

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
 Data File : BF113117.D
 Acq On : 19 Mar 2019 4:08
 Operator : JU/SJ
 Sample : K1947-06
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-025-B035-031319

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	5.351	550	555	571	rBV	2791918	2974048	93.24%	9.649%
2	6.381	724	730	746	rBV	2861660	3187218	99.92%	10.341%
3	6.504	746	751	754	rBV	3370222	3066820	96.15%	9.950%
4	6.569	759	762	774	rVB	26150	53641	1.68%	0.174%
5	6.728	786	789	793	rBV	863350	698770	21.91%	2.267%
6	6.886	812	816	819	rBV	2835896	2456732	77.02%	7.971%
7	7.292	879	885	897	rBV	1897299	1913456	59.99%	6.208%
8	8.010	1003	1007	1013	rBV	759529	744187	23.33%	2.415%
9	9.086	1185	1190	1209	rBV	3289659	3189659	100.00%	10.349%
10	9.480	1253	1257	1266	rBV	316957	348054	10.91%	1.129%
11	9.763	1297	1305	1315	rBV	749816	813779	25.51%	2.640%
12	10.545	1434	1438	1454	rBV	1719948	1885856	59.12%	6.119%
13	11.239	1552	1556	1566	rBV	739273	754650	23.66%	2.448%
14	11.774	1644	1647	1656	rBV2	81943	121297	3.80%	0.394%
15	12.563	1778	1781	1792	rBV3	23973	39960	1.25%	0.130%
16	12.651	1792	1796	1800	rBV	35692	33050	1.04%	0.107%
17	12.821	1820	1825	1828	rBV	3220179	2922853	91.64%	9.483%
18	13.304	1897	1907	1917	rBV	82358	197382	6.19%	0.640%
19	13.380	1917	1920	1922	rBV	38206	40990	1.29%	0.133%
20	13.727	1976	1979	1983	rBV	81760	67236	2.11%	0.218%
21	13.792	1983	1990	1999	rBV5	65498	235979	7.40%	0.766%
