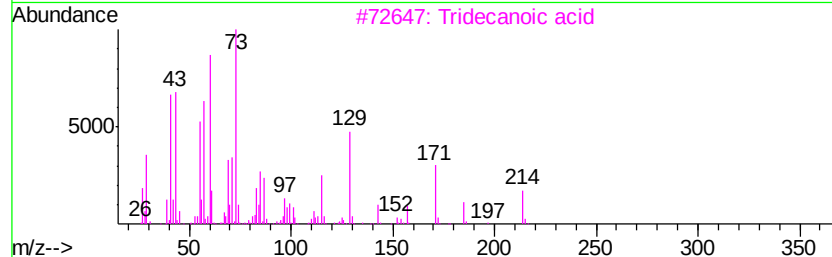
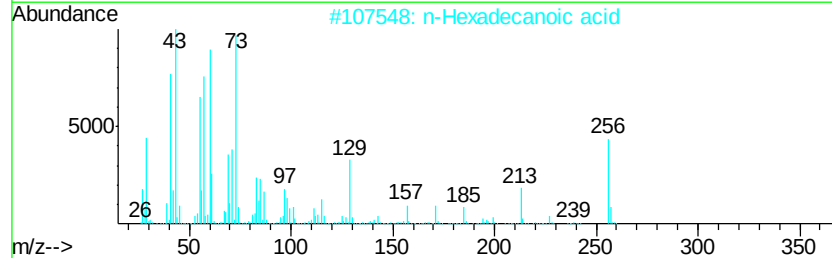
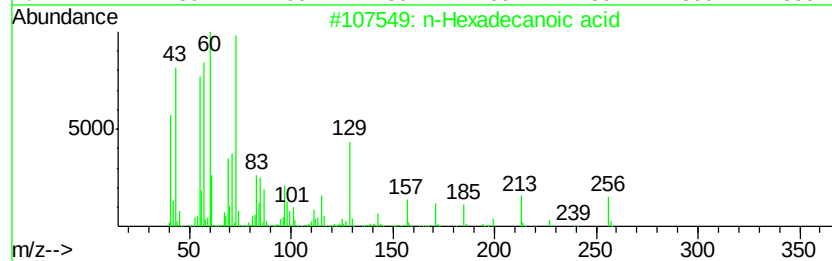
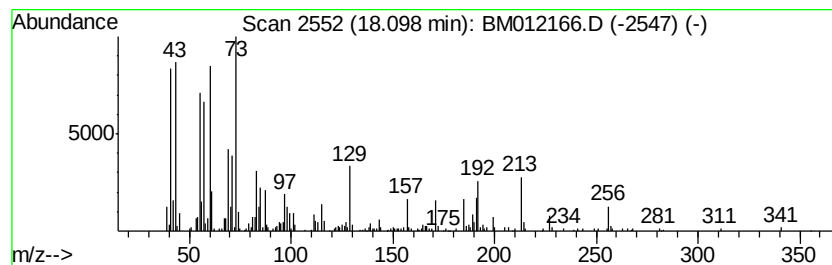
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	4.56 ng/ul	496218	Phenanthrene-d10	17.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	89
5		Octadecanoic acid	284	C18H36O2	000057-11-4	76



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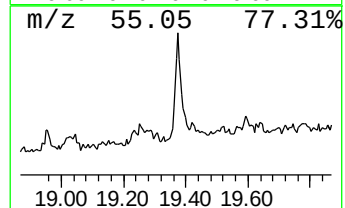
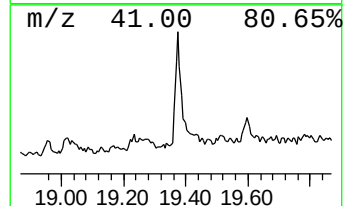
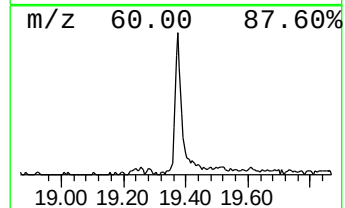
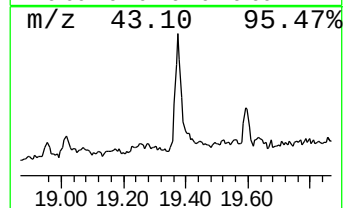
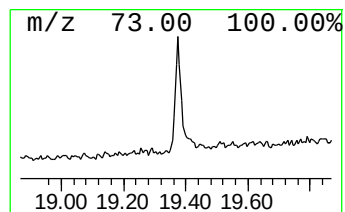
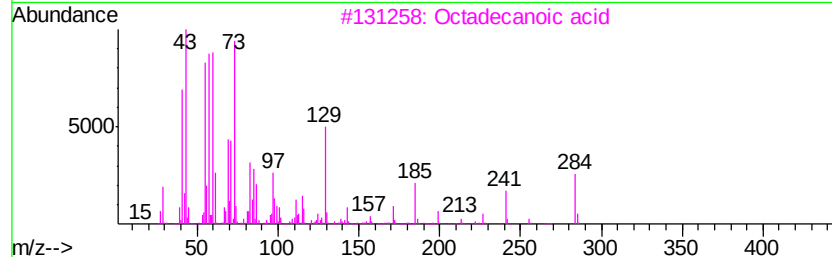
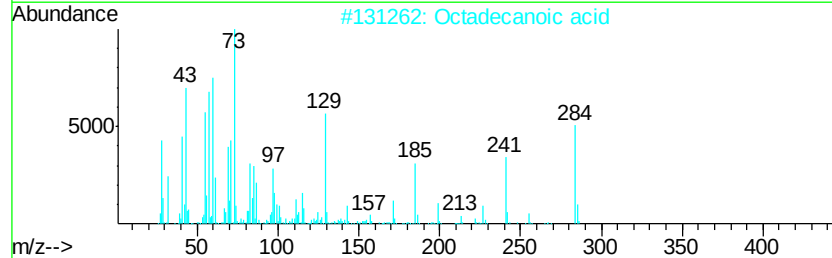
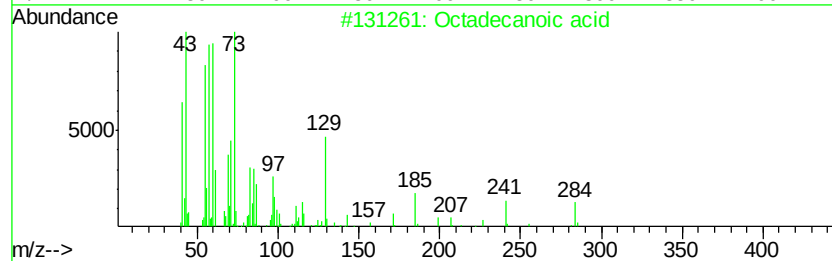
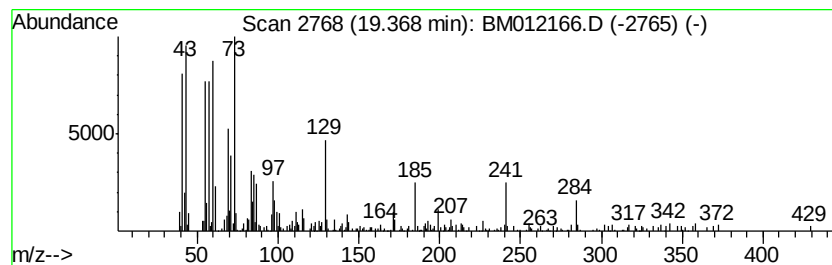
