

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
 Data File : BF112851.D
 Acq On : 5 Mar 2019 13:13
 Operator : JU/SJ
 Sample : K1704-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-SW068-022719

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	551	556	559	rBV	3653717	3863466	84.59%	9.944%
2	6.381	724	730	748	rBV	3741415	4222504	92.45%	10.868%
3	6.516	748	753	756	rBV	4272488	4109607	89.97%	10.578%
4	6.745	788	792	795	rBV	1222455	1024618	22.43%	2.637%
5	6.904	814	819	822	rBV	3345132	3162694	69.24%	8.140%
6	7.304	882	887	890	rBV	2616555	2557110	55.98%	6.582%
7	8.028	1005	1010	1016	rBV	1160678	1235322	27.05%	3.180%
8	9.104	1188	1193	1203	rBV	4433446	4567535	100.00%	11.756%
9	9.492	1256	1259	1266	rBV	242573	236936	5.19%	0.610%
10	9.775	1303	1307	1322	rVB	1489471	1403510	30.73%	3.612%
11	10.557	1436	1440	1456	rBV	2738913	2811008	61.54%	7.235%
12	11.010	1512	1517	1523	rVB	84839	116652	2.55%	0.300%
13	11.251	1554	1558	1566	rBV	1410841	1308048	28.64%	3.367%
14	11.792	1646	1650	1657	rBV2	183047	271125	5.94%	0.698%
