

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
 Data File : BF113049.D
 Acq On : 14 Mar 2019 15:00
 Operator : JU/SJ
 Sample : K1866-13
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-MH-13-COMP

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	5.345	549	554	558	rBV	4088145	4573504	77.58%	7.764%
2	6.010	663	667	670	rBV	109947	95481	1.62%	0.162%
3	6.375	723	729	732	rBV	4115848	4893047	83.00%	8.306%
4	6.504	745	751	754	rBV	4563025	4815846	81.69%	8.175%
5	6.728	785	789	792	rBV	1296218	1100777	18.67%	1.869%
6	6.887	811	816	819	rBV	3839319	3675716	62.35%	6.240%
7	7.287	879	884	887	rBV	2692137	3115870	52.86%	5.289%
8	7.716	953	957	967	rVB4	42641	65289	1.11%	0.111%
9	8.010	1002	1007	1013	rBV	1416374	1497312	25.40%	2.542%
10	9.086	1184	1190	1193	rBV	4970778	5170124	87.70%	8.777%
11	9.475	1252	1256	1260	rBV	549723	466311	7.91%	0.792%
12	9.757	1298	1304	1308	rBV	1825849	1796374	30.47%	3.049%
13	9.886	1322	1326	1335	rBV	71776	83998	1.42%	0.143%
14	10.545	1432	1438	1449	rBV	3950010	4304799	73.02%	7.308%
15	11.233	1551	1555	1558	rBV	1900680	1965135	33.34%	3.336%
16	11.780	1642	1648	1656	rBV	1601757	1987849	33.72%	3.374%
17	12.439	1756	1760	1763	rBV	223858	242693	4.12%	0.412%
18	12.557	1774	1780	1792	rBV	821056	1140395	19.35%	1.936%
19	12.669	1793	1799	1802	rVB	200791	221396	3.76%	0.376%
20	12.821	1817	1825	1828	rBV	5455173	5894971	100.00%	10.007%
21	12.998	1848	1855	1859	rBV3	44057	80209	1.36%	0.136%
22	13.057	1859	1865	1870	rBV3	124478	186009	3.16%	0.316%
23	13.227	1890	1894	1897	rBV2	61498	63022	1.07%	0.107%