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Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	2.82 ng/ul	366434	Chrysene-d12	21.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	99
5		Octadecanoic acid	284	C18H36O2	000057-11-4	95



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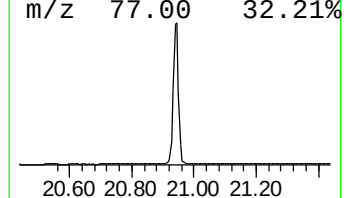
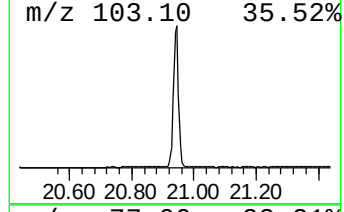
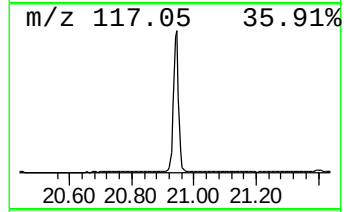
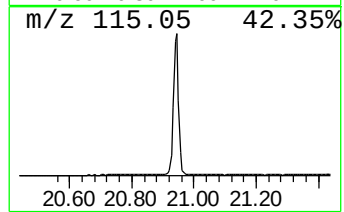
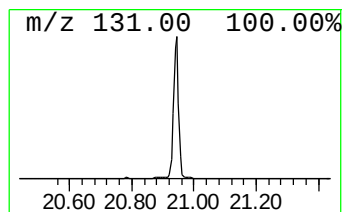
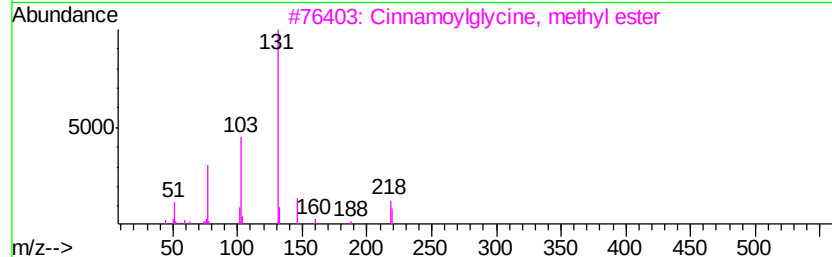
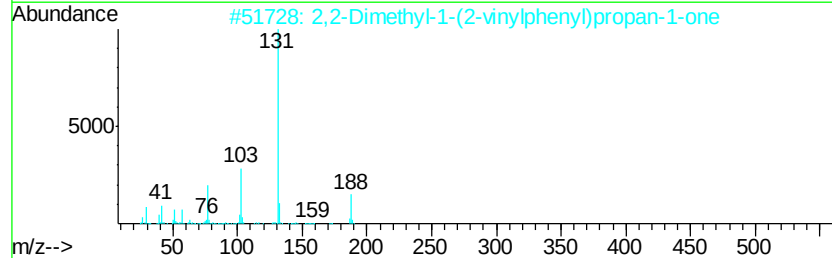
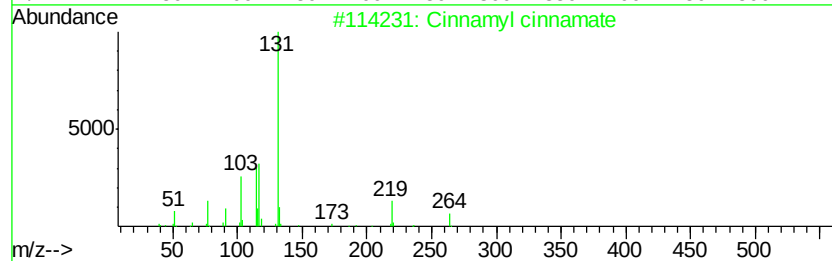
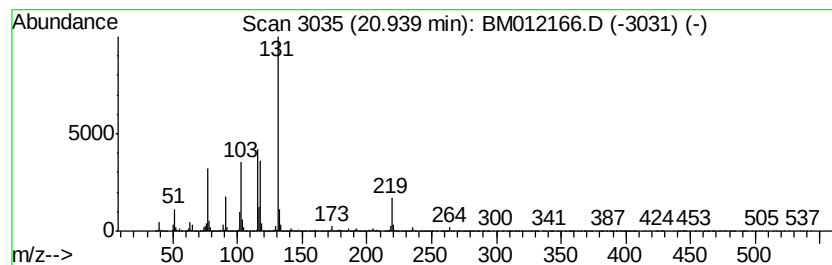
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	59.69 ng/ul	7751590	Chrysene-d12	21.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cinnamyl cinnamate	264 C18H16O2	000122-69-0 64	
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188 C13H16O	1000210-99-9 60	