15	11.851	1657	1660	1668	rVB4	48726	77717	1.70%	0.200%
16	12.580	1780	1784	1796	rBV3	75325	160328	3.51%	0.413%
17	12.833	1823	1827	1831	rBV	3766730	3761195	82.35%	9.681%
18	13.422	1920	1927	1929	rBV2	35577	47247	1.03%	0.122%
19	13.739	1977	1981	1988	rBV2	193159	278414	6.10%	0.717%
20	13.880	2001	2005	2012	rBV	1189953	1152001	25.22%	2.965%
21	14.063	2033	2036	2042	rBV	89096	87889	1.92%	0.226%
22	14.369	2085	2088	2093	rBV	111069	113457	2.48%	0.292%
23	14.663	2135	2138	2142	rVB	147964	134235	2.94%	0.346%
24	14.733	2147	2150	2157	rVB	90010	100194	2.19%	0.258%
25	14.980	2189	2192	2207	rVB	240617	415913	9.11%	1.071%
26	15.292	2240	2245	2250	rBV	905528	1118609	24.49%	2.879%
27	15.339	2250	2253	2259	rVB	146896	183345	4.01%	0.472%
28	15.751	2319	2323	2327	rVB	137784	182999	4.01%	0.471%
29	16.221	2400	2403	2415	rVB3	82751	148188	3.24%	0.381%

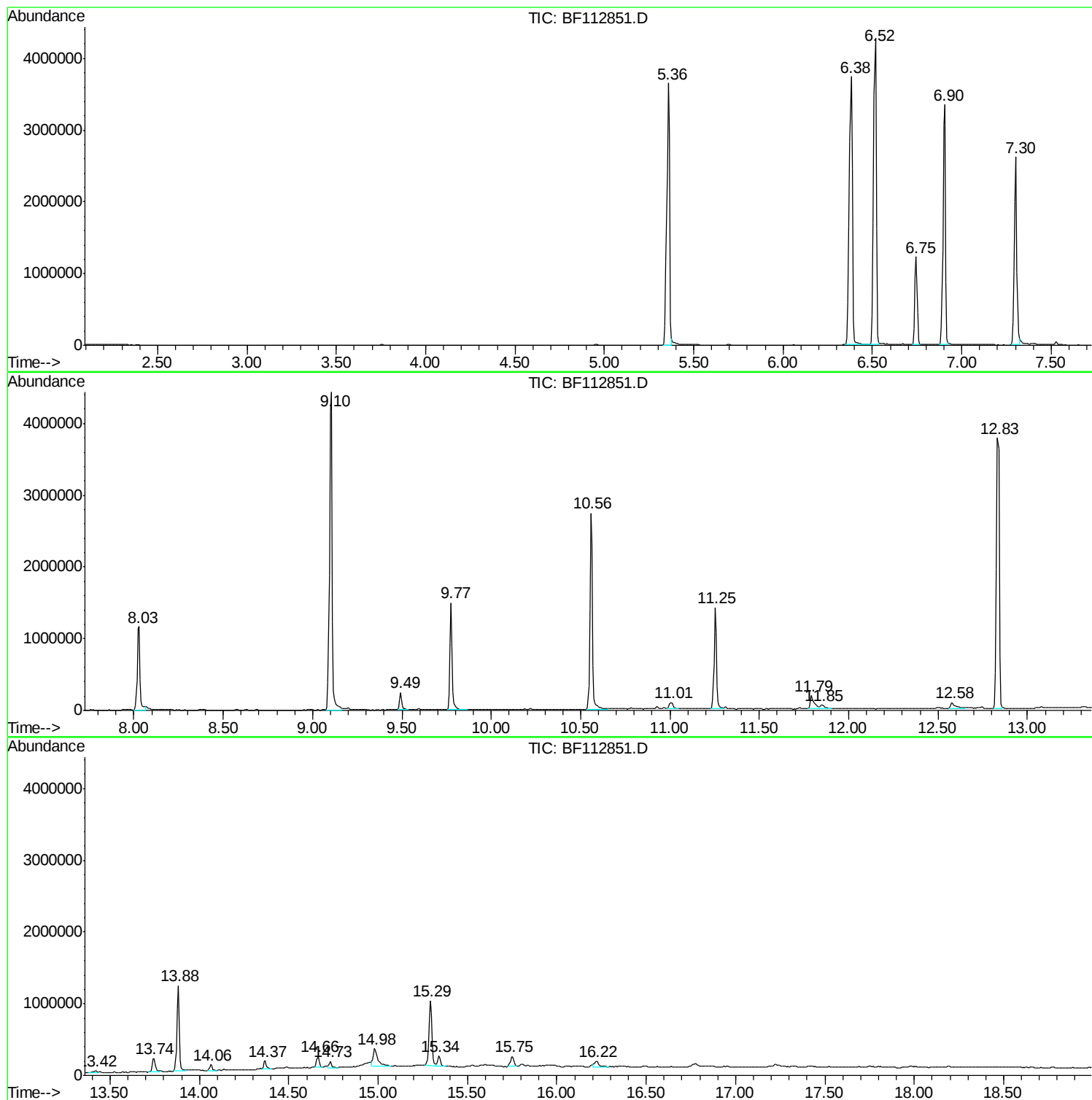
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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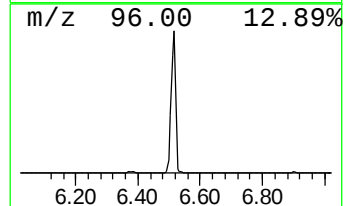