24	13.286	1899	1904	1905	rBV3	43553	61296	1.04%	0.104%
25	13.398	1920	1923	1926	rVB	152895	126279	2.14%	0.214%
26	13.574	1950	1953	1957	rBV2	130861	157914	2.68%	0.268%
27	13.663	1966	1968	1973	rBV2	108003	112846	1.91%	0.192%
28	13.721	1974	1978	1987	rVB	1000766	1180585	20.03%	2.004%
29	13.863	1997	2002	2005	rBV	2335391	2236513	37.94%	3.797%
30	14.039	2028	2032	2038	rBV	323818	327711	5.56%	0.556%
31	14.345	2077	2084	2092	rBV	449790	669769	11.36%	1.137%
32	14.615	2126	2130	2131	rBV	175224	192358	3.26%	0.327%
33	14.639	2131	2134	2141	rVB	605207	630172	10.69%	1.070%
34	14.868	2170	2173	2176	rBV	85767	103425	1.75%	0.176%

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

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

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35	14.957	2183	2188	2192	rBV	587423	716225	12.15%	1.216%
36	15.151	2218	2221	2227	rBV3	44998	67340	1.14%	0.114%
37	15.204	2228	2230	2235	rVV	68194	79134	1.34%	0.134%
38	15.274	2236	2242	2245	rVV	1653467	2165186	36.73%	3.676%
39	15.310	2245	2248	2255	rVB	499756	623479	10.58%	1.058%
40	15.709	2311	2316	2321	rBV	489209	735584	12.48%	1.249%
41	15.768	2321	2326	2338	rVB2	237609	519082	8.81%	0.881%
42	16.174	2390	2395	2400	rBV	172703	320787	5.44%	0.545%
43	16.721	2483	2488	2495	rVB2	114237	204722	3.47%	0.348%
44	17.186	2562	2567	2576	rVB8	100661	241872	4.10%	0.411%

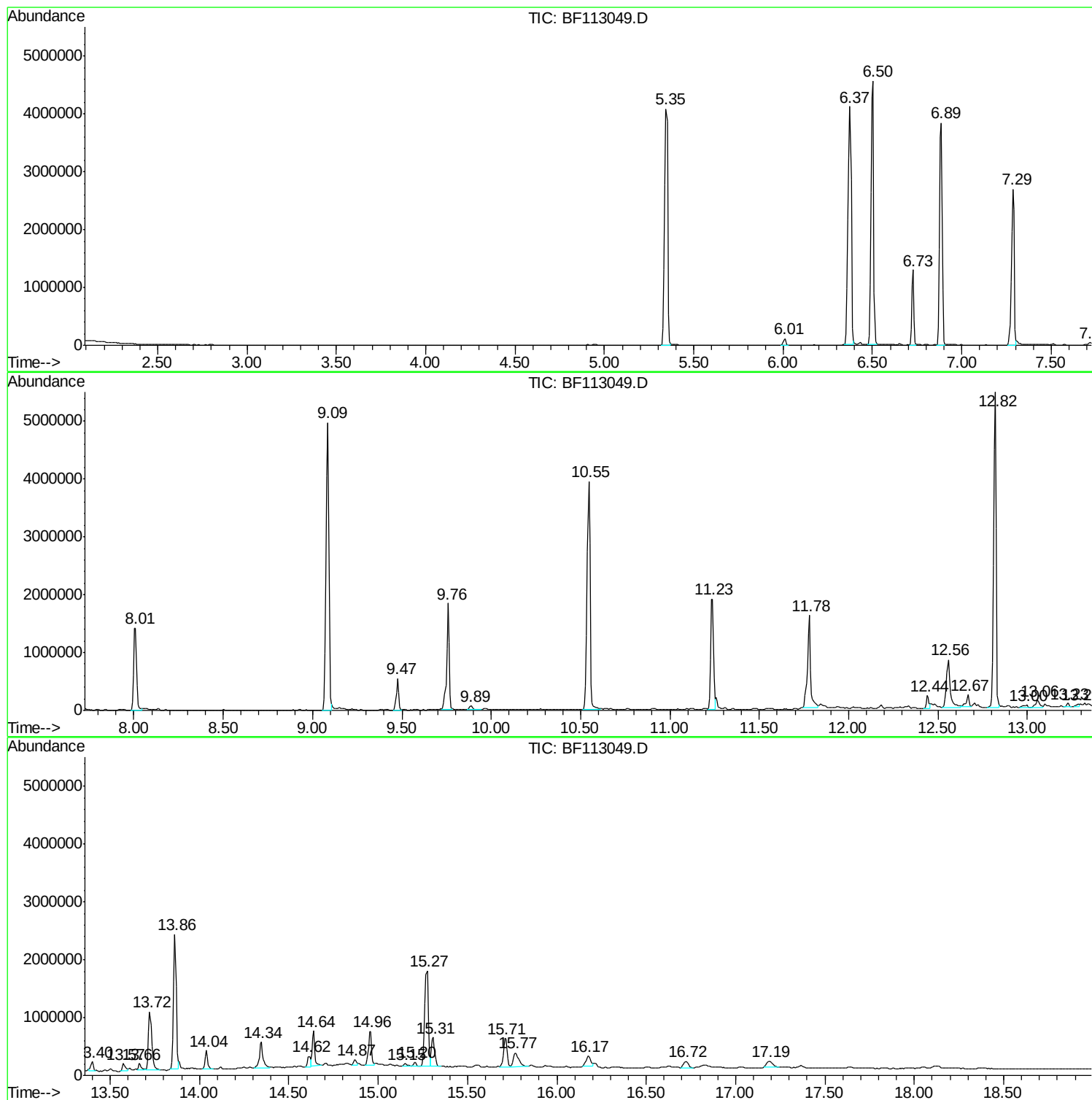
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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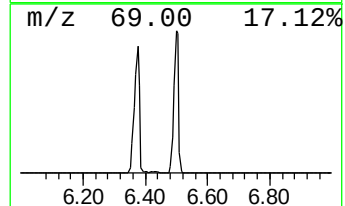