3	Cinnamoylglycine, methyl ester	219 C12H13NO3	040778-04-9 50	
4	1-Phenyl-4-methyl-1-pentyn-3-ol	174 C12H14O	005923-02-4 47	
5	trans-1-Cinnamoylimidazole	198 C12H10N2O	001138-15-4 47	



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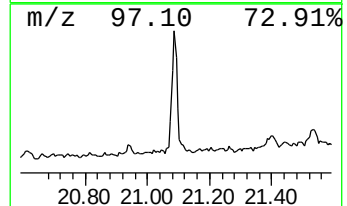
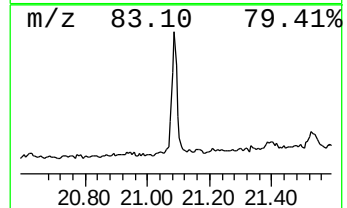
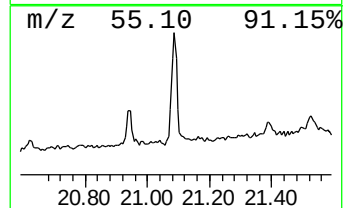
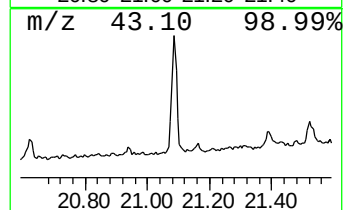
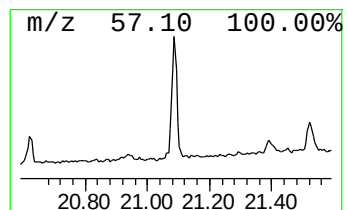
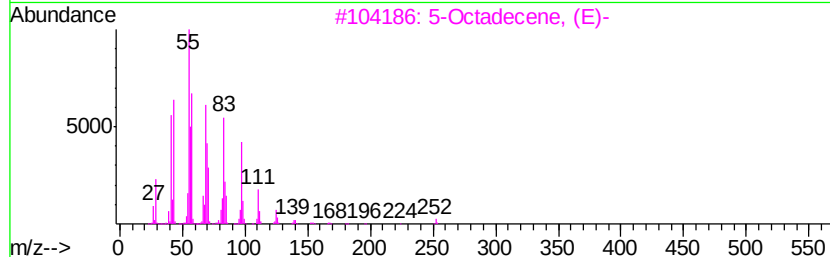
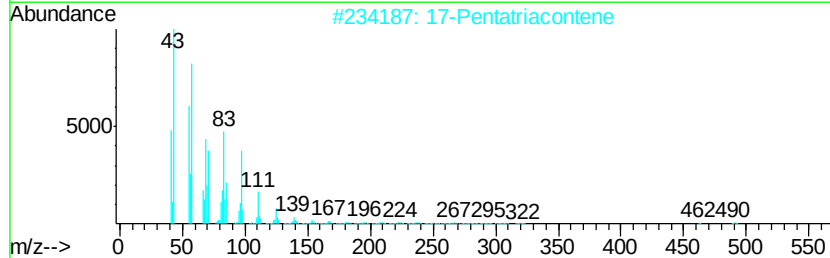
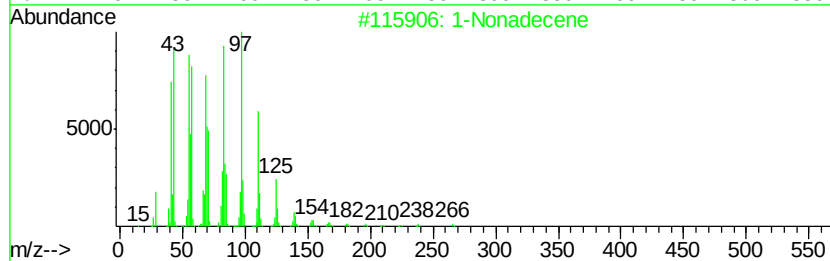
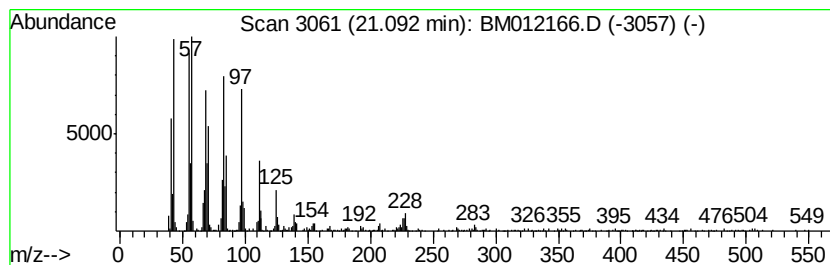
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Peak Number 5 (DEL) Alkane: Cyclic Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.09	5.22 ng/ul	677941	Chrysene-d12	21.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	17-Pentatriacontene	491	C35H70	006971-40-0	95