22	13.868	1999	2003	2012	rVB	822408	878244	27.53%	2.849%
23	13.974	2017	2021	2024	rBV4	26921	39363	1.23%	0.128%
24	14.045	2029	2033	2037	rVB	166799	160476	5.03%	0.521%
25	14.345	2077	2084	2090	rBV	394543	374009	11.73%	1.213%
26	14.639	2130	2134	2138	rVB	680217	596542	18.70%	1.935%
27	14.709	2143	2146	2150	rVB	38631	36006	1.13%	0.117%
28	14.774	2154	2157	2162	rVB3	29724	32919	1.03%	0.107%
29	14.957	2184	2188	2194	rVB	685534	713287	22.36%	2.314%
30	15.280	2238	2243	2245	rBV	414495	531360	16.66%	1.724%
31	15.309	2245	2248	2257	rVB	564227	667739	20.93%	2.167%
32	15.715	2311	2317	2329	rBV	314896	482438	15.13%	1.565%
33	16.186	2391	2397	2411	rVB2	160926	335245	10.51%	1.088%
34	16.733	2485	2490	2499	rVB2	66604	132111	4.14%	0.429%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.368	2596	2598	2607	rVB3	31878	62227	1.95%	0.202%
36	18.786	2837	2839	2845	rBV7	19656	33499	1.05%	0.109%

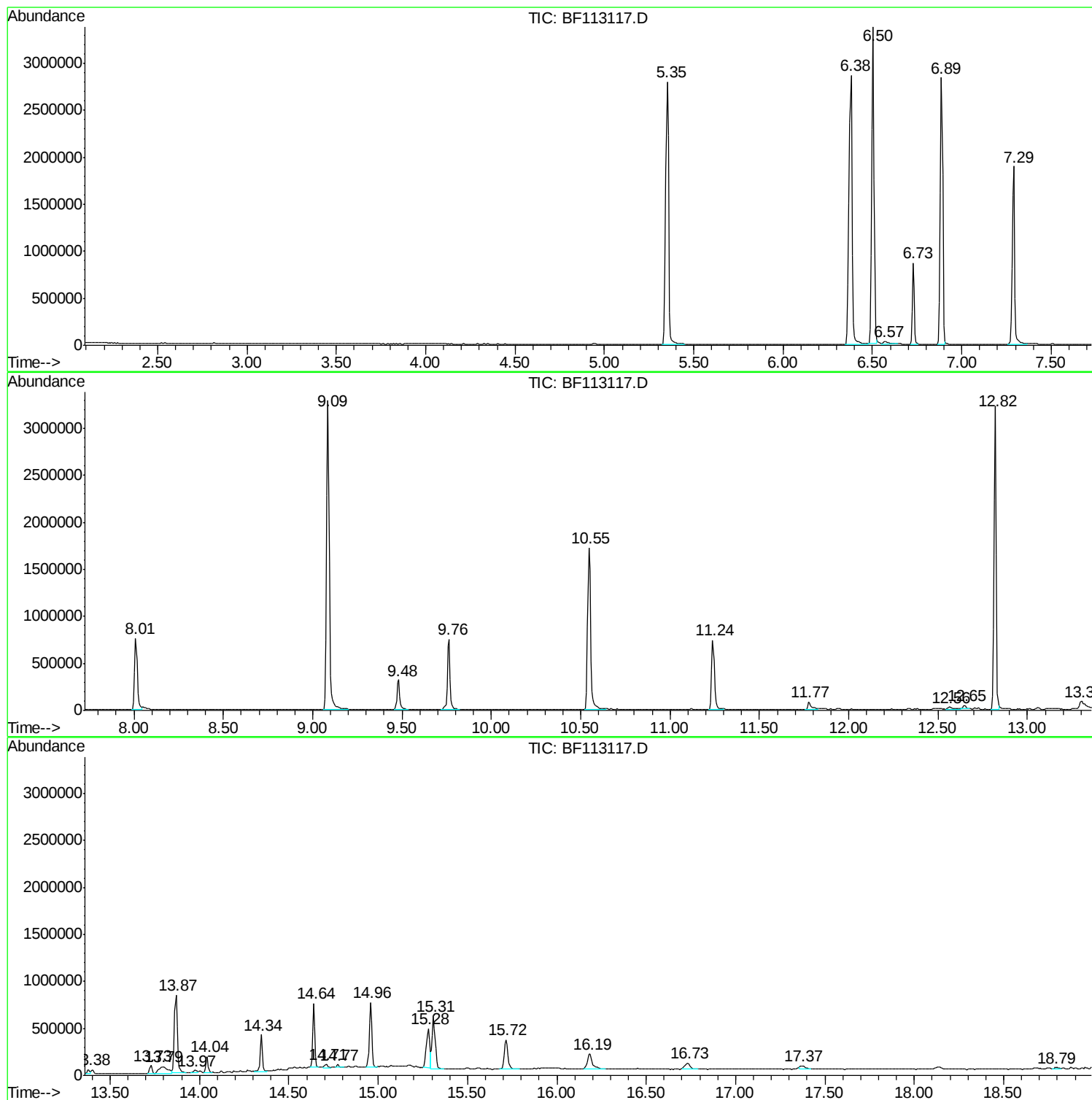
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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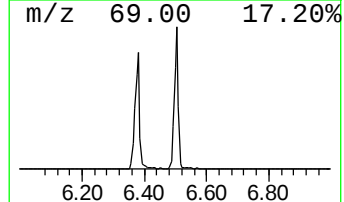
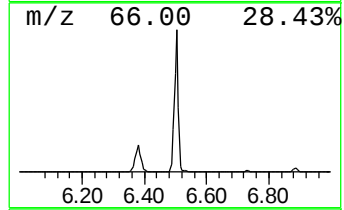
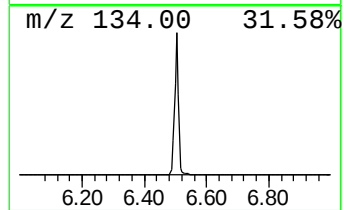
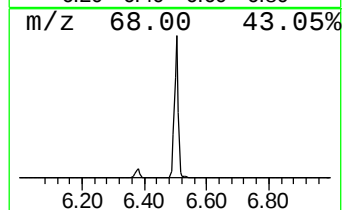
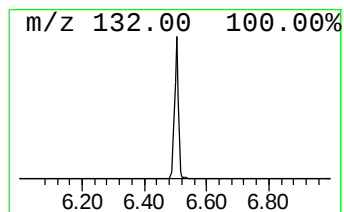
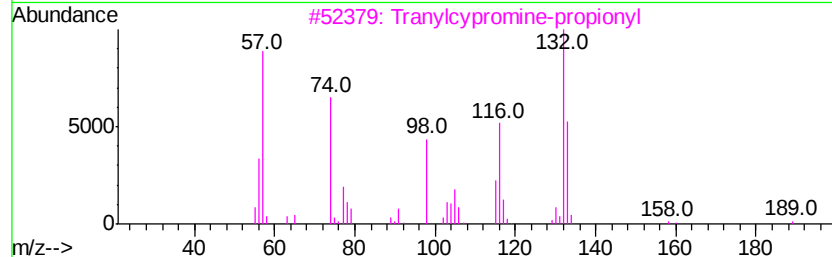
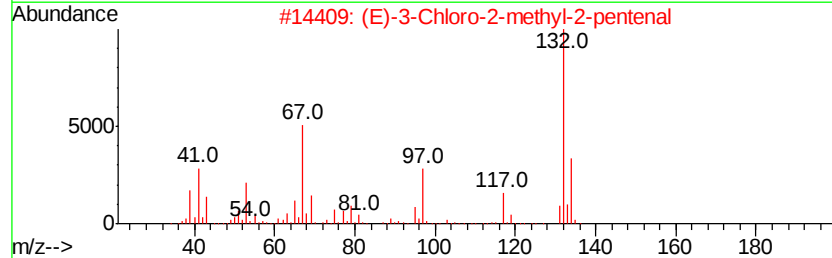
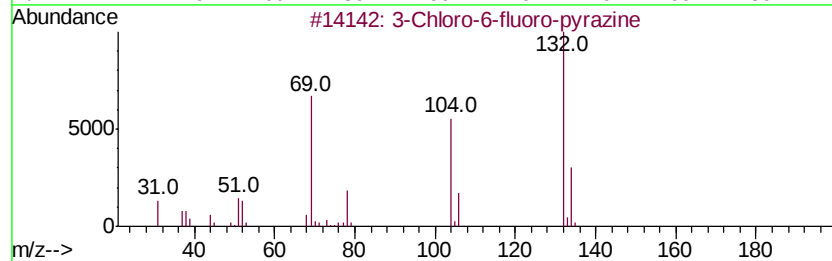
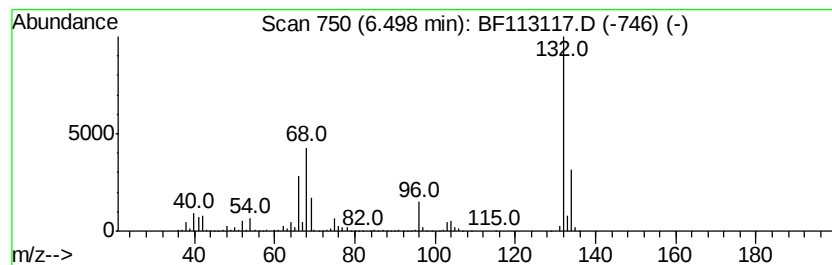