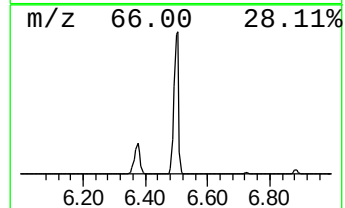
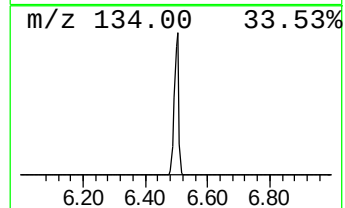
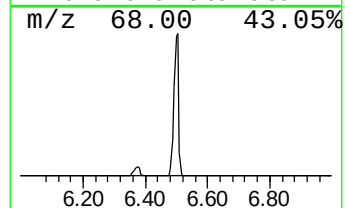
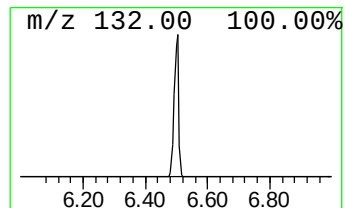
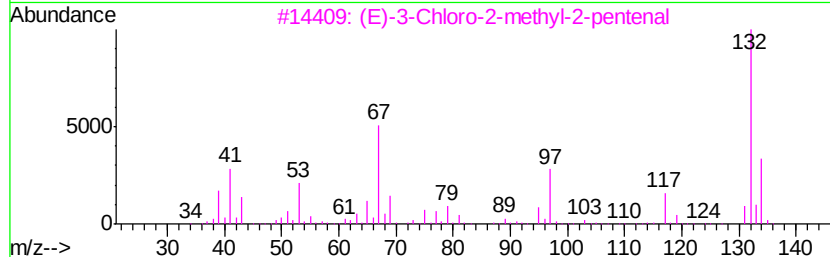
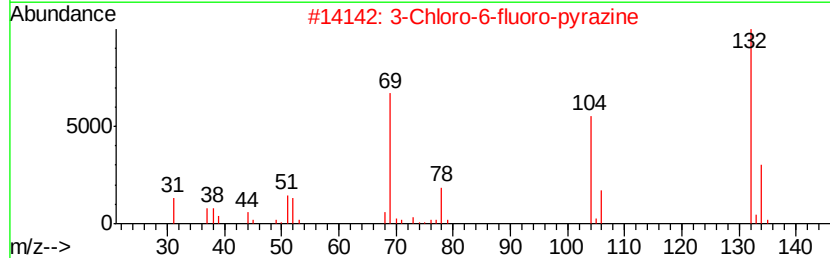
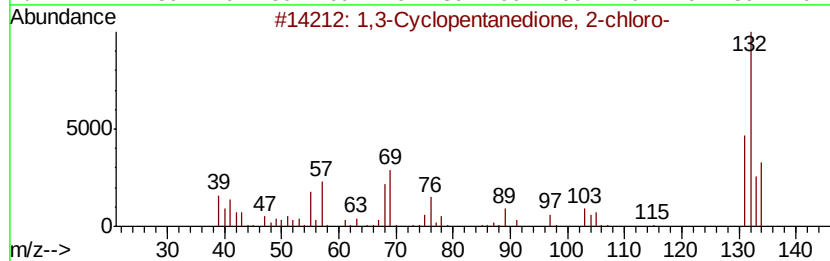
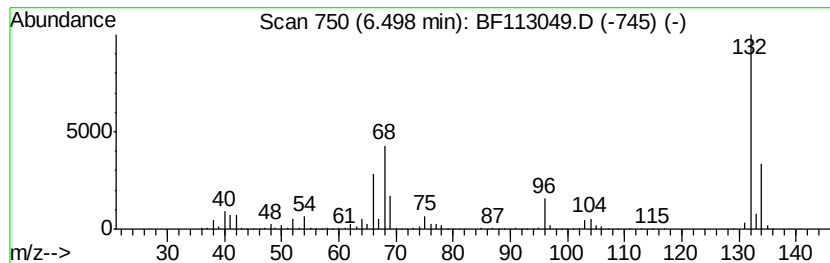
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	87.50 ng	4815850	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	47
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Xenon	132	Xe	007440-63-3	9



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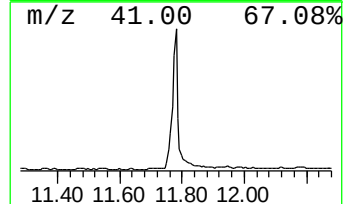
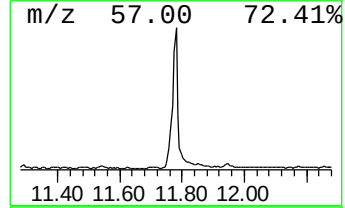
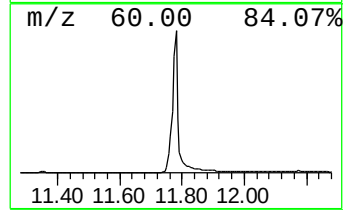
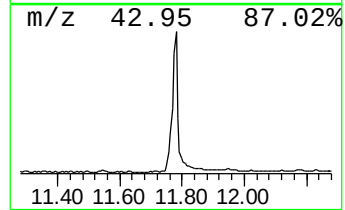
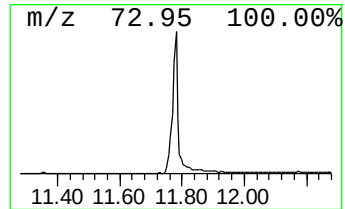
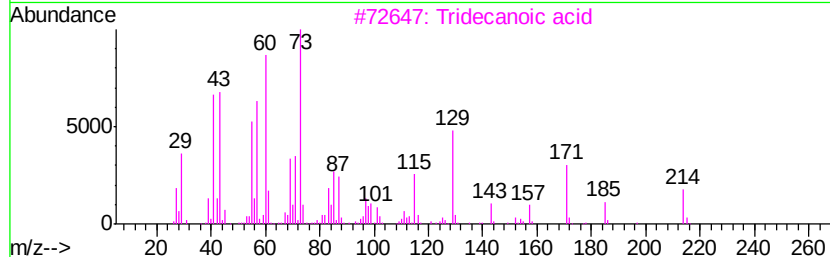
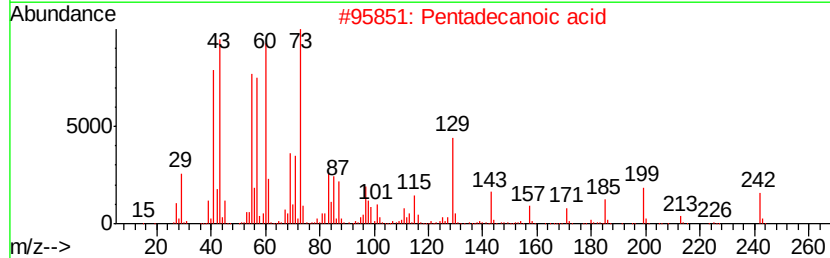
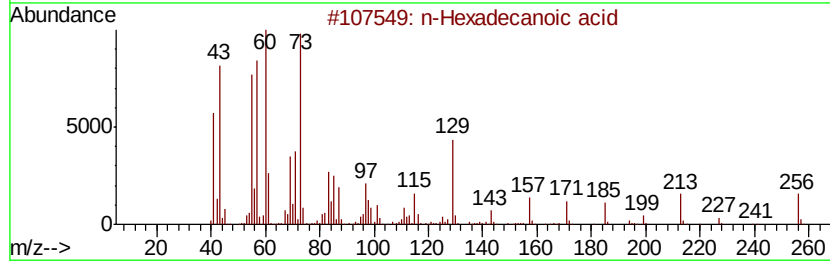
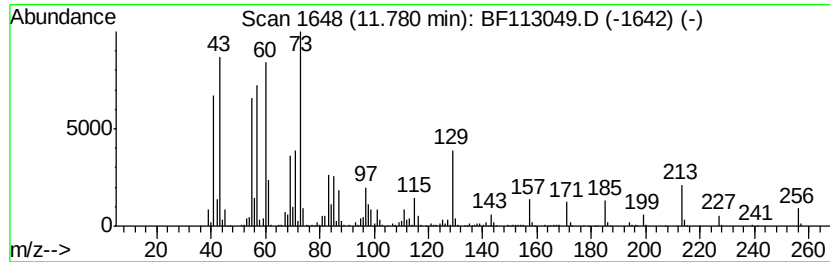
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	20.23 ng	1987850	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	92
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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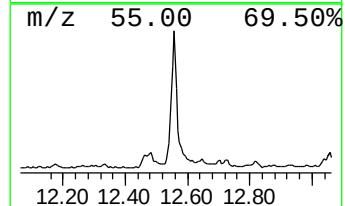
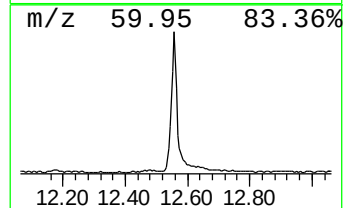
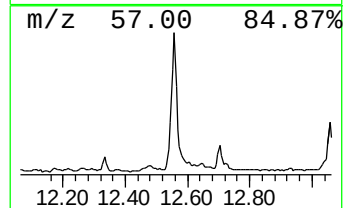
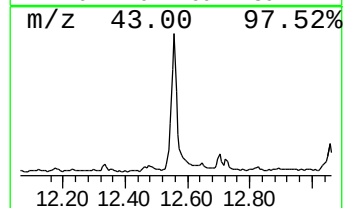
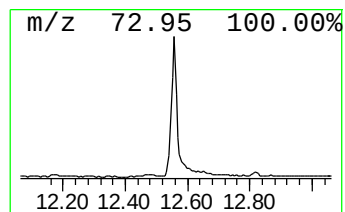
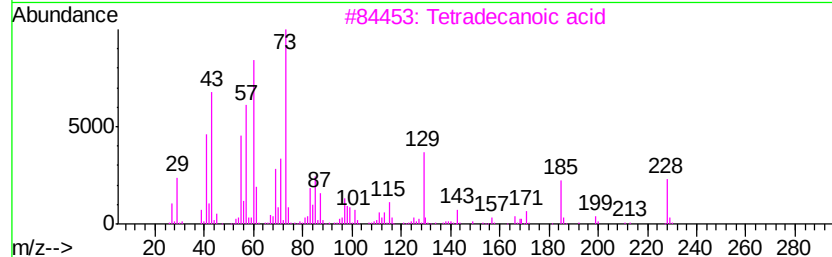
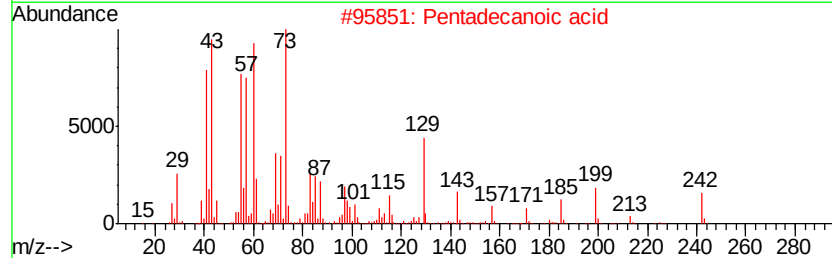
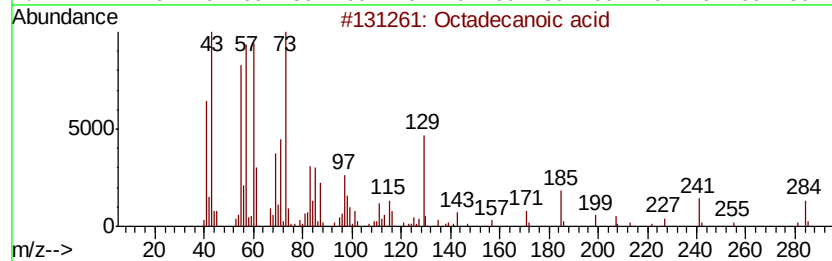