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
5	2,6,10,14-Tetramethyl-7-(3-methy...	348	C25H48	1000370-41-6	91



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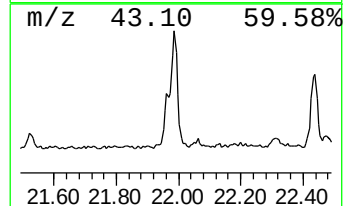
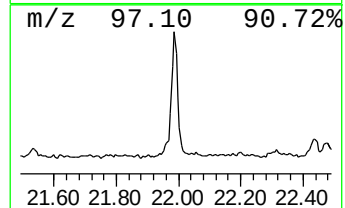
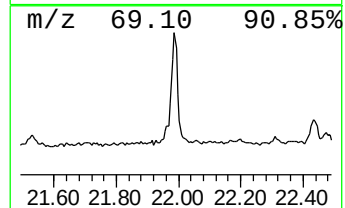
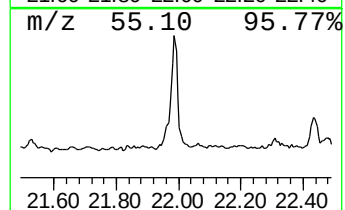
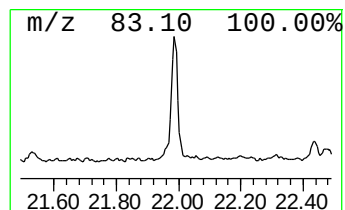
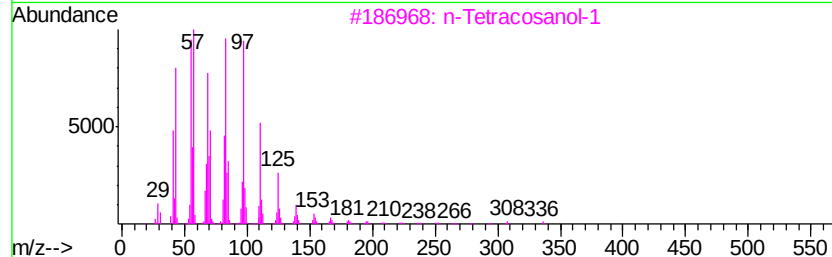
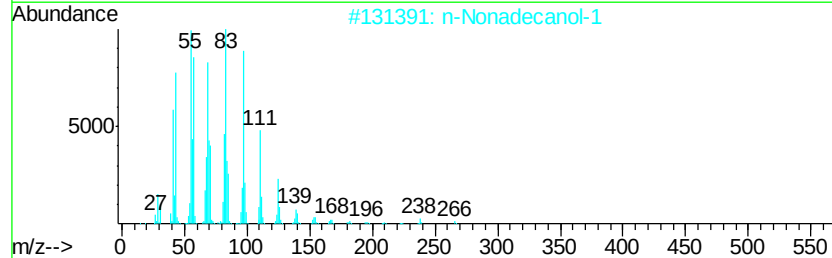
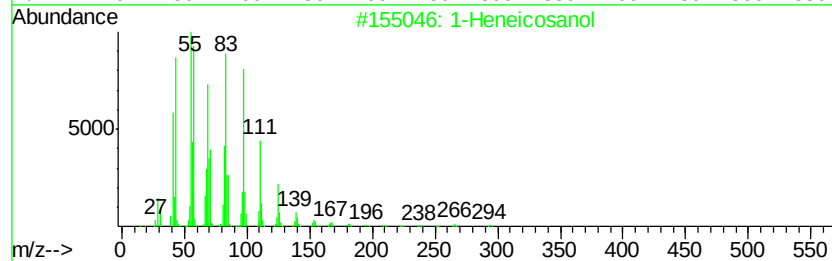
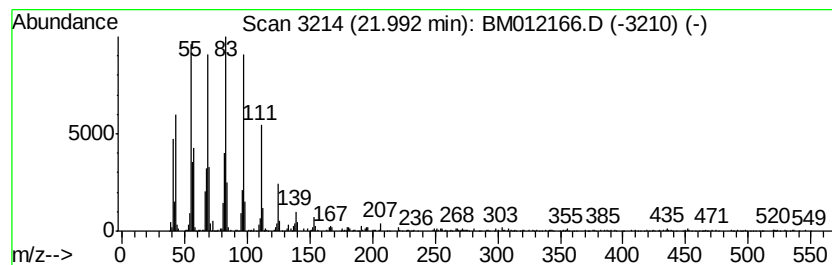
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	10.59 ng/ul	1375160	Chrysene-d12	21.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		1-Heptacosanol	396	C27H56O	002004-39-9	90



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM101317\
Data File : BM012166.D