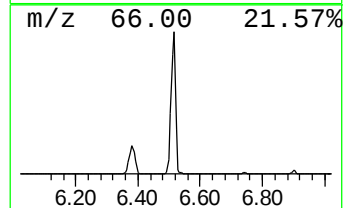
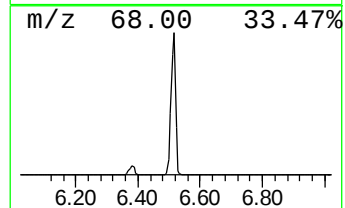
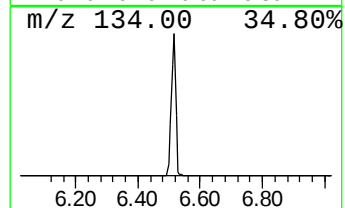
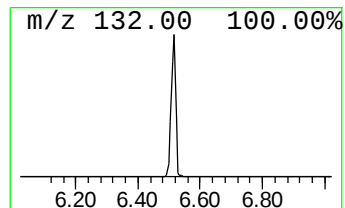
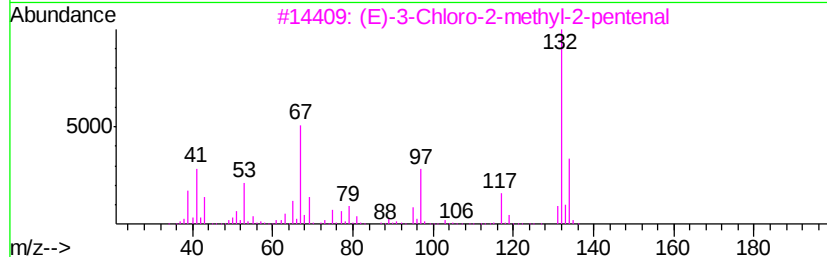
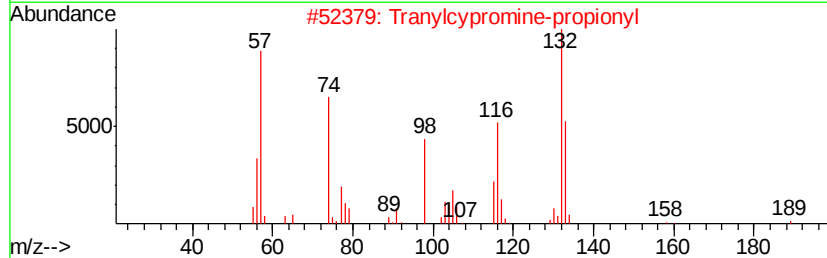
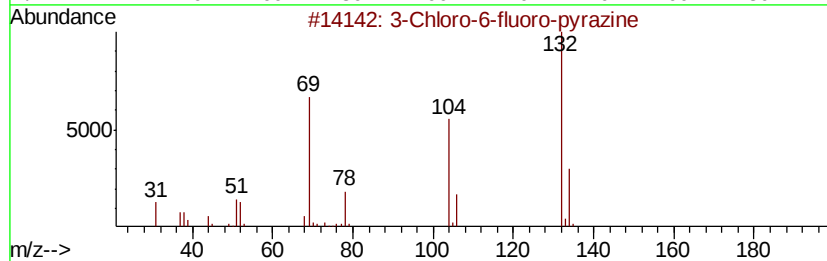
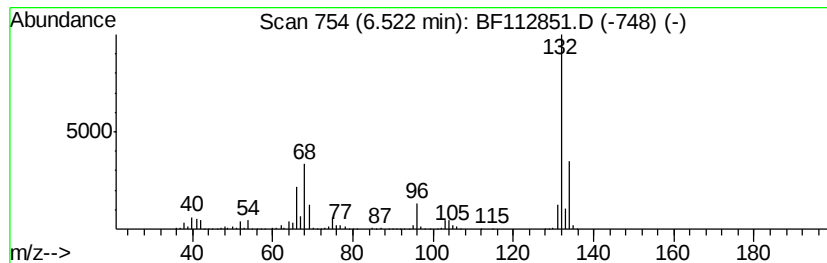
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	80.22 ng	4109610	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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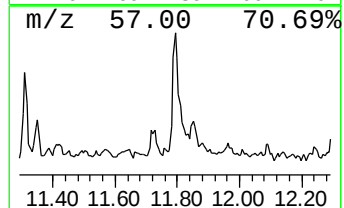
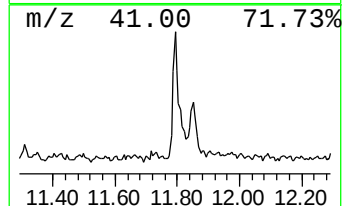
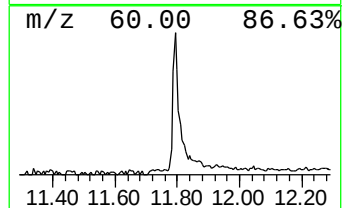
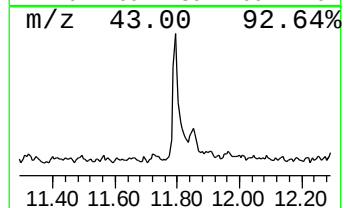
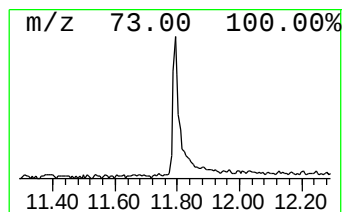
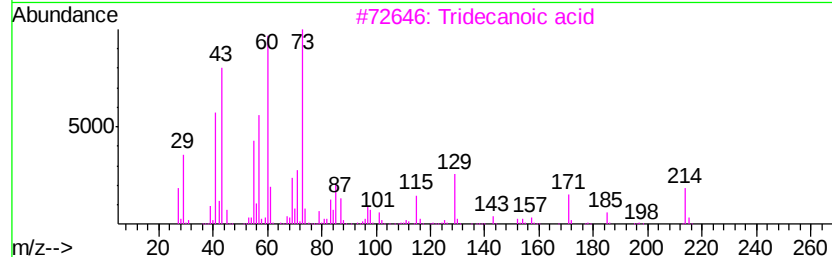
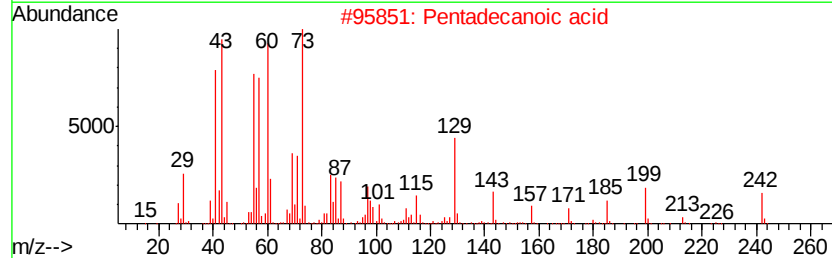
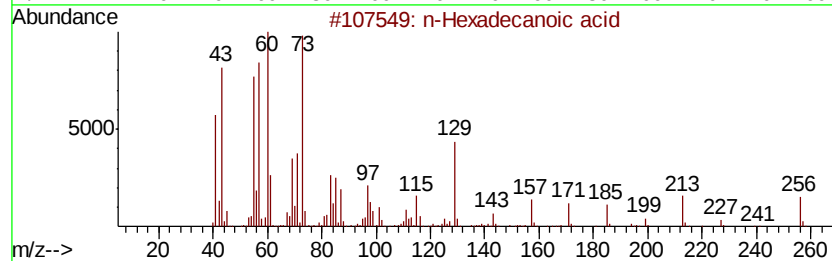
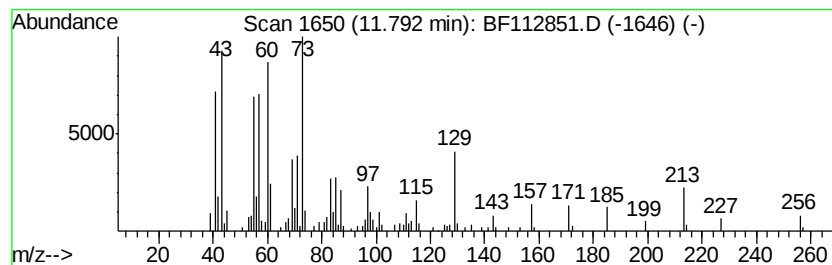
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.79	4.15 ng	271125	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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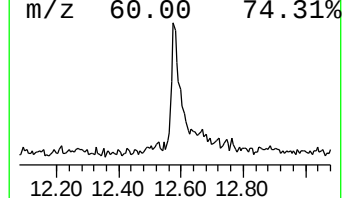