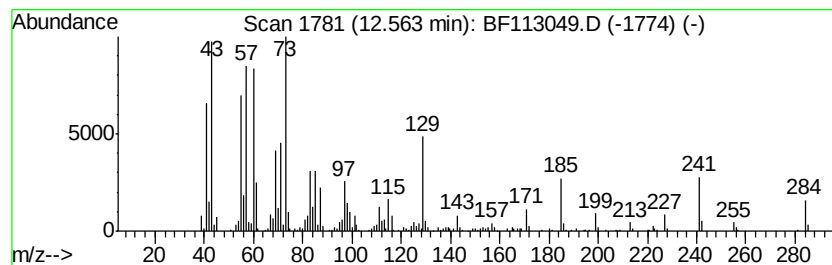
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	10.20 ng	1140400	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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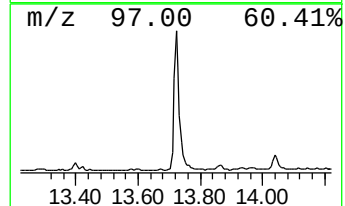
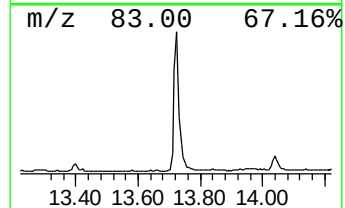
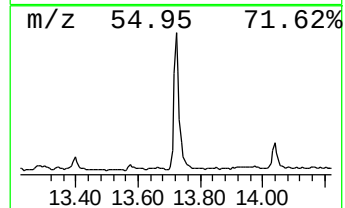
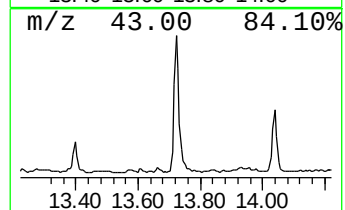
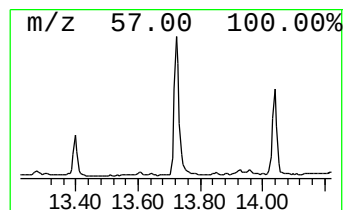
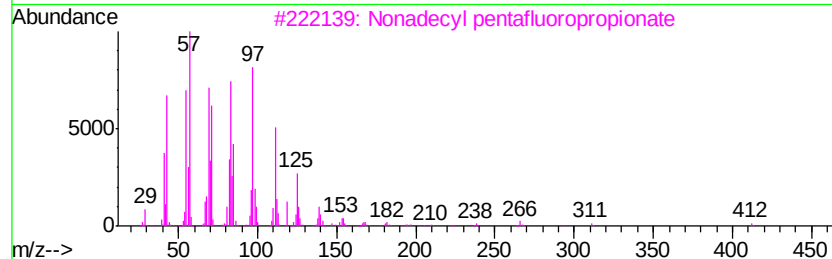
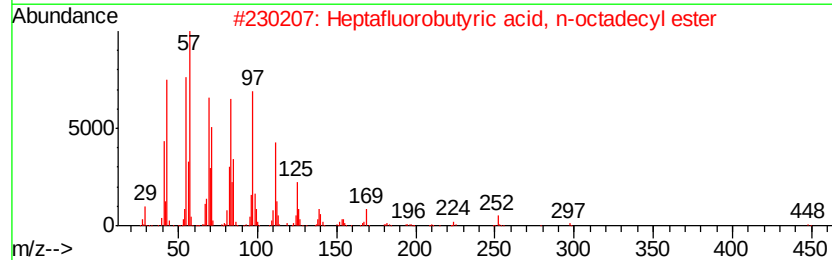
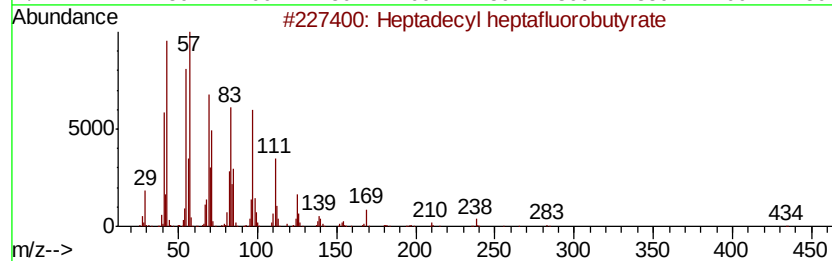
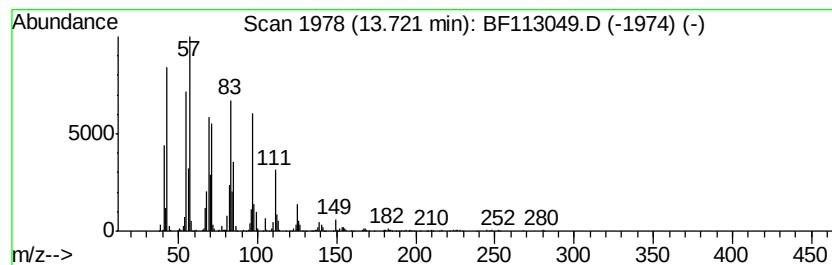
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.56 ng	1180590	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	94
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5		Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	91



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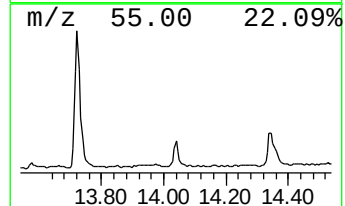
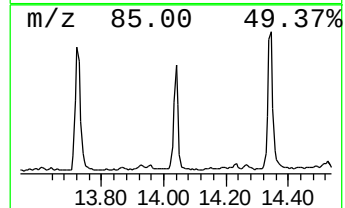
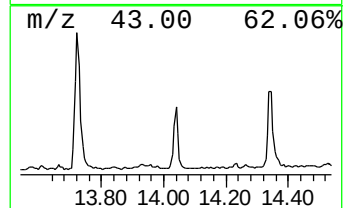
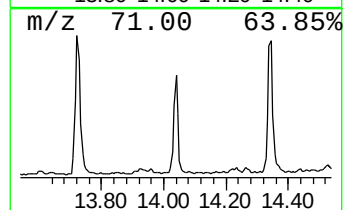
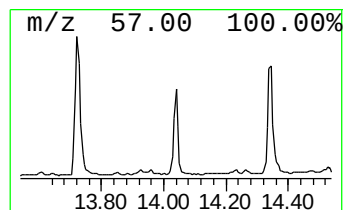
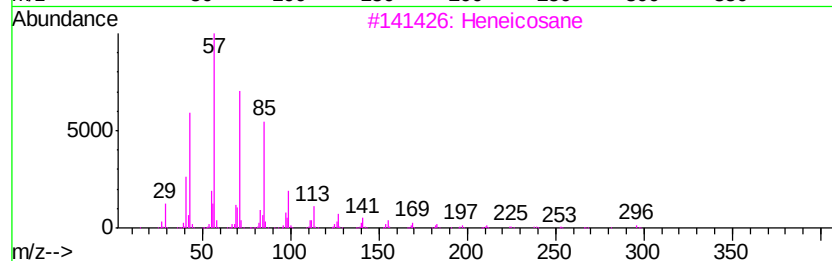
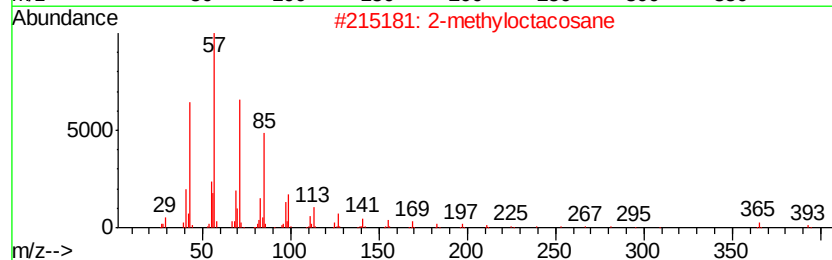
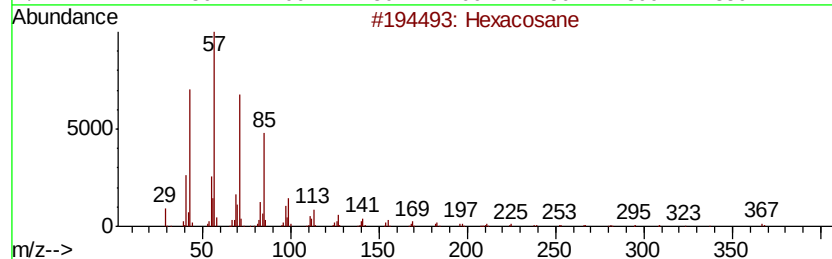
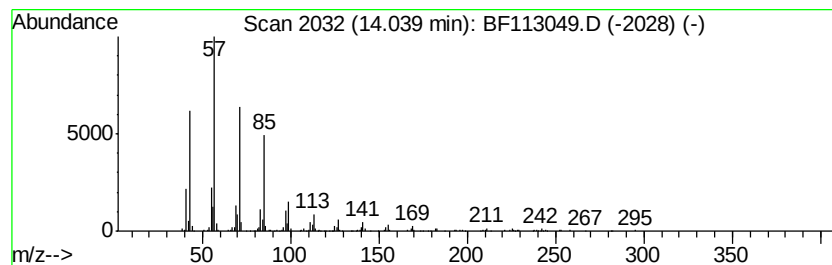
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 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.93 ng	327711	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Triacotane	422	C30H62	000638-68-6	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113049.D
Acq On : 14 Mar 2019 15:00
Operator : JU/SJ