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	87.78 ng	3066820	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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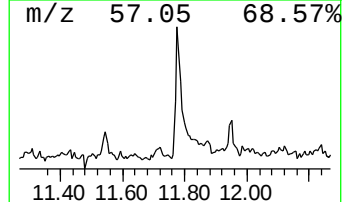
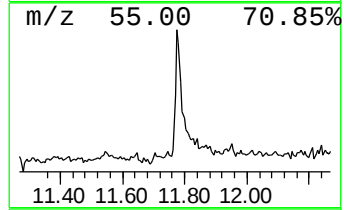
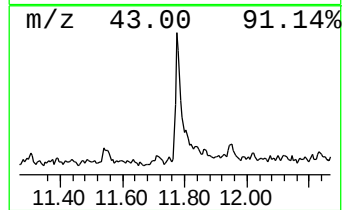
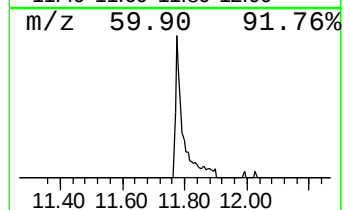
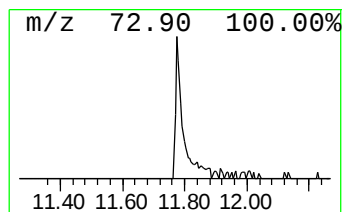
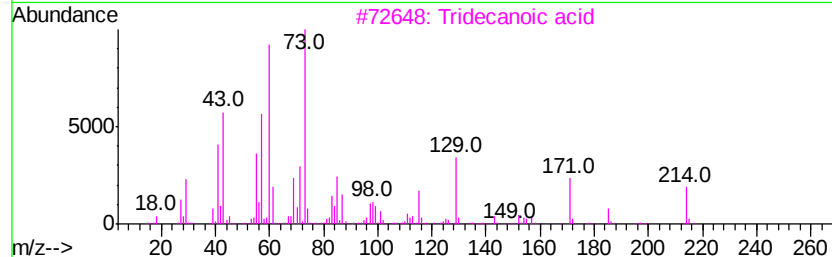
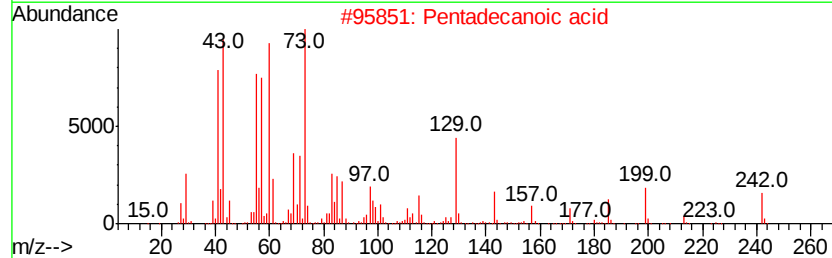
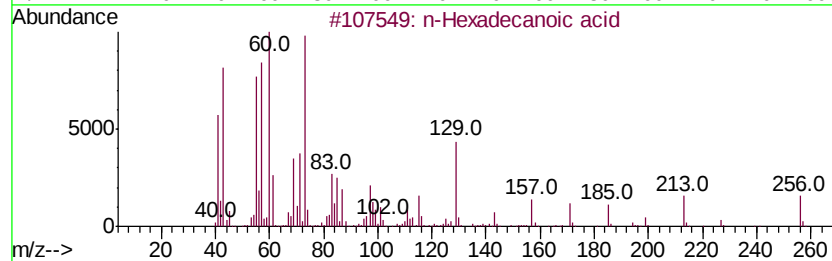
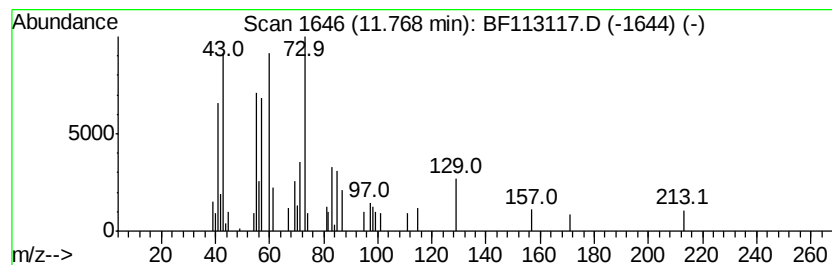
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	3.21 ng	121297	Phenanthrene-d10	11.24	
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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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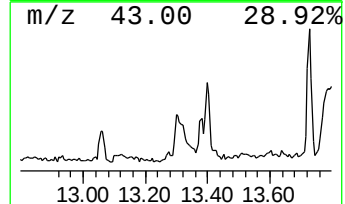
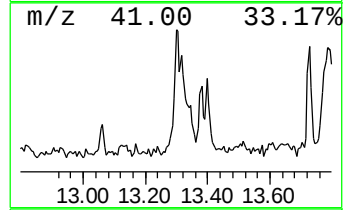
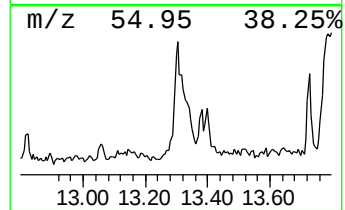
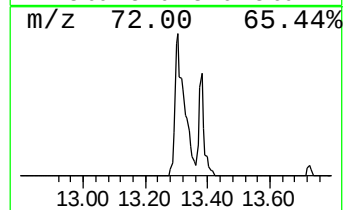
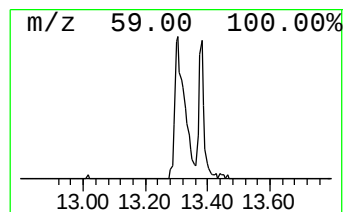
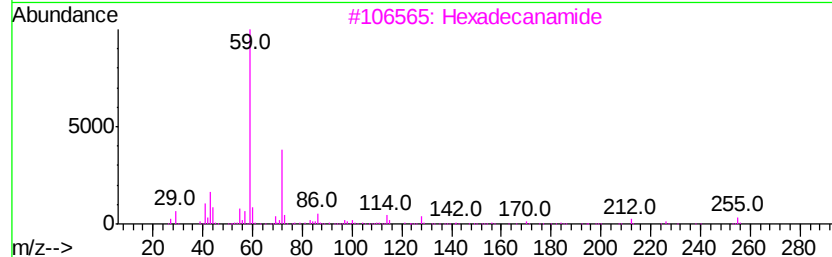
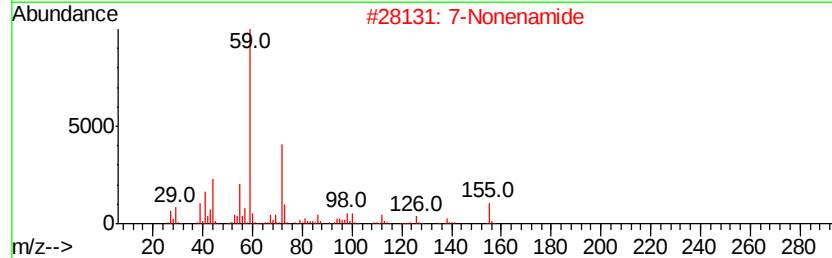
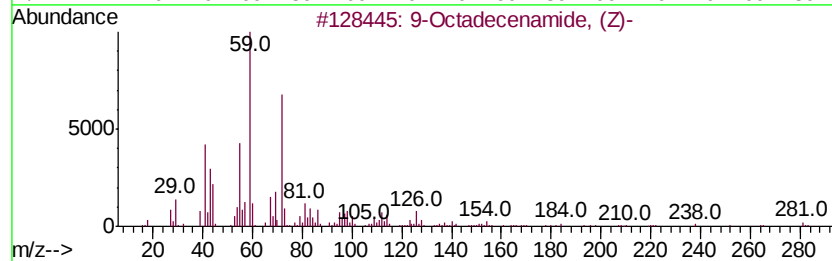
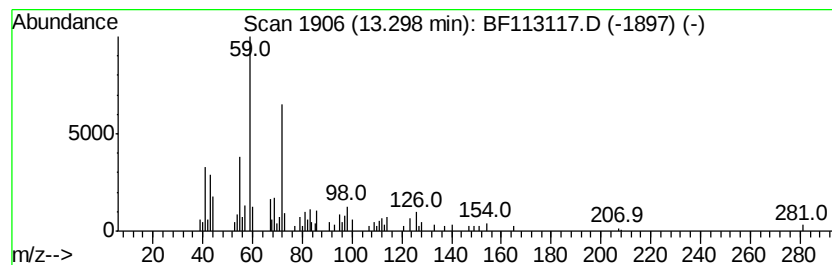
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.30	4.49 ng	197382	Chrysene-d12		13.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	7-Nonenamide	155	C9H17NO	090949-53-4	72
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Tetradecanamide	227	C14H29NO	000638-58-4	59
5	Octanamide	143	C8H17NO	000629-01-6	53