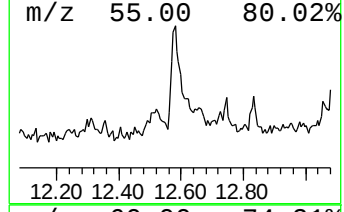
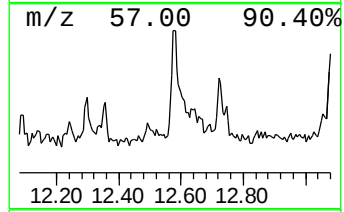
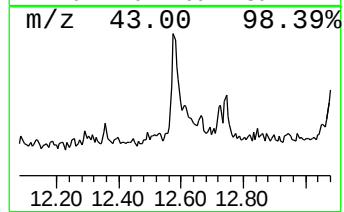
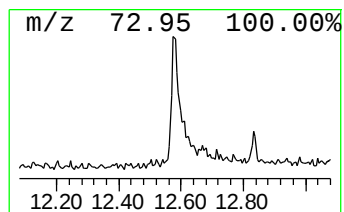
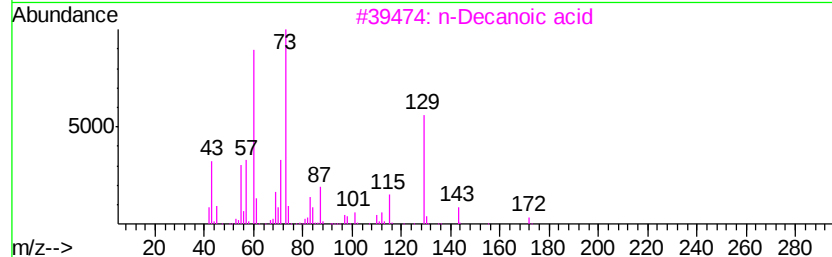
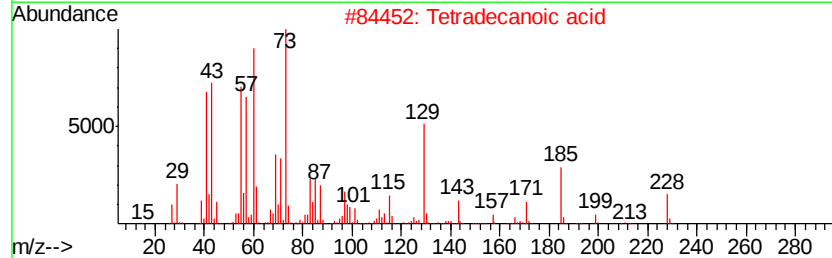
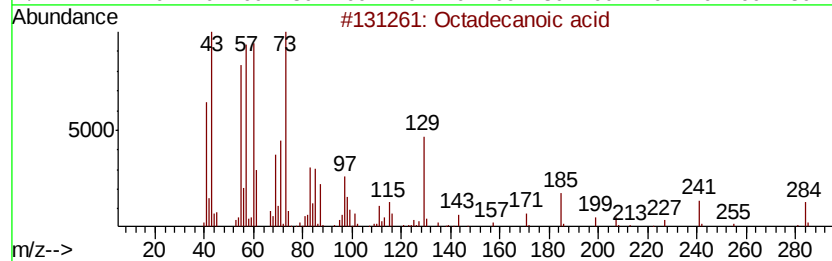
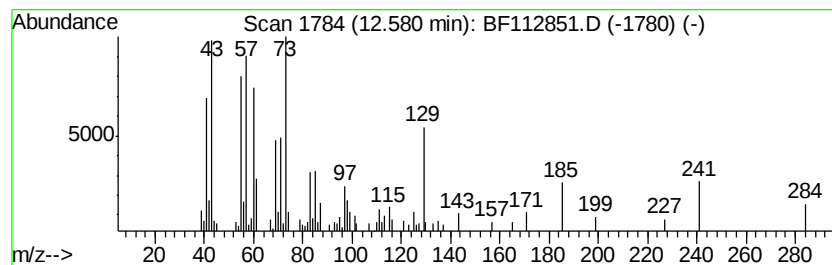
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Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.58	2.78 ng	160328	Chrysene-d12		13.88	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3		n-Decanoic acid	172	C10H20O2	000334-48-5	49
4		3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	18
5		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	11



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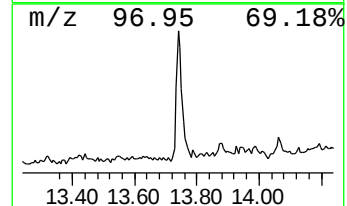
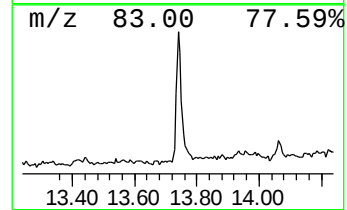
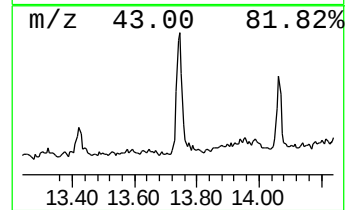
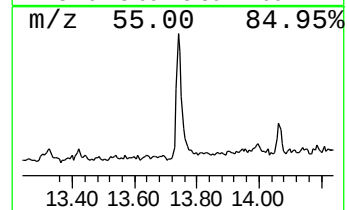
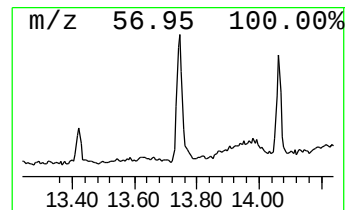
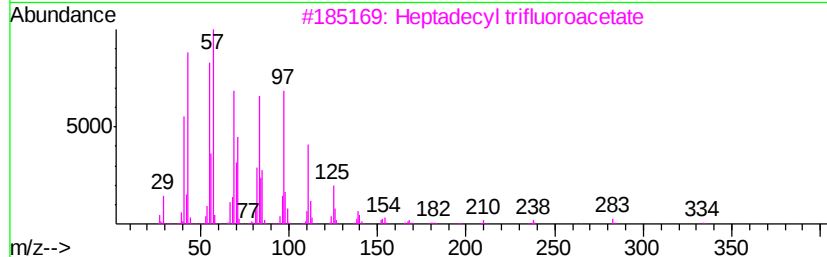