Acq On : 14 Oct 2017 10:28
Operator : SJ/JU
Sample : I5548-16
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AF6

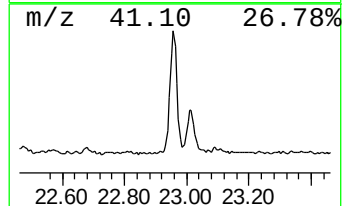
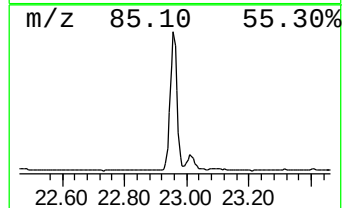
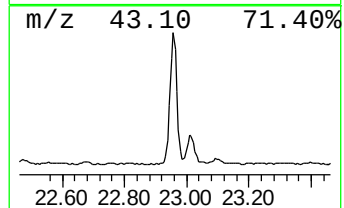
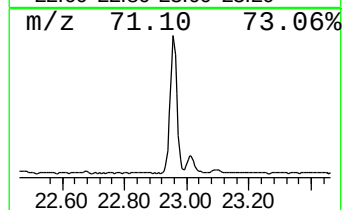
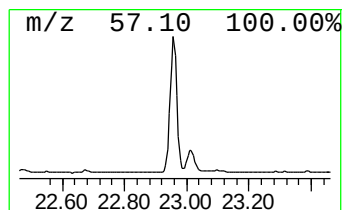
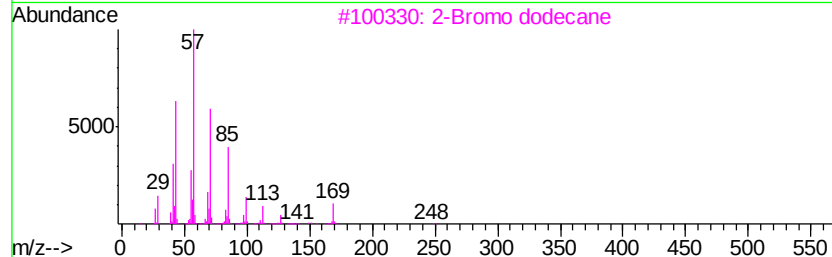
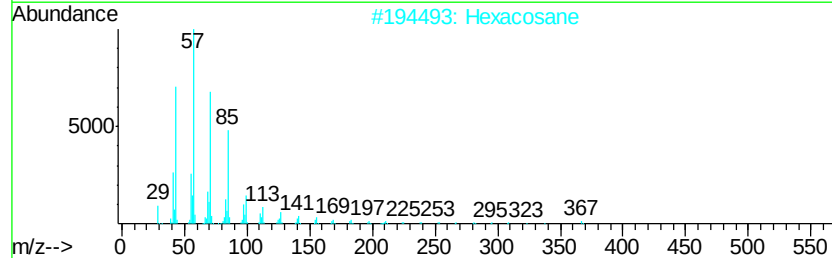
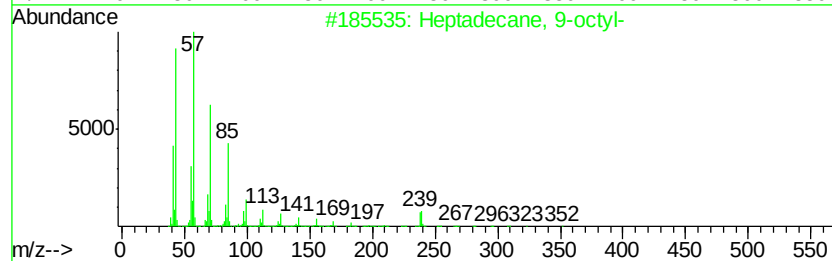
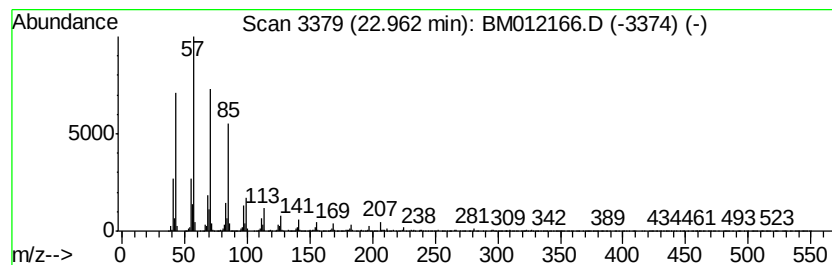
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chain Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	21.98 ng/ul	2576200	Perylene-d12	23.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2		Hexacosane	366	C26H54	000630-01-3	94
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4		Heptacosane	380	C27H56	000593-49-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM101317\