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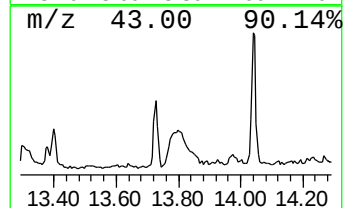
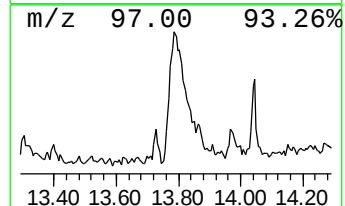
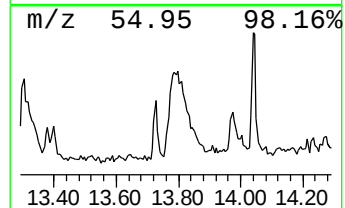
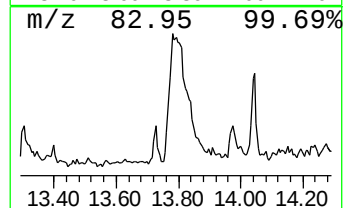
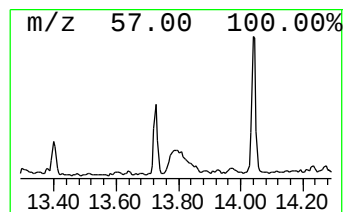
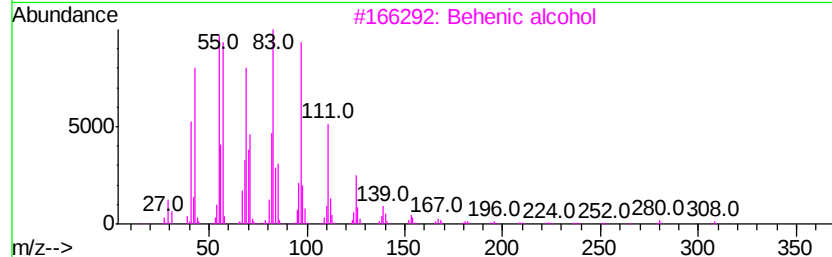
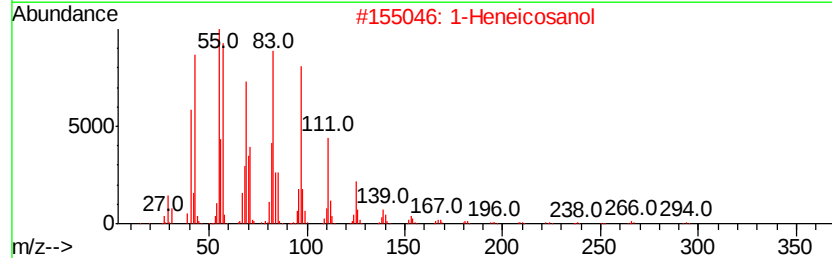
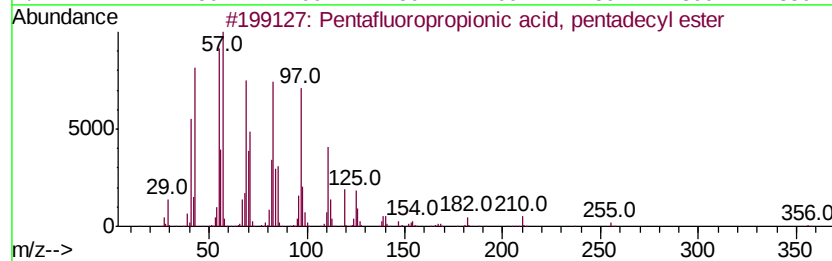
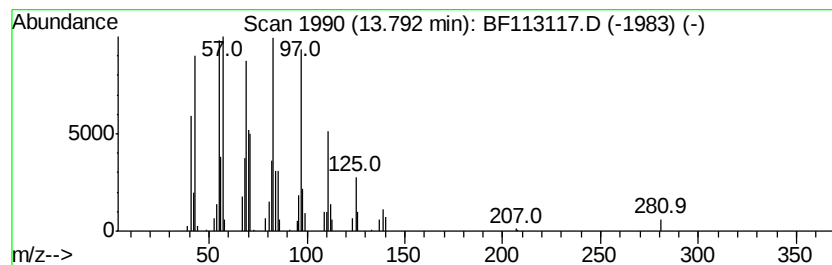
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	5.37 ng	235979	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Behenic alcohol	326	C22H46O	000661-19-8	95
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95



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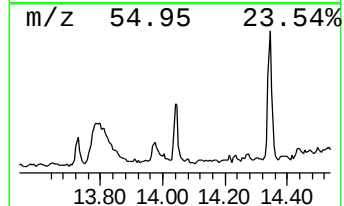
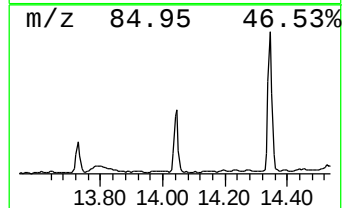
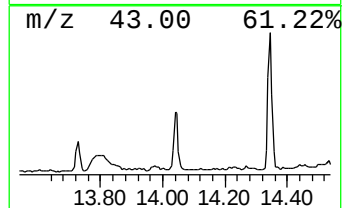
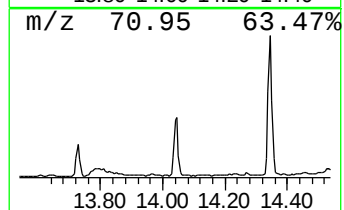
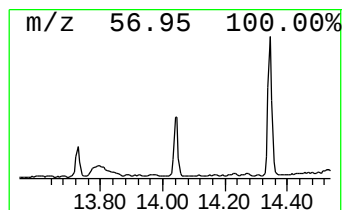
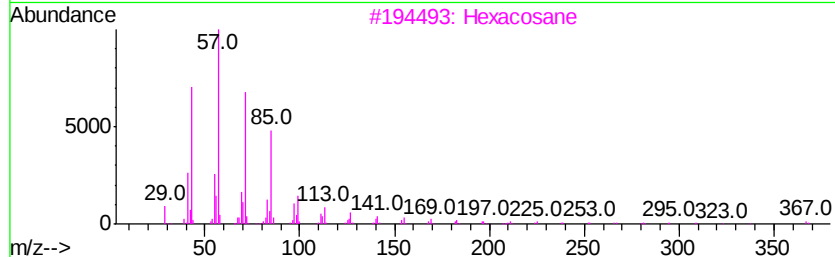
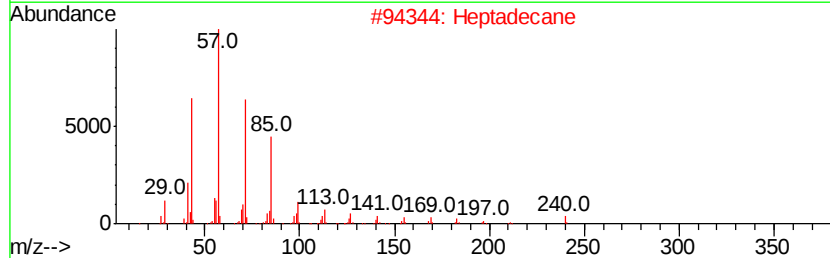
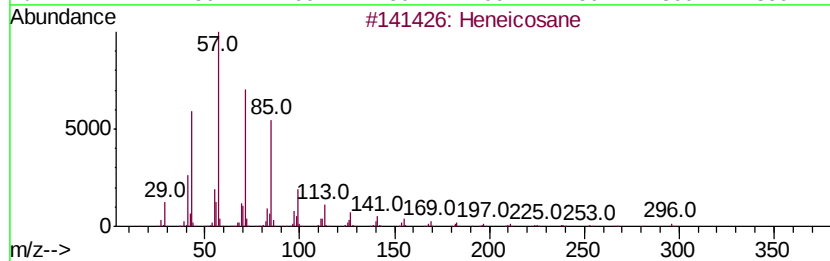
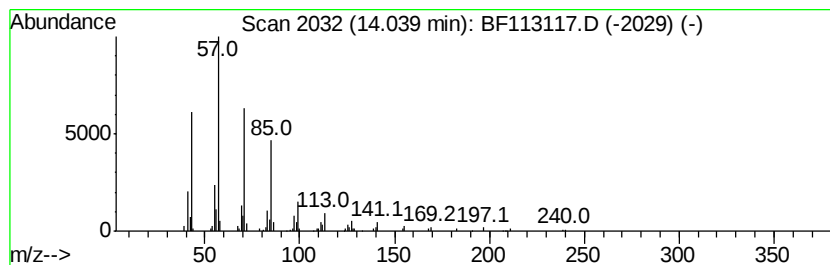
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.65 ng	160476	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	triacontane	422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
Sample : K1947-06
Misc :
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Instrument :
BNA_F
ClientSampleId :
PST-025-B035-031319

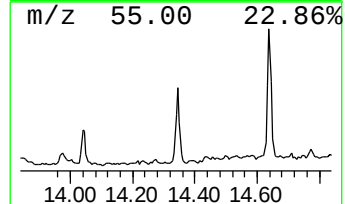
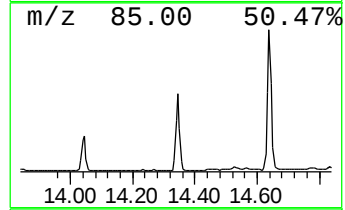