Sample : K1866-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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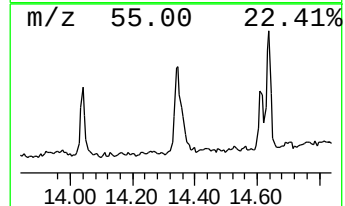
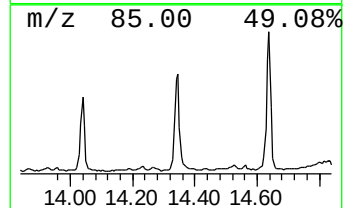
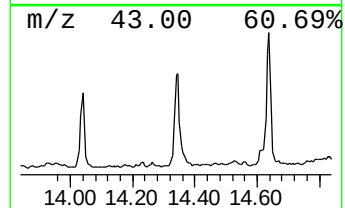
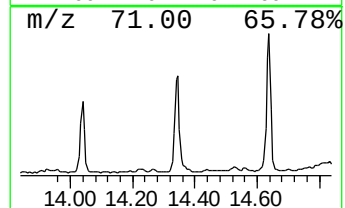
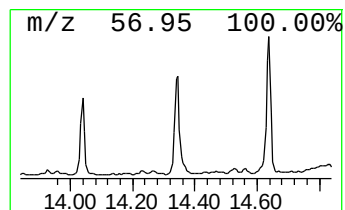
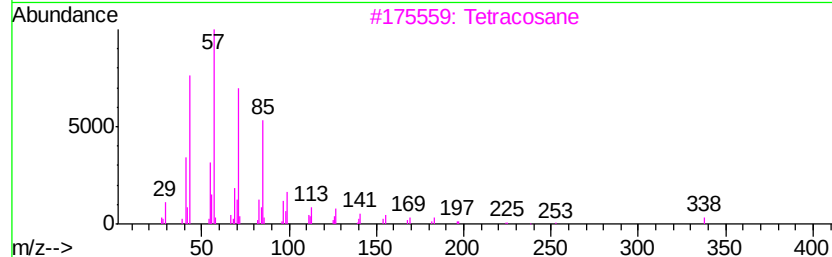
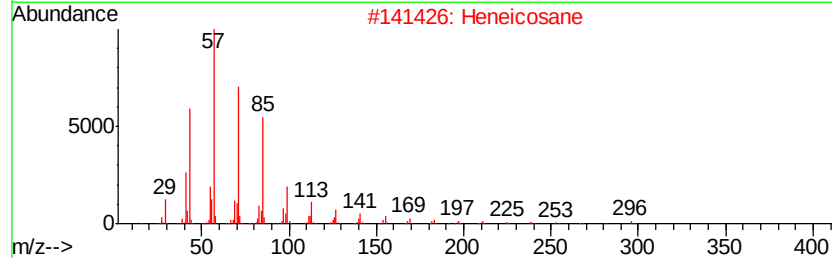
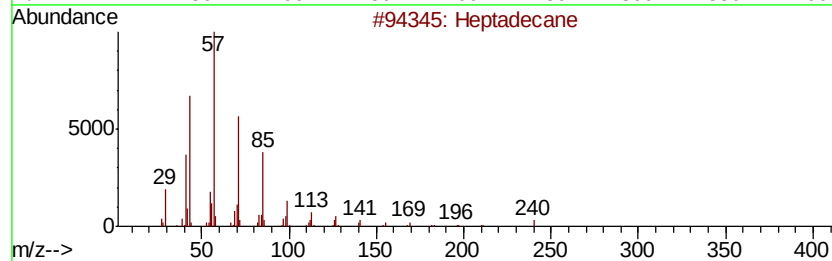
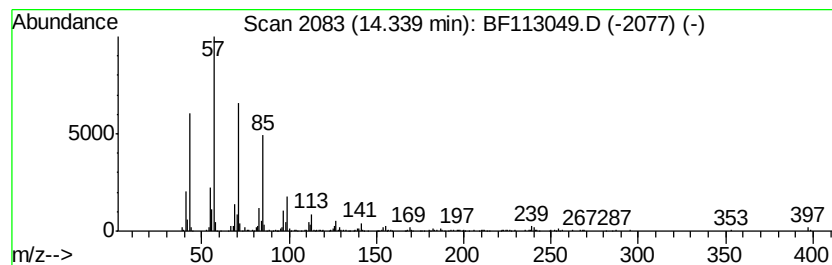
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	5.99 ng	669769	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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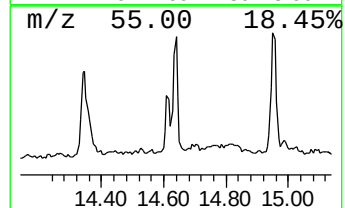
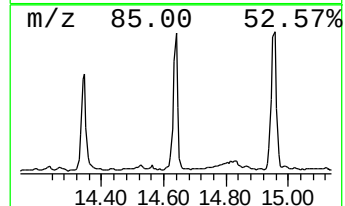
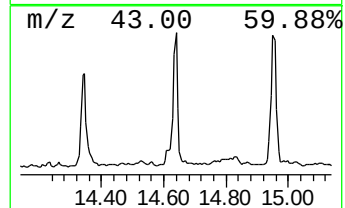
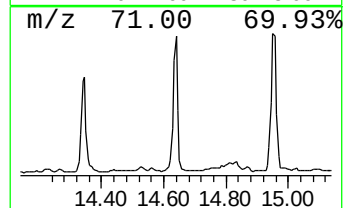
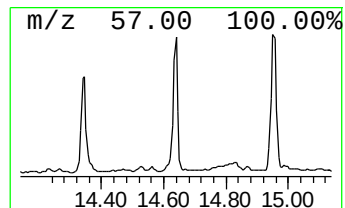
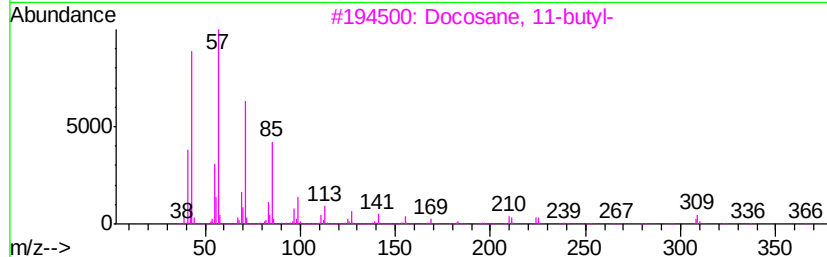
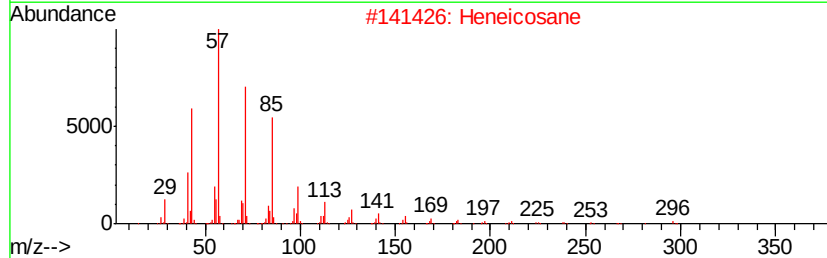
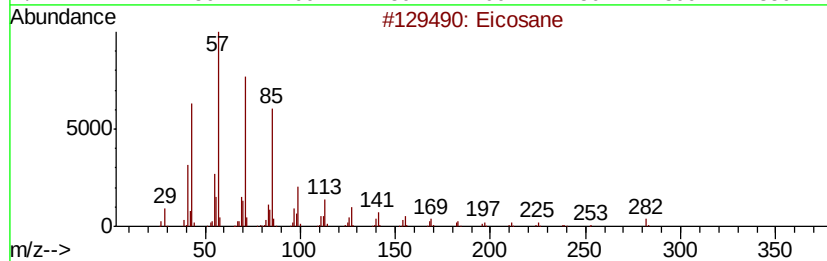
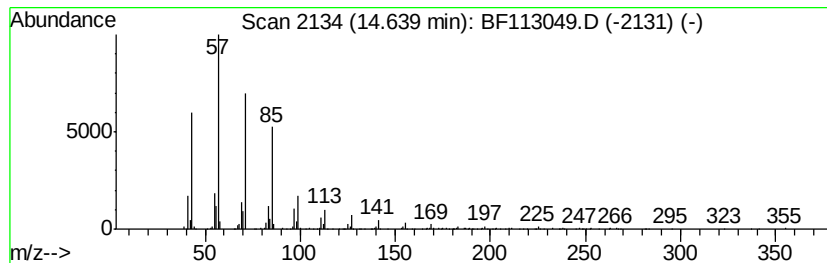
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	5.82 ng	630172	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	Heneicosane		296	C21H44	000629-94-7	91
3	Docosane, 11-butyl-		366	C26H54	013475-76-8	90
4	Octadecane		254	C18H38	000593-45-3	86
5	Heptacosane		380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Sample : K1866-13
Misc :
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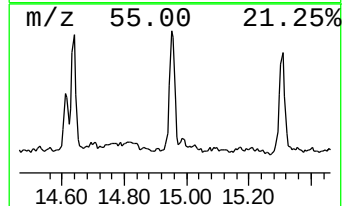
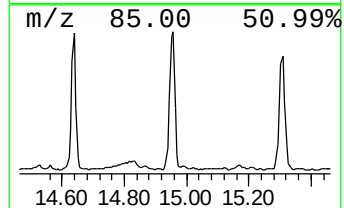
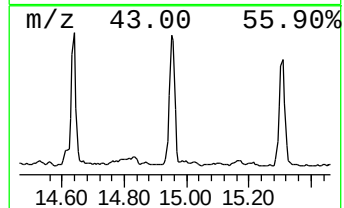