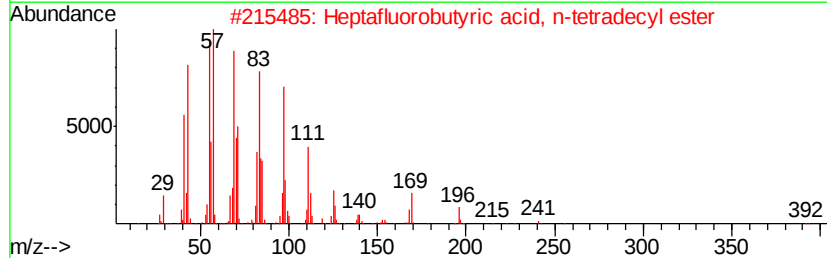
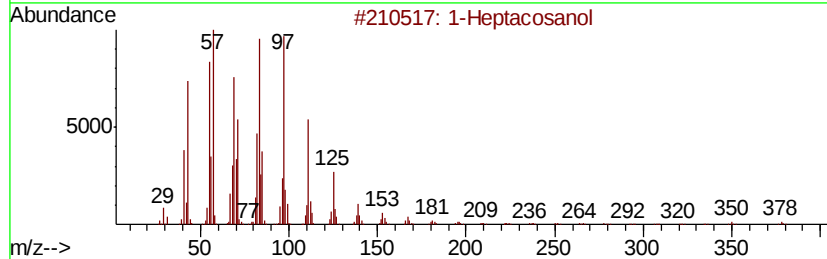
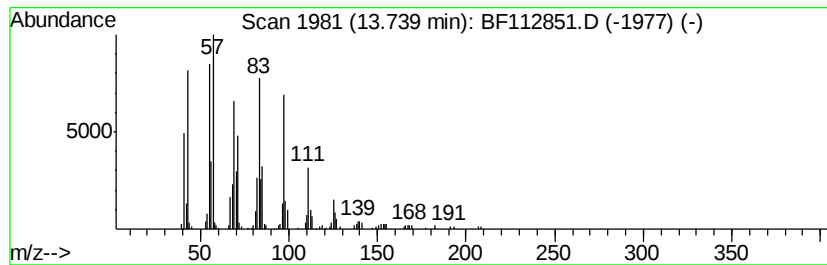
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Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.74	4.83 ng	278414	Chrysene-d12		13.88	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	91
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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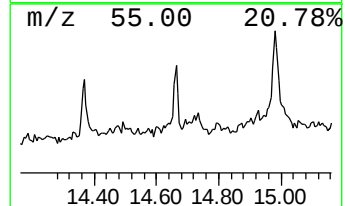
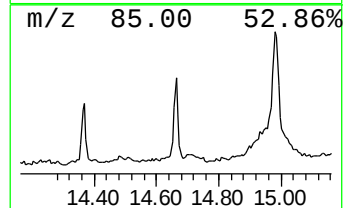
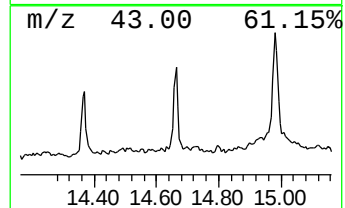
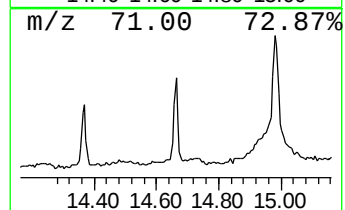
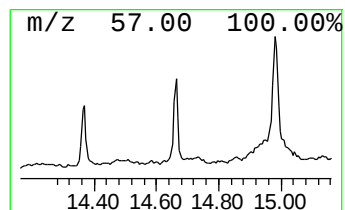
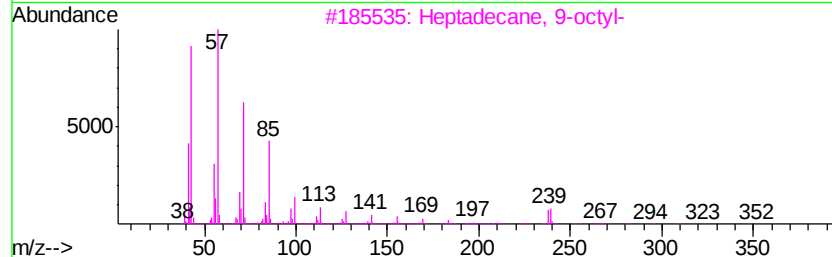
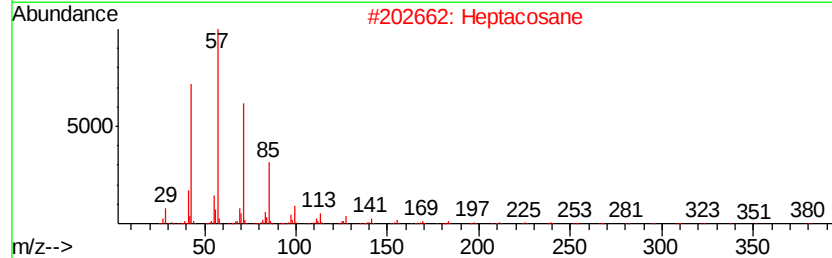
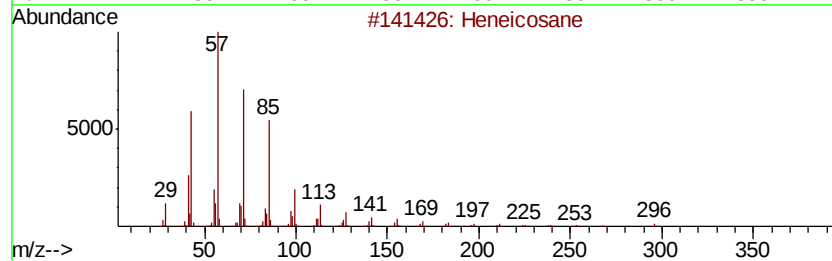
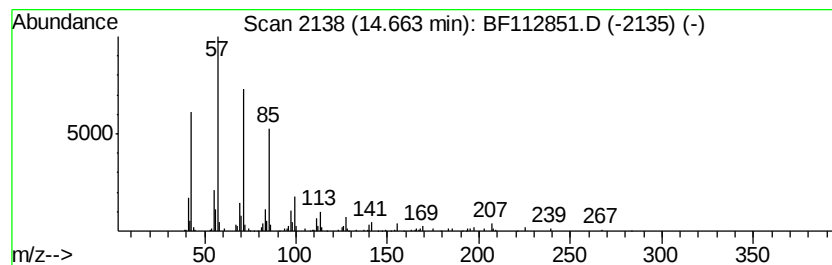
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Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.40 ng	134235	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	90
2	Heptacosane	380 C27H56	000593-49-7	87