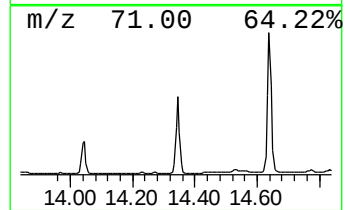
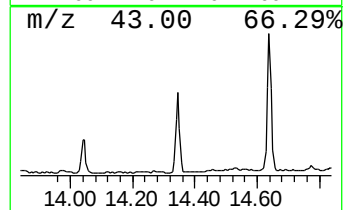
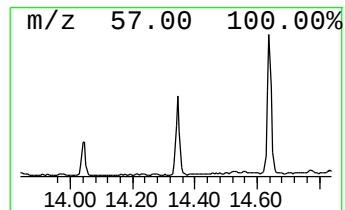
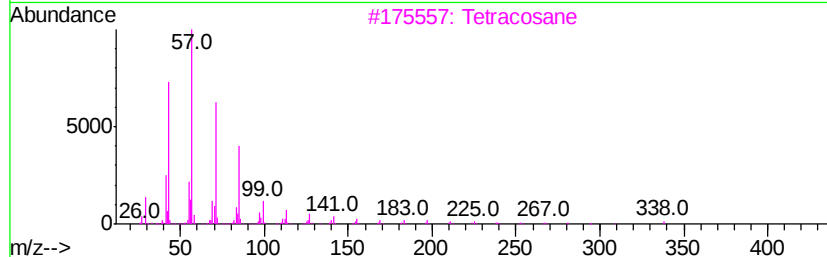
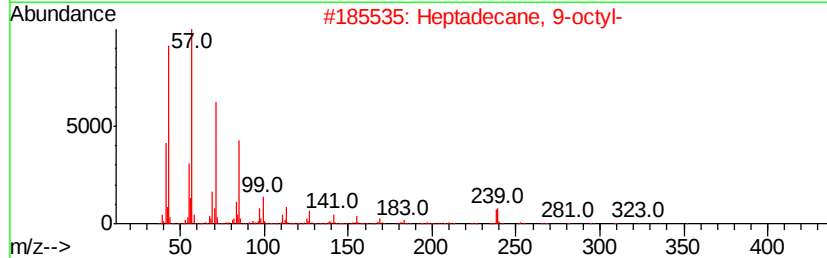
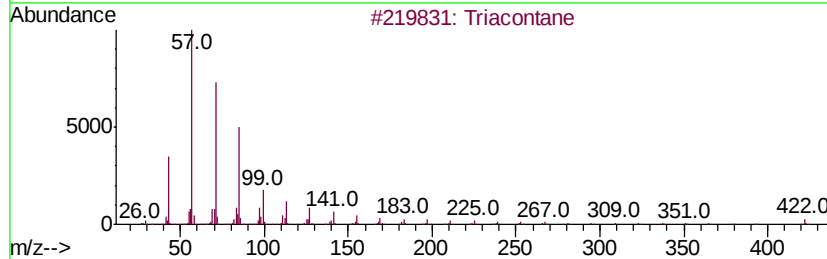
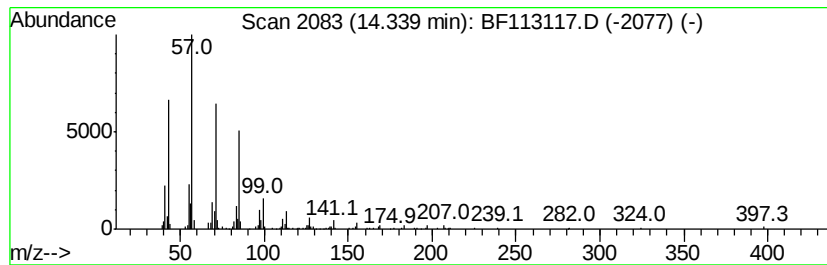
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	8.52 ng	374009	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
Sample : K1947-06
Misc :
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ClientSampleId :
PST-025-B035-031319

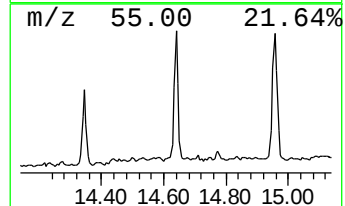
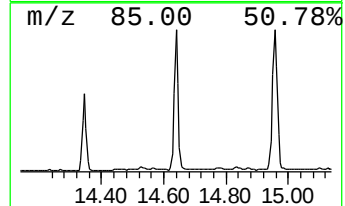
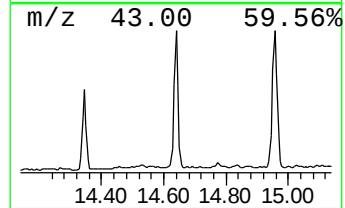
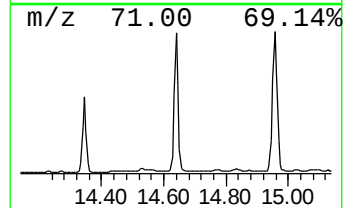
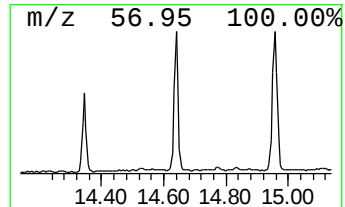
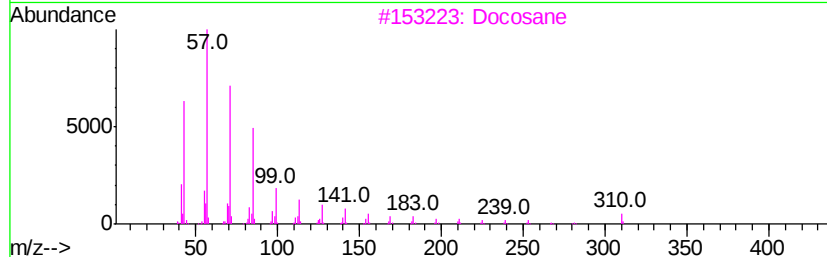
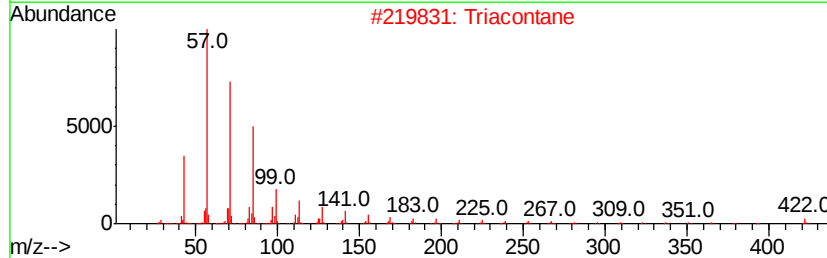
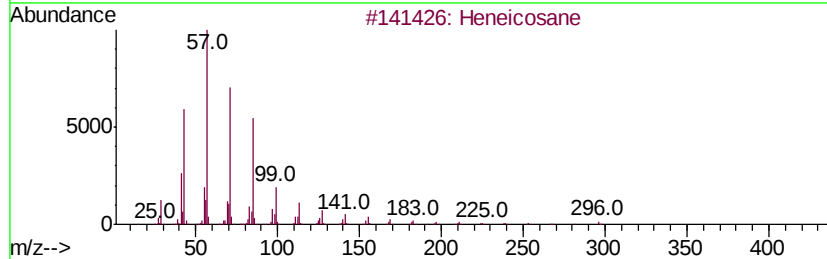
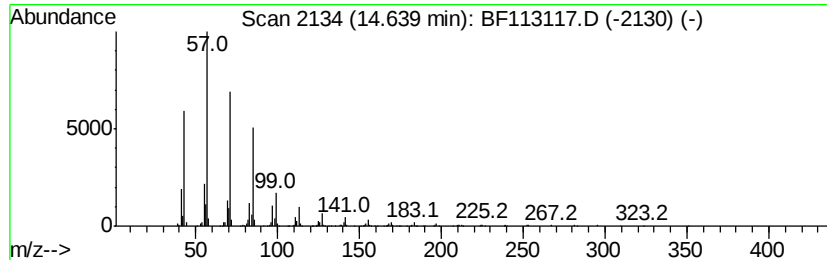
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	22.45 ng	596542	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Docosane	310	C22H46	000629-97-0	87
4		Hexadecane	226	C16H34	000544-76-3	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
Sample : K1947-06
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ClientSampleId :
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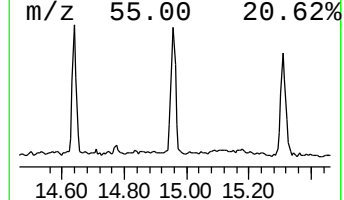
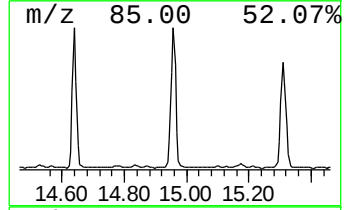
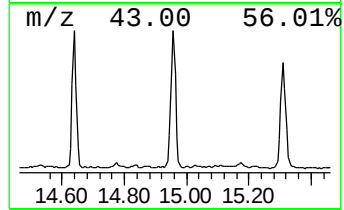
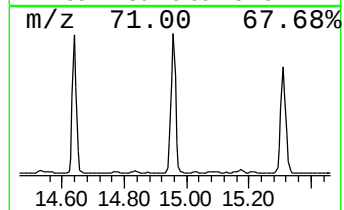