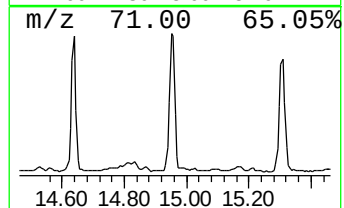
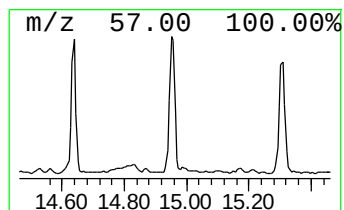
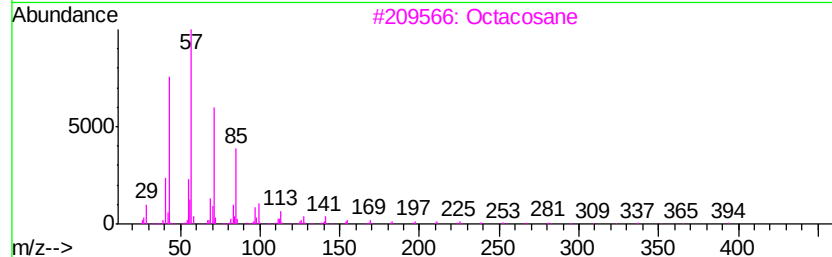
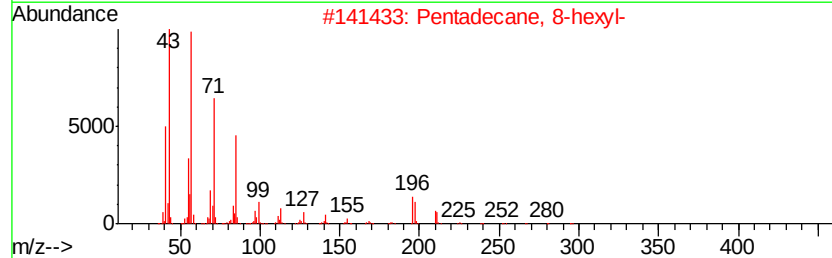
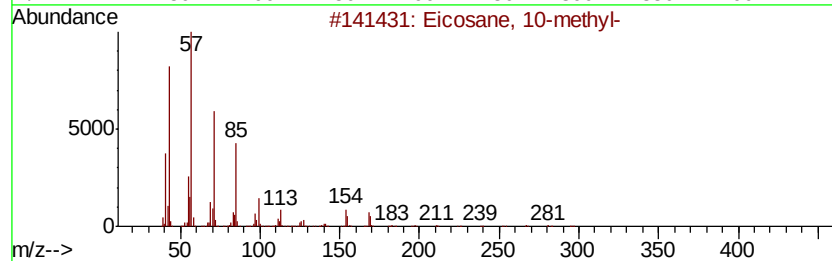
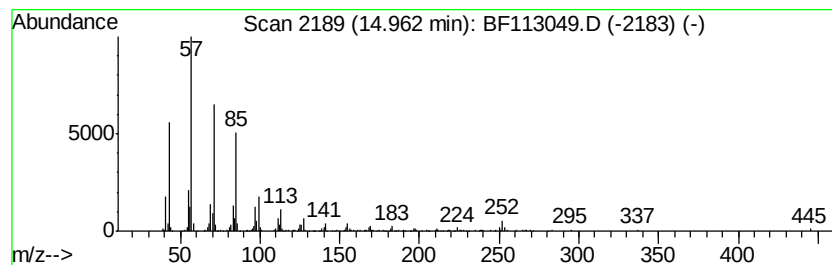
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.62 ng	716225	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane, 10-methyl-	296 C21H44	054833-23-7	93
2	Pentadecane, 8-hexyl-	296 C21H44	013475-75-7	93
3	Octacosane	394 C28H58	000630-02-4	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Tetracosane	338 C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113049.D
Acq On : 14 Mar 2019 15:00
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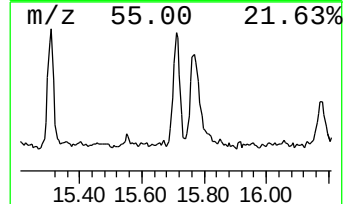
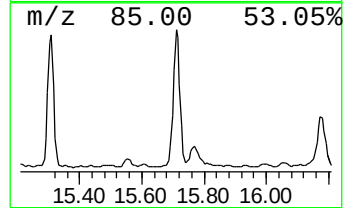
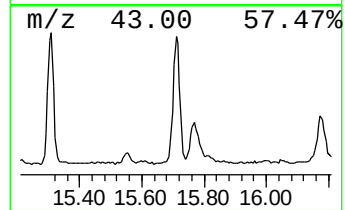
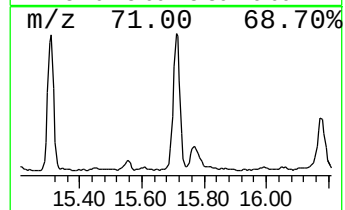
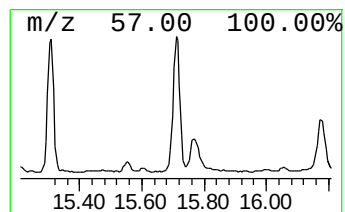
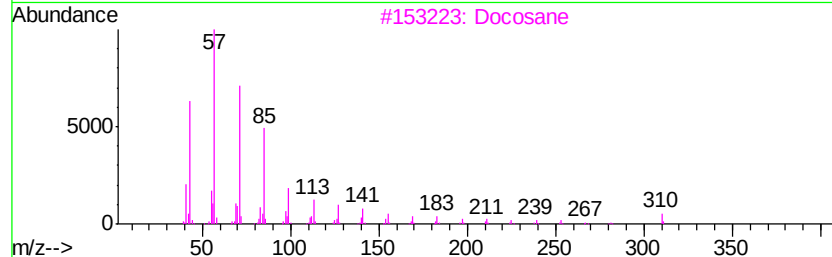
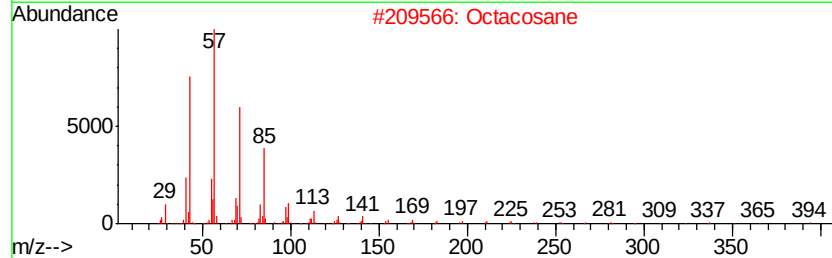
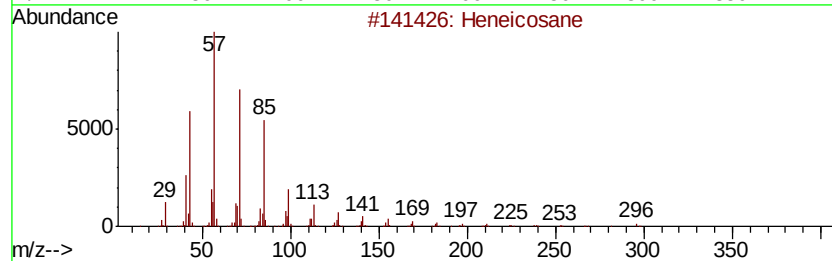
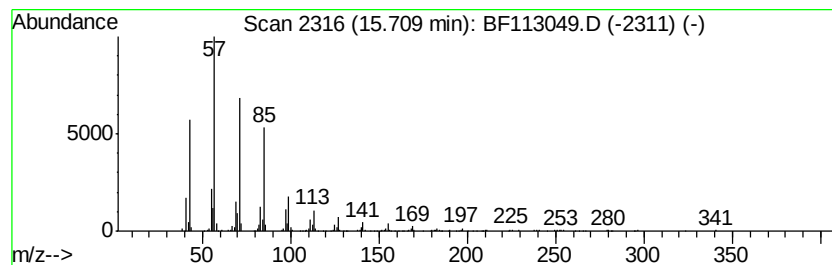
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	6.79 ng	735584	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Docosane	310	C22H46	000629-97-0	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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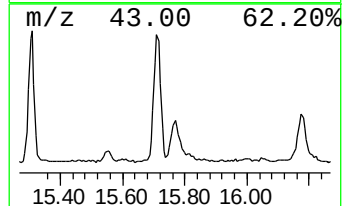
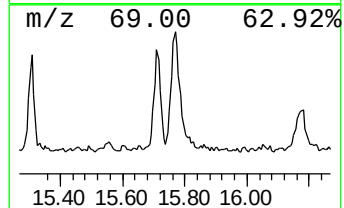
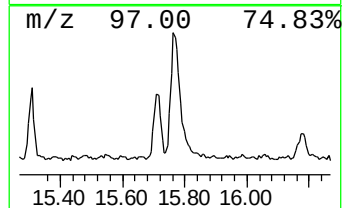
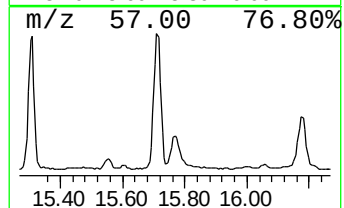
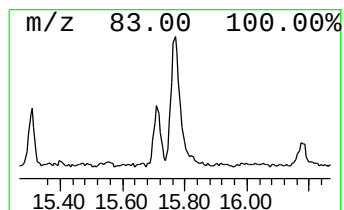