Data File : BM012166.D
Acq On : 14 Oct 2017 10:28
Operator : SJ/JU
Sample : I5548-16
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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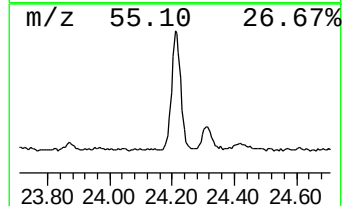
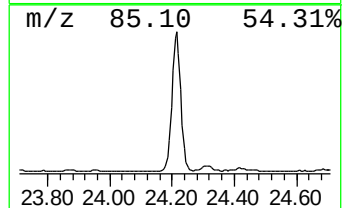
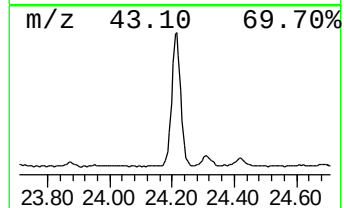
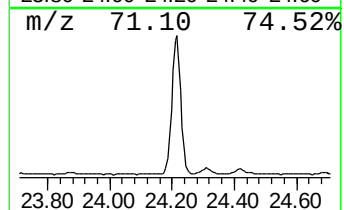
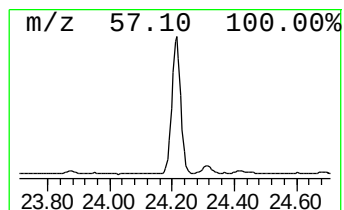
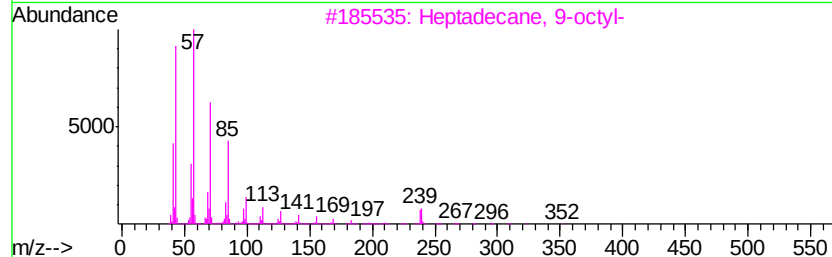
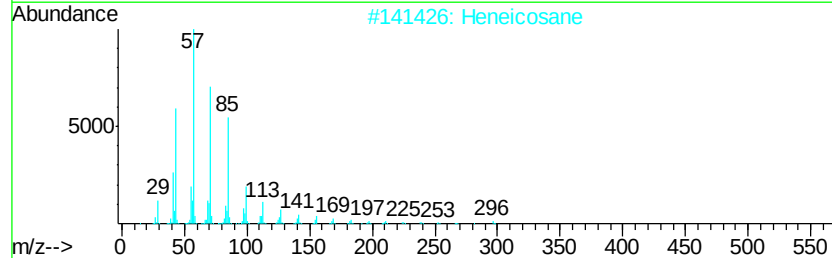
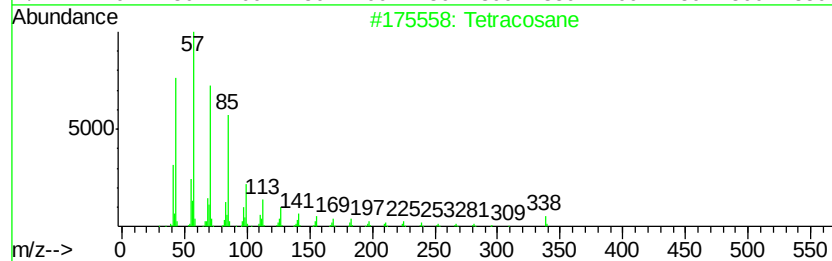
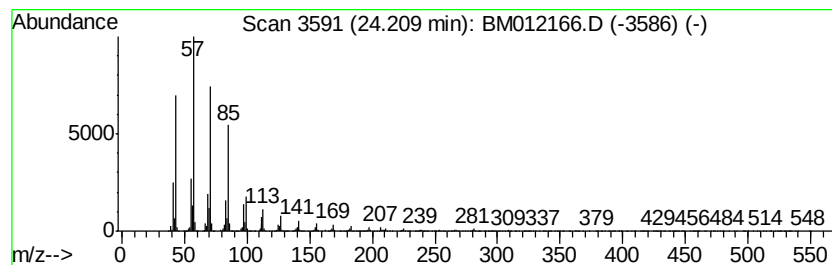
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.21	42.38 ng/ul	4965880	Perylene-d12	23.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	98
2		Heneicosane	296	C21H44	000629-94-7	96
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM101317\
Data File : BM012166.D