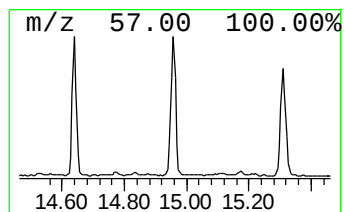
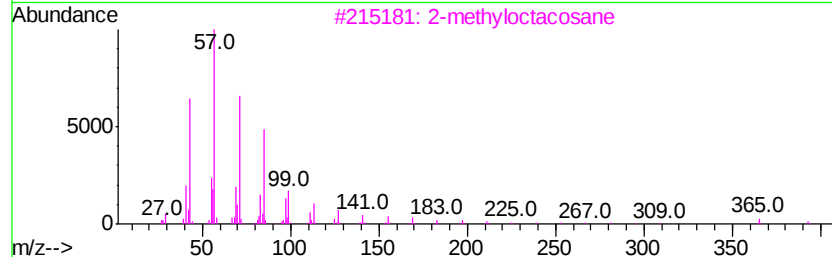
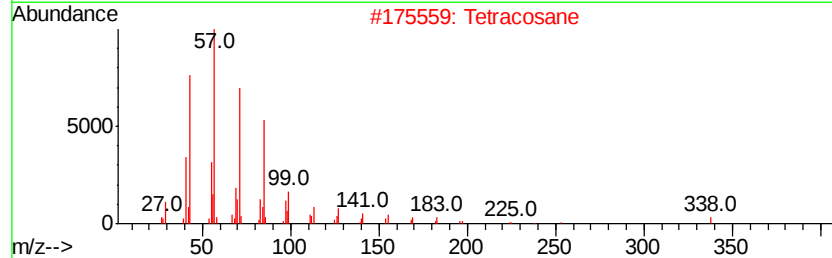
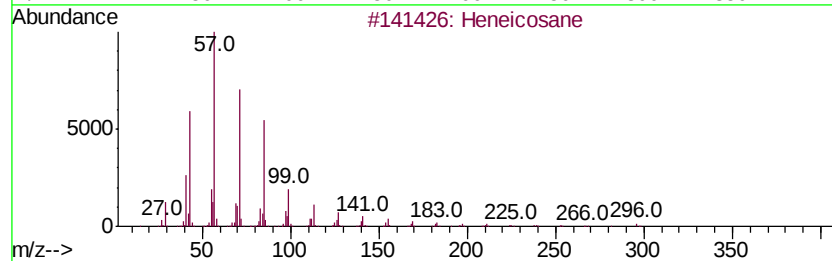
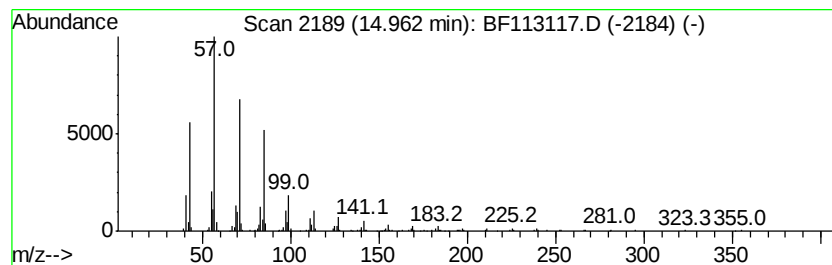
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	26.85 ng	713287	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexadecane	226	C16H34	000544-76-3	87
5		Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
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ClientSampleId :
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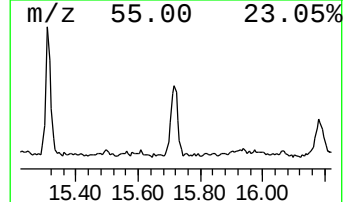
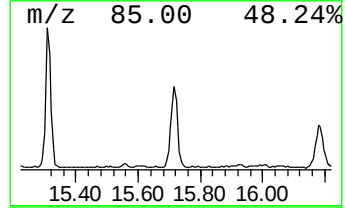
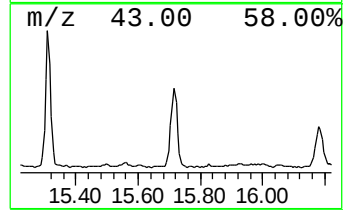
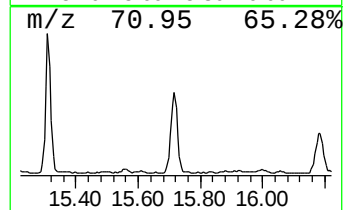
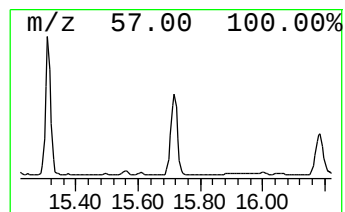
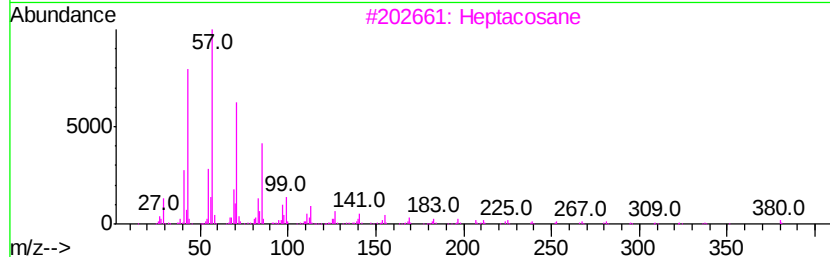
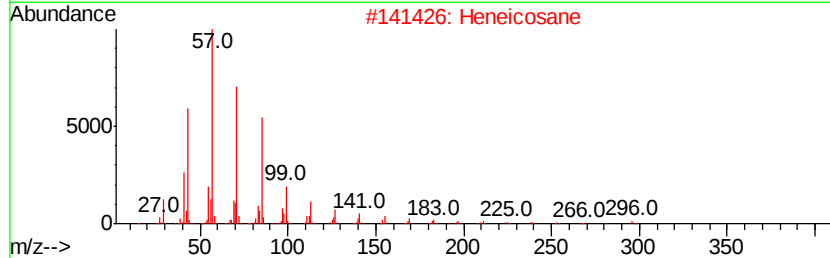
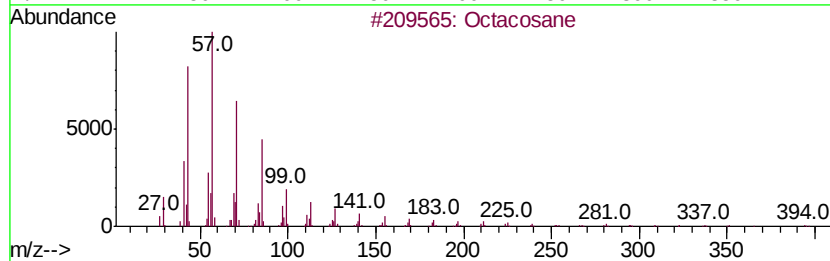
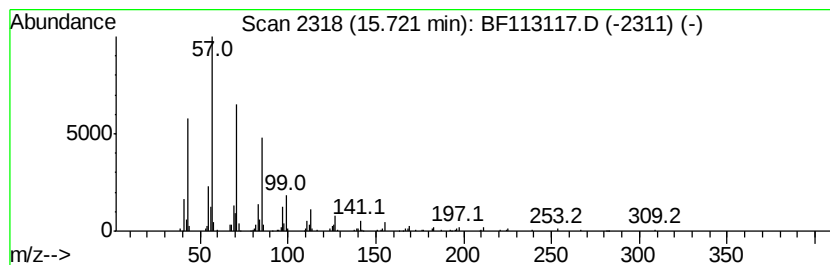
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	18.16 ng	482438	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Docosane	310	C22H46	000629-97-0	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
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Misc :
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Instrument :
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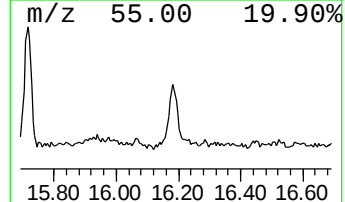
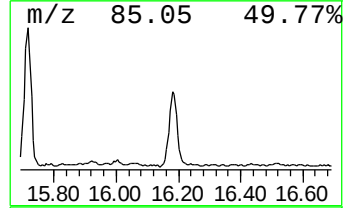
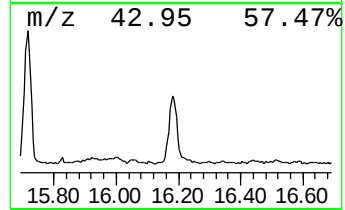
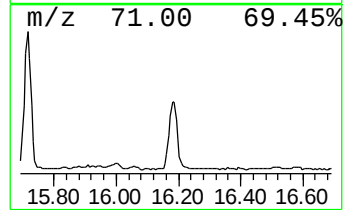