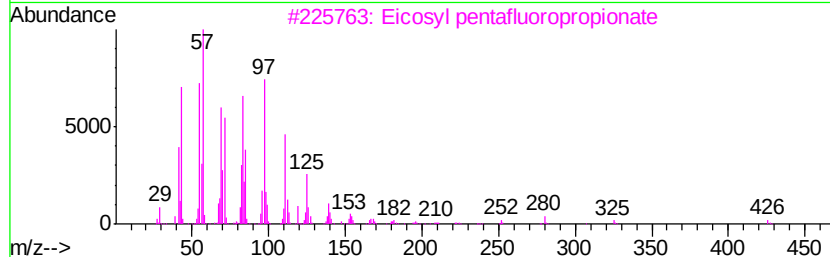
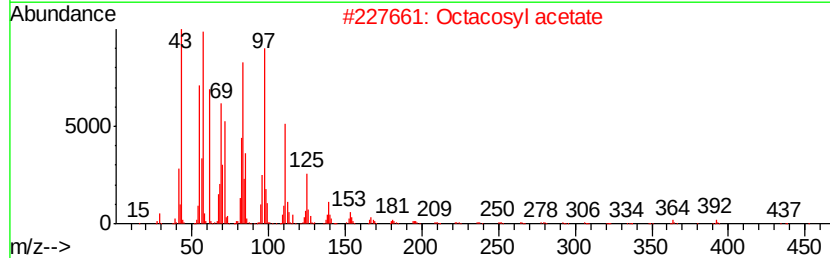
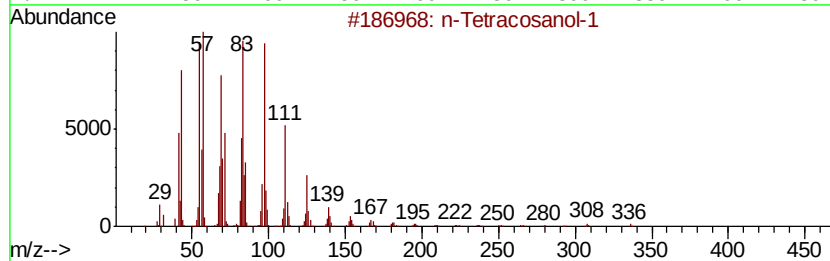
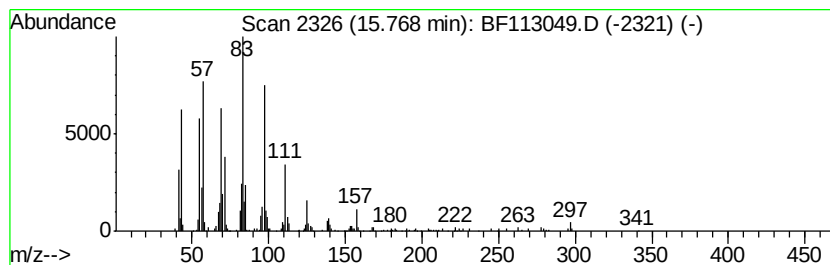
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	4.79 ng	519082	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Tetracosanol-1	354 C24H50O	000506-51-4 90
2		Octacosyl acetate	452 C30H60O2	018206-97-8 64
3		Eicosyl pentafluoropropionate	444 C23H41F5O2	1000351-80-8 60
4		Heneicosyl heptafluorobutyrte	508 C25H43F7O2	1000351-83-8 60
5		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 60



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Data File : BF113049.D
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Misc :
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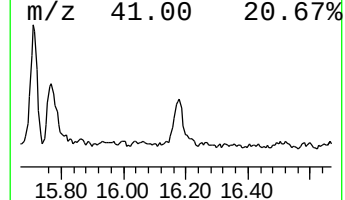
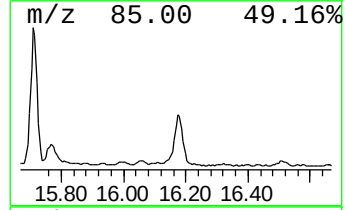
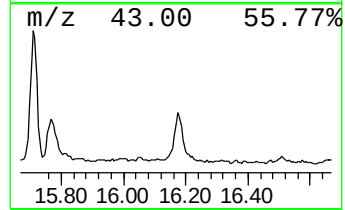
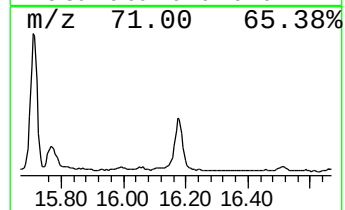
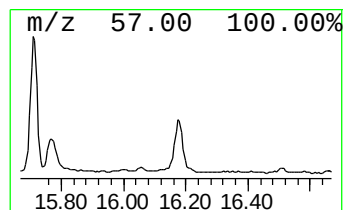
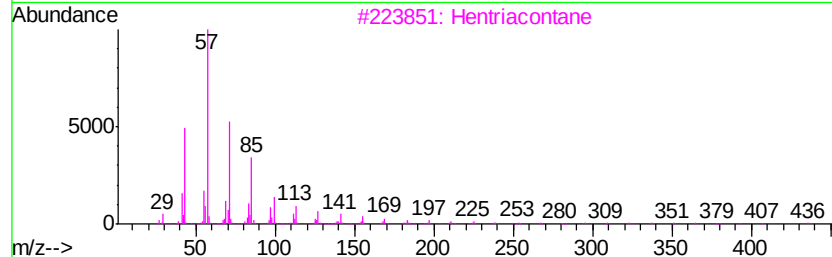
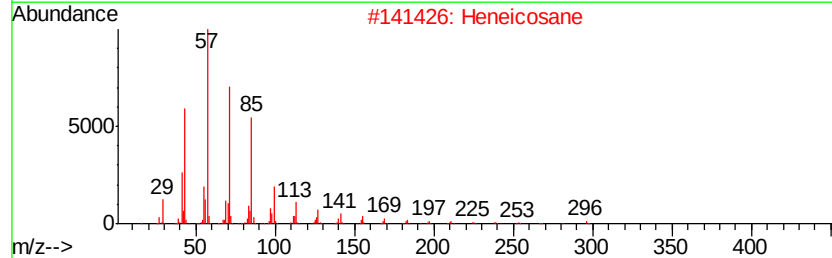
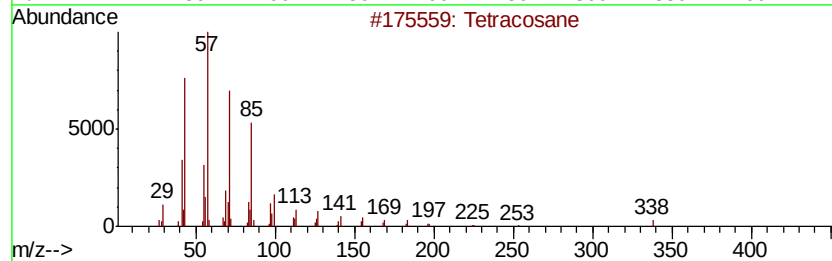
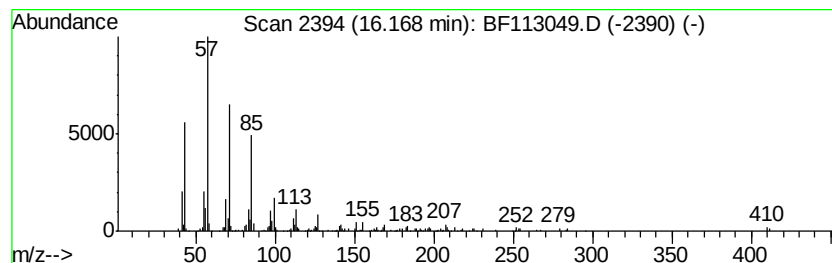
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.96 ng	320787	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Nonadecane	268	C19H40	000629-92-5	86
5			Octadecane	254	C18H38	000593-45-3	83



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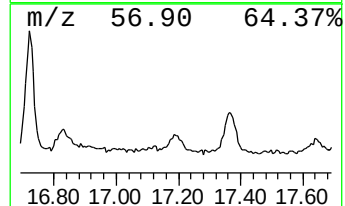
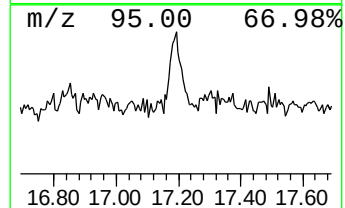
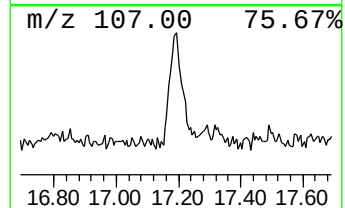
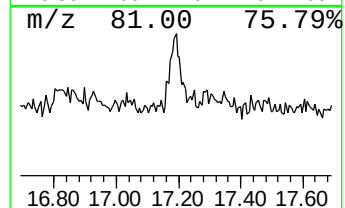