Acq On : 14 Oct 2017 10:28
Operator : SJ/JU
Sample : I5548-16
Misc :
ALS Vial : 23 Sample Multiplier: 1

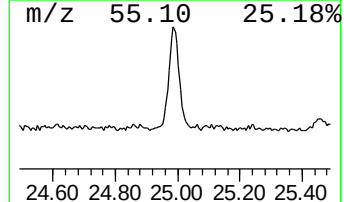
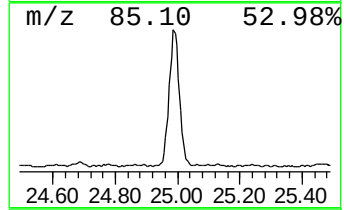
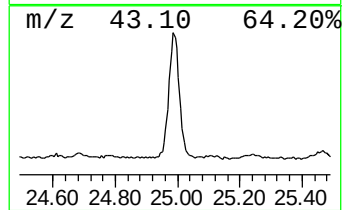
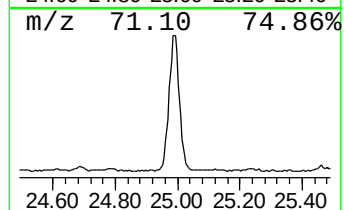
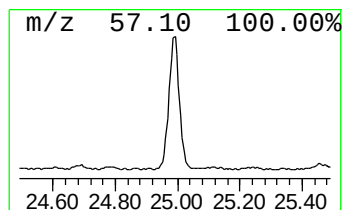
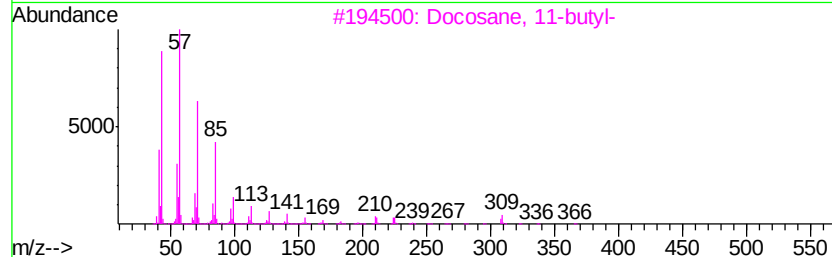
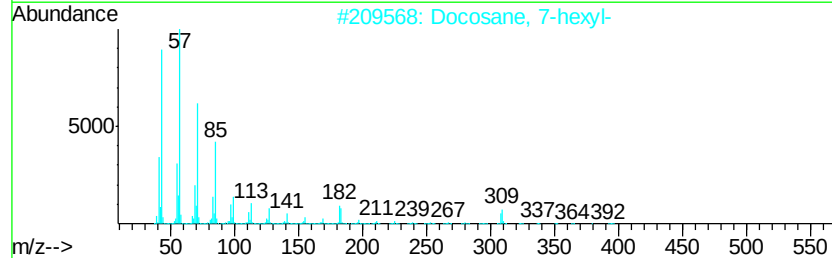
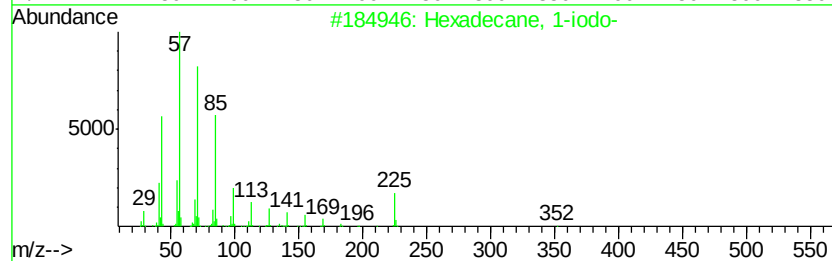
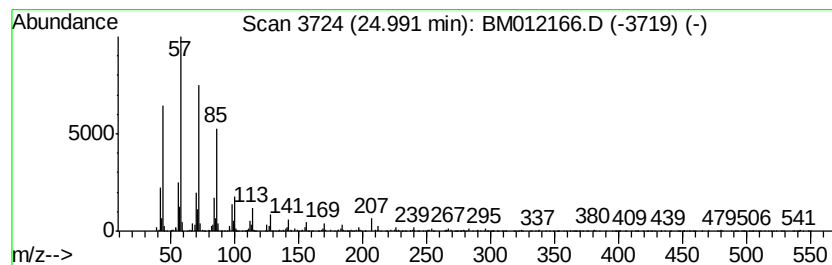
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 Hexadecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.99	21.99 ng/ul	2577420	Perylene-d12	23.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane, 1-iodo-	352 C16H33I	000544-77-4	95
2	Docosane, 7-hexyl-	394 C28H58	055373-86-9	95
3	Docosane, 11-butyl-	366 C26H54	013475-76-8	95
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	93
5	Octadecane	254 C18H38	000593-45-3	93



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM101317\
Data File : BM012166.D
Acq On : 14 Oct 2017 10:28
Operator : SJ/JU
Sample : I5548-16
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AF6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM101217.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	18.10	4.6	ng/ul	496218	4	17.22	2174920	20.0
Octadecanoic acid	19.37	2.8	ng/ul	366434	5	21.40	2597400	20.0
Cinnamyl cinnamate	20.94	59.7	ng/ul	7751590	5	21.40	2597400	20.0
(DEL) Alkane: Cyclic	21.09	5.2	ng/ul	677941	5	21.40	2597400	20.0
1-Heneicosanol	21.99	10.6	ng/ul	1375160	5	21.40	2597400	20.0
(DEL) Alkane: Str...	22.96	22.0	ng/ul	2576200	6	23.72	2343670	20.0
Tetracosane	24.21	42.4	ng/ul	4965880	6	23.72	2343670	20.0
Hexadecane, 1-iodo-	24.99	22.0	ng/ul	2577420	6	23.72	2343670	20.0