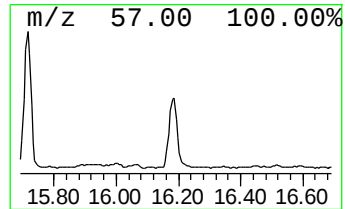
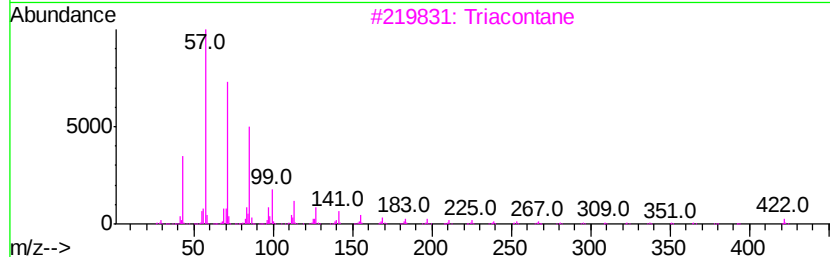
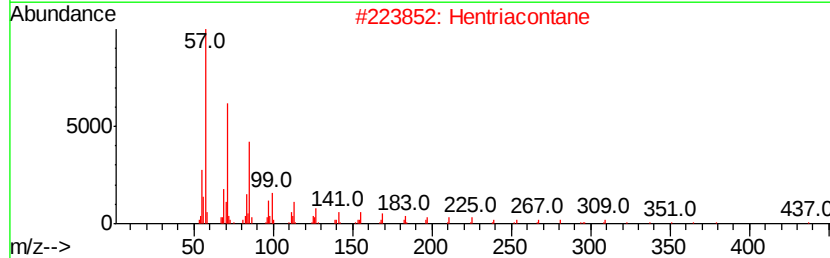
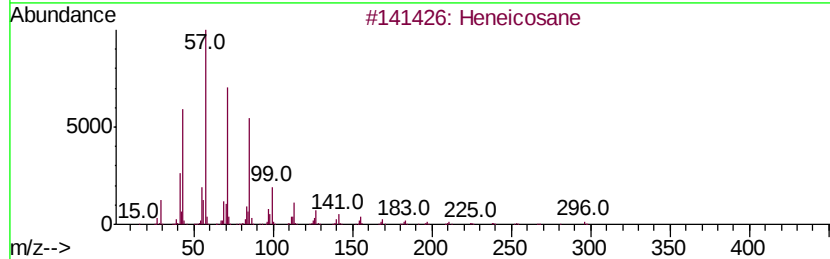
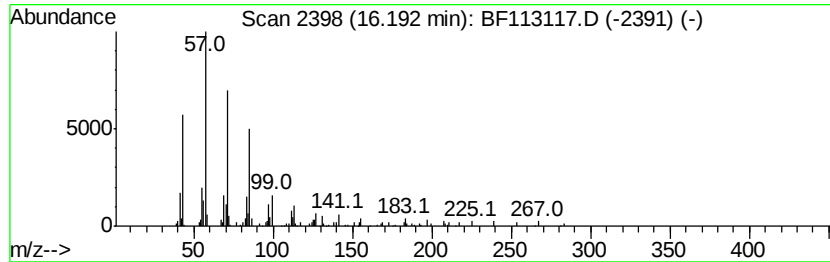
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	12.62 ng	335245	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
 Data File : BF113117.D
 Acq On : 19 Mar 2019 4:08
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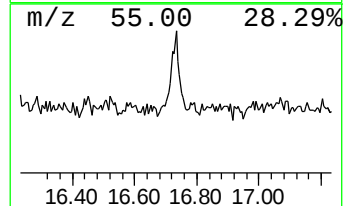
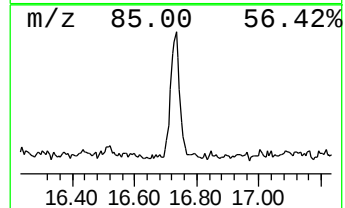
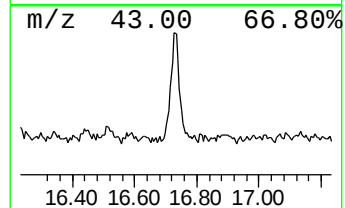
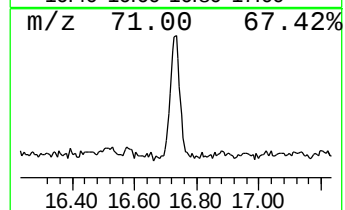
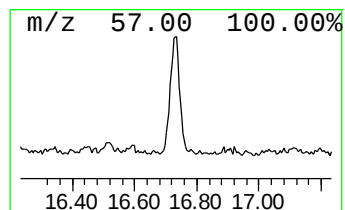
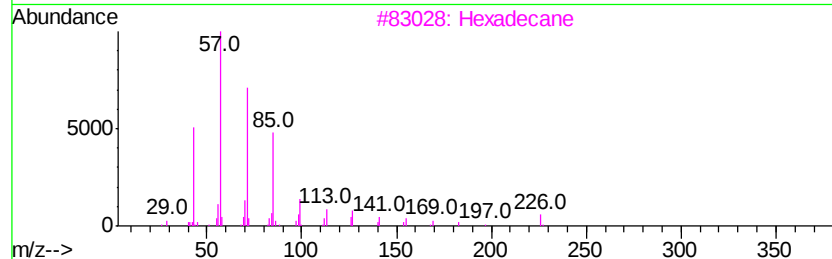
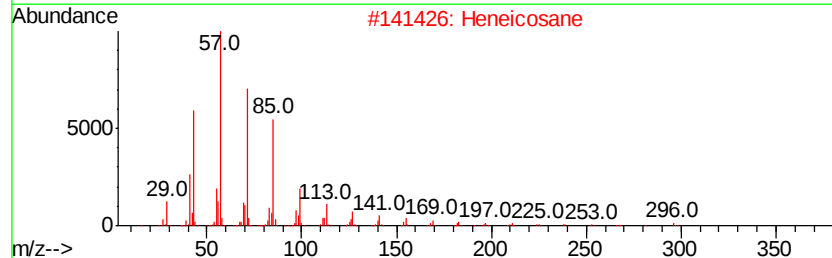
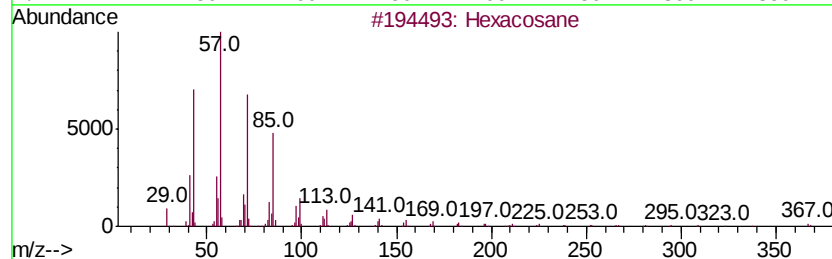
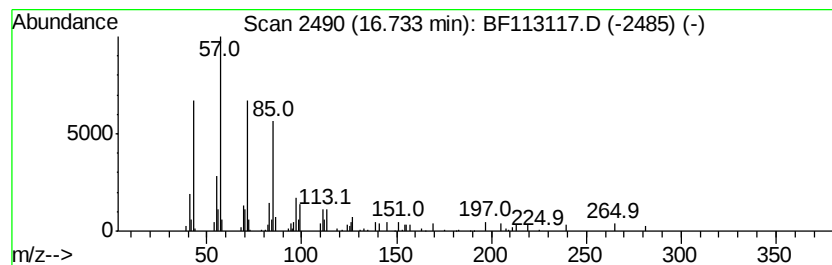
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	4.97 ng	132111	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Heneicosane	296	C21H44	000629-94-7	83
3		Hexadecane	226	C16H34	000544-76-3	81
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113117.D
Acq On : 19 Mar 2019 4:08
Operator : JU/SJ
Sample : K1947-06
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ALS Vial : 37 Sample Multiplier: 1

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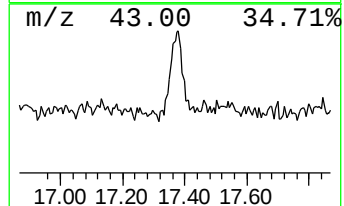
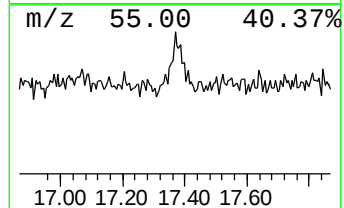
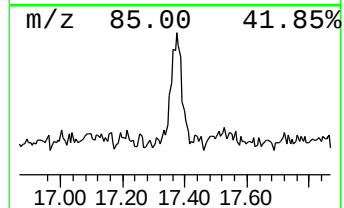
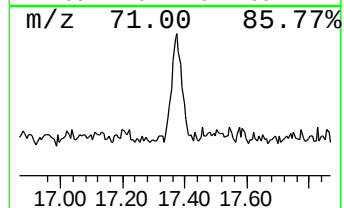