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
4	Docosane	310 C22H46	000629-97-0	87
5	Octadecane	254 C18H38	000593-45-3	83



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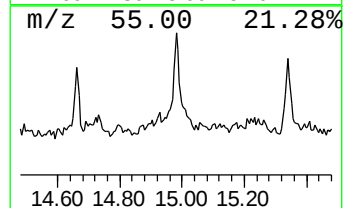
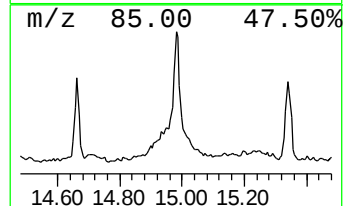
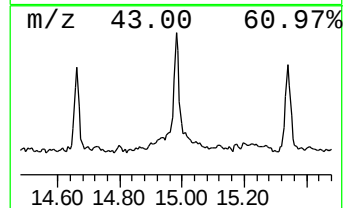
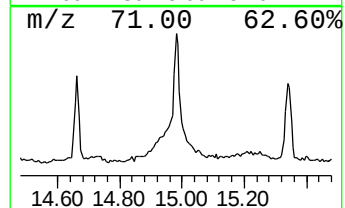
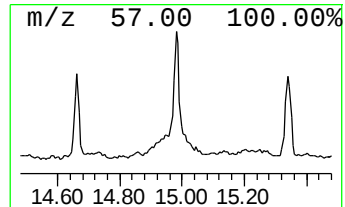
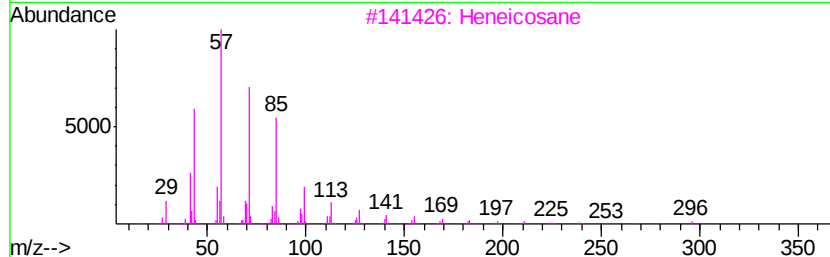
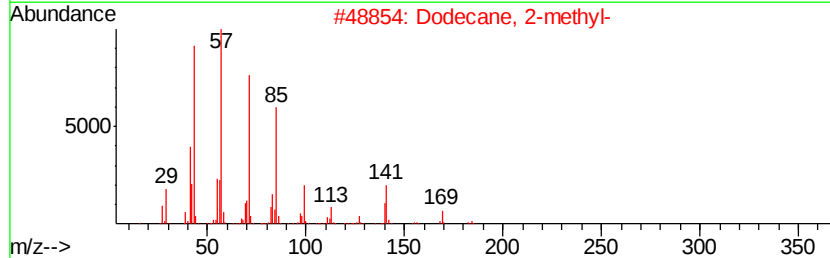
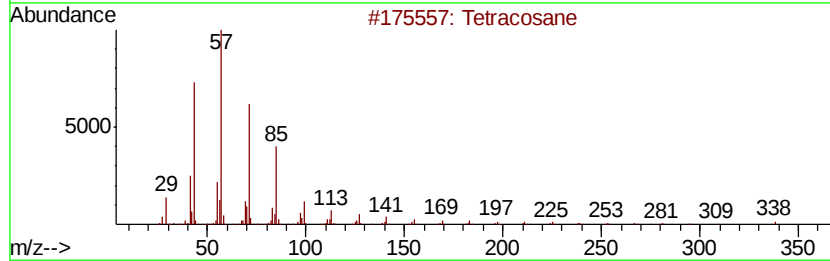
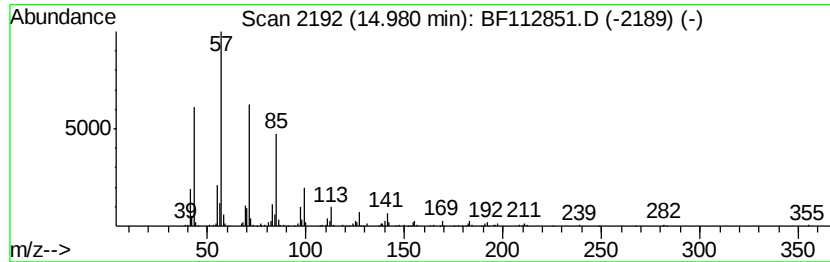
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	7.44 ng	415913	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	90
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112851.D
Acq On : 5 Mar 2019 13:13
Operator : JU/SJ
Sample : K1704-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

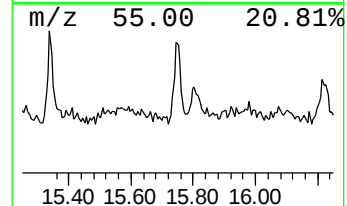
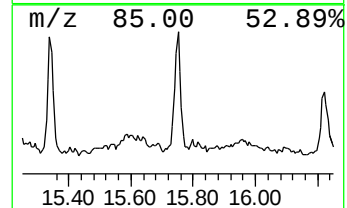
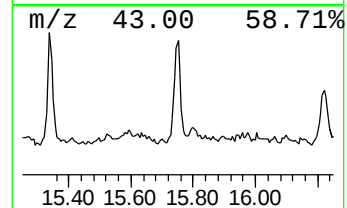
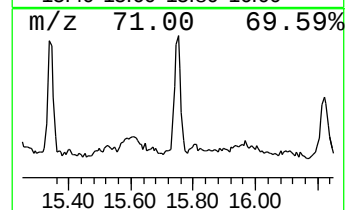
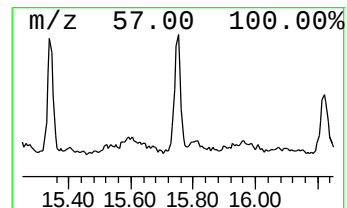