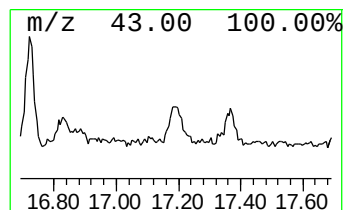
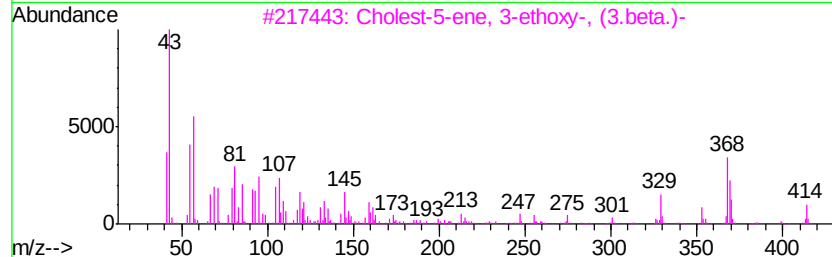
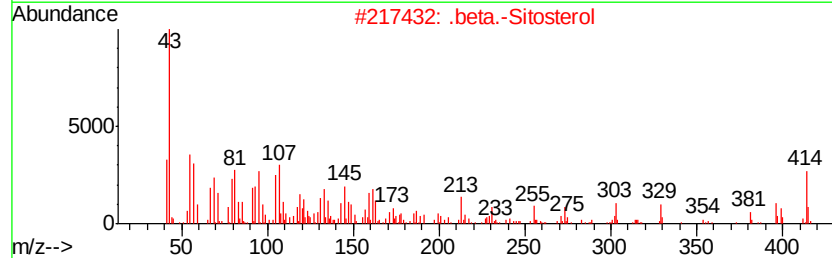
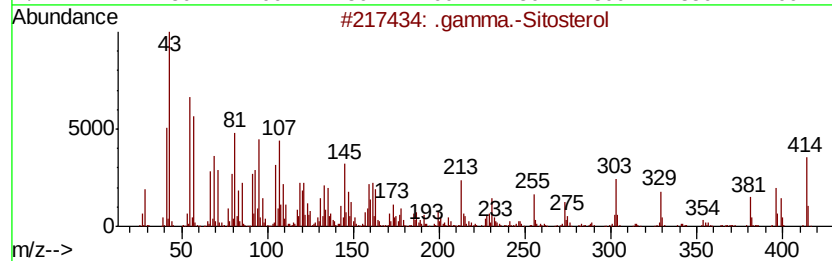
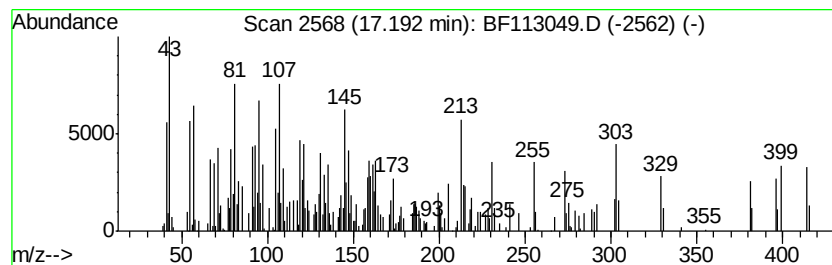
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .gamma.-Sitosterol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	2.23 ng	241872	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 97
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 89
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 38
4		5-O-Tolylcarbamoyl-3H-imidazole-...	273 C14H15N3O3	313251-31-9 30
5		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
 Data File : BF113049.D
 Acq On : 14 Mar 2019 15:00
 Operator : JU/SJ
 Sample : K1866-13
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-MH-13-COMP

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
unknown6.50	6.50	87.5	ng	4815850	1	6.73	1100780	20.0
n-Hexadecanoic acid	11.78	20.2	ng	1987850	4	11.24	1965140	20.0
Octadecanoic acid	12.56	10.2	ng	1140400	5	13.86	2236510	20.0
Heptadecyl heptaf...	13.72	10.6	ng	1180590	5	13.86	2236510	20.0
Hexacosane	14.04	2.9	ng	327711	5	13.86	2236510	20.0
Heptadecane	14.34	6.0	ng	669769	5	13.86	2236510	20.0
Eicosane	14.64	5.8	ng	630172	6	15.27	2165190	20.0
Eicosane, 10-methyl-	14.96	6.6	ng	716225	6	15.27	2165190	20.0
Octacosane	15.71	6.8	ng	735584	6	15.27	2165190	20.0
n-Tetracosanol-1	15.77	4.8	ng	519082	6	15.27	2165190	20.0
Tetracosane	16.17	3.0	ng	320787	6	15.27	2165190	20.0
.gamma.-Sitosterol	17.19	2.2	ng	241872	6	15.27	2165190	20.0