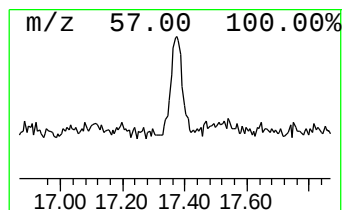
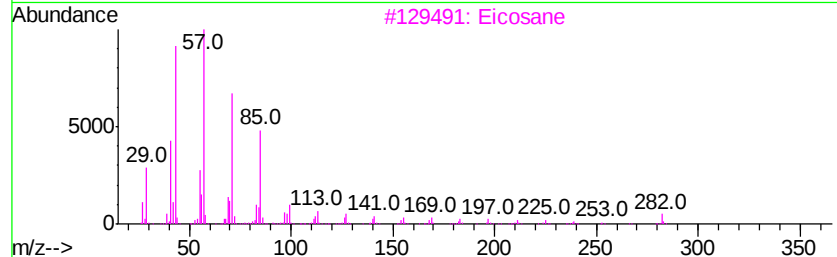
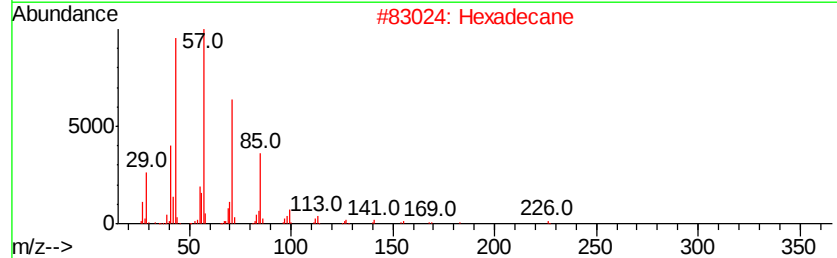
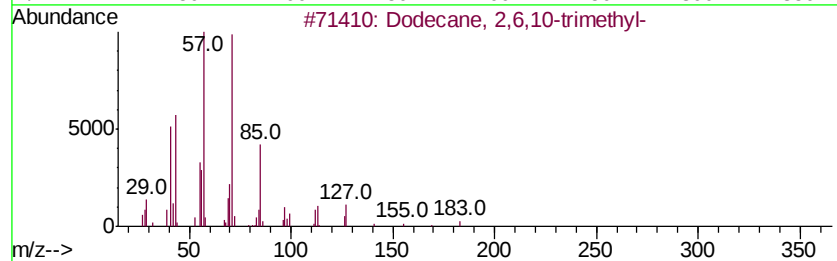
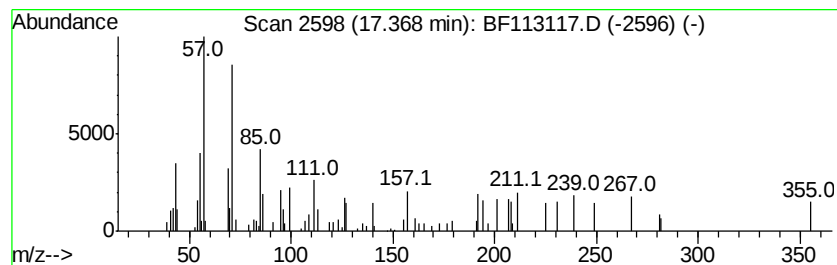
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.37 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	2.34 ng	62227	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	38
2			Hexadecane	226	C16H34	000544-76-3	38
3			Eicosane	282	C20H42	000112-95-8	38
4			Oxalic acid, 2-ethylhexyl isohex...	286	C16H30O4	1000309-38-8	38
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
 Data File : BF113117.D
 Acq On : 19 Mar 2019 4:08
 Operator : JU/SJ
 Sample : K1947-06
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-025-B035-031319

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	87.8	ng	3066820	1	6.73	698770	20.0
n-Hexadecanoic acid	11.77	3.2	ng	121297	4	11.24	754650	20.0
9-Octadecenamide,...	13.30	4.5	ng	197382	5	13.87	878244	20.0
Pentafluoropropio...	13.79	5.4	ng	235979	5	13.87	878244	20.0
Heneicosane	14.04	3.6	ng	160476	5	13.87	878244	20.0
Triacontane	14.34	8.5	ng	374009	5	13.87	878244	20.0
Tetratetracontane	14.64	22.4	ng	596542	6	15.28	531360	20.0
2-methyloctacosane	14.96	26.9	ng	713287	6	15.28	531360	20.0
Octacosane	15.72	18.2	ng	482438	6	15.28	531360	20.0
Heptadecane, 9-oc...	16.19	12.6	ng	335245	6	15.28	531360	20.0
Hexacosane	16.73	5.0	ng	132111	6	15.28	531360	20.0
unknown17.37	17.37	2.3	ng	62227	6	15.28	531360	20.0