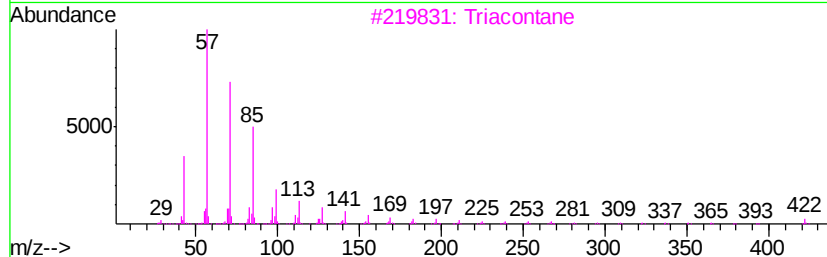
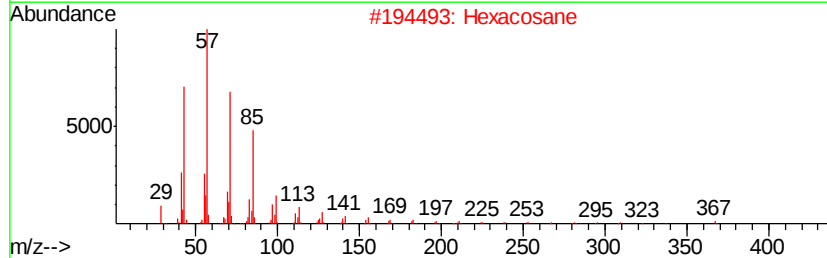
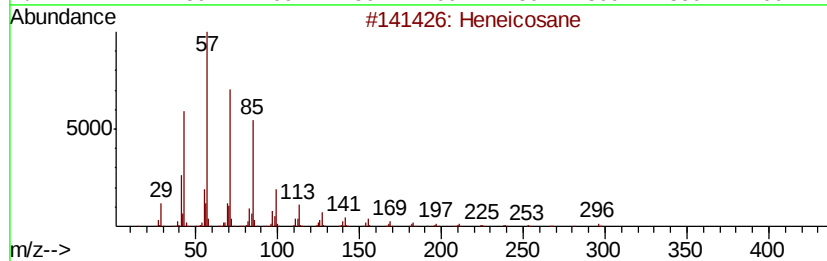
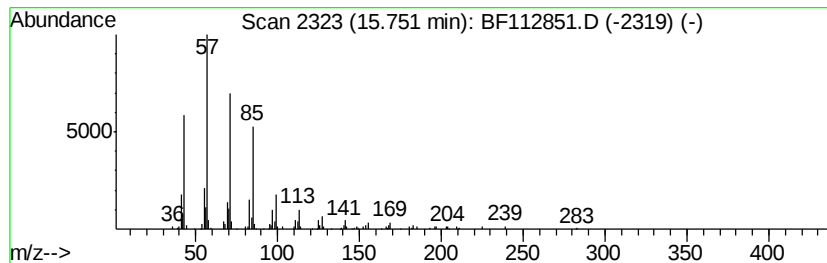
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ClientSampleId :
PST-028-SW068-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	3.27 ng	182999	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Hexacosane	366 C26H54	000630-01-3	91
3	triacontane	422 C30H62	000638-68-6	91
4	Docosane	310 C22H46	000629-97-0	91
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112851.D
Acq On : 5 Mar 2019 13:13
Operator : JU/SJ
Sample : K1704-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-SW068-022719

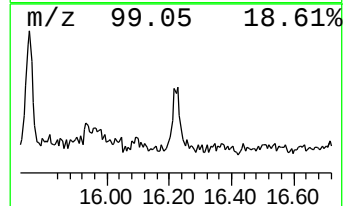
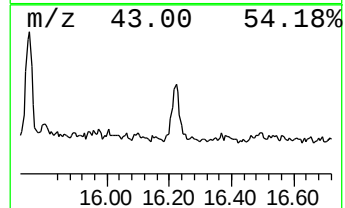
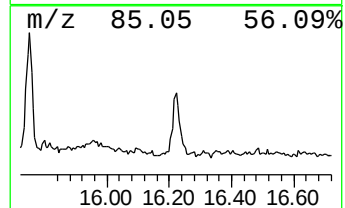
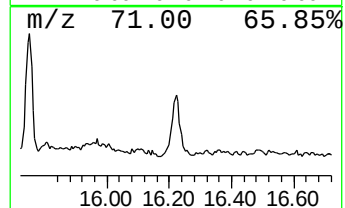
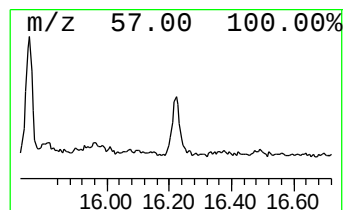
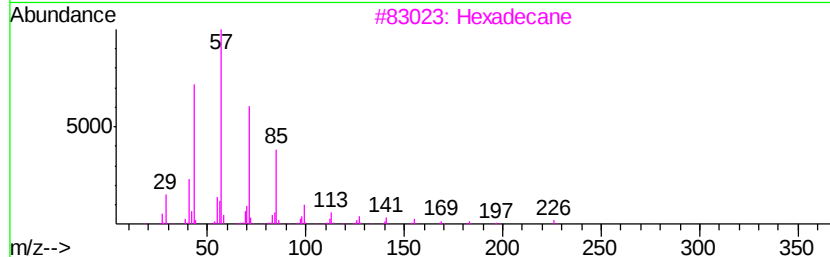
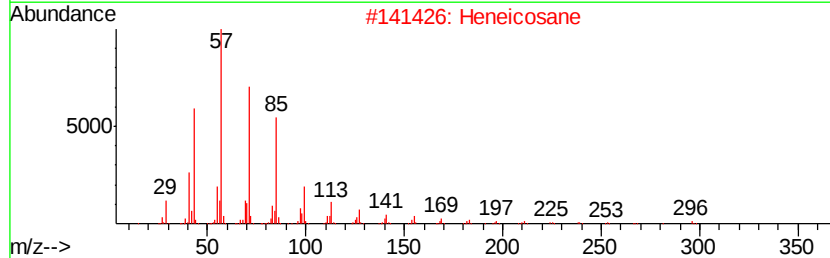
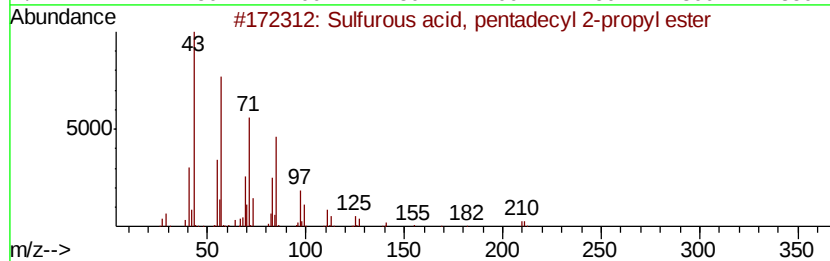
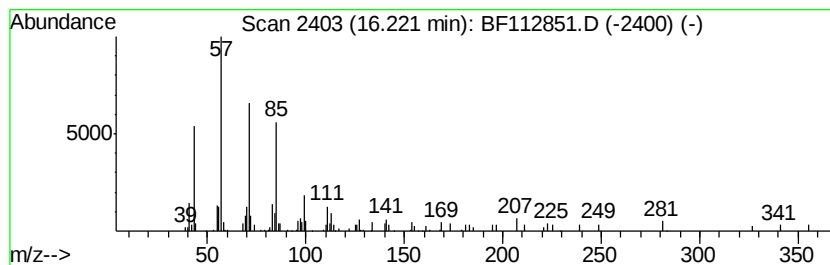
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, pentadecyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.65 ng	148188	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	86
2		Heneicosane	296	C21H44	000629-94-7	83
3		Hexadecane	226	C16H34	000544-76-3	80
4		Hexacosane	366	C26H54	000630-01-3	80
5		Octadecane	254	C18H38	000593-45-3	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112851.D
Acq On : 5 Mar 2019 13:13
Operator : JU/SJ
Sample : K1704-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-SW068-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
unknown6.52	6.52	80.2	ng	4109610	1	6.75	1024620	20.0
n-Hexadecanoic acid	11.79	4.2	ng	271125	4	11.25	1308050	20.0
Octadecanoic acid	12.58	2.8	ng	160328	5	13.88	1152000	20.0
1-Heptacosanol	13.74	4.8	ng	278414	5	13.88	1152000	20.0
Heneicosane	14.66	2.4	ng	134235	6	15.29	1118610	20.0
Tetracosane	14.98	7.4	ng	415913	6	15.29	1118610	20.0
Hexacosane	15.75	3.3	ng	182999	6	15.29	1118610	20.0
Sulfurous acid, p...	16.22	2.6	ng	148188	6	15.29	1118610	20.0