

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
 Data File : BF113119.D
 Acq On : 19 Mar 2019 5:02
 Operator : JU/SJ
 Sample : K1947-08
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-025-B128-031319

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	558	rBV	3012764	2970228	71.14%	8.761%
2	6.381	724	730	746	rBV	2867573	3388505	81.16%	9.995%
3	6.504	746	751	754	rBV	3412366	3213999	76.98%	9.480%
4	6.563	759	761	770	rVB	33485	50530	1.21%	0.149%
5	6.728	785	789	793	rBV	926846	742418	17.78%	2.190%
6	6.887	812	816	819	rBV	2952281	2539962	60.84%	7.492%
7	7.293	879	885	897	rBV	1973512	2070852	49.60%	6.108%
8	8.010	1003	1007	1027	rBV	902234	895427	21.45%	2.641%
9	9.086	1185	1190	1205	rBV	4254251	4174946	100.00%	12.315%
10	9.475	1253	1256	1271	rVB	309733	344026	8.24%	1.015%
11	9.763	1301	1305	1316	rVB	807581	880882	21.10%	2.598%
12	10.545	1434	1438	1452	rBV	1793905	1899175	45.49%	5.602%
13	11.239	1552	1556	1565	rBV	803298	814148	19.50%	2.401%
14	11.775	1644	1647	1650	rBV	106557	115145	2.76%	0.340%
15	12.822	1820	1825	1828	rBV	2954515	2755430	66.00%	8.128%
16	13.304	1903	1907	1914	rBV3	49969	66479	1.59%	0.196%
17	13.727	1973	1979	1983	rBV	115066	112846	2.70%	0.333%
18	13.786	1983	1989	1999	rVV5	89000	320227	7.67%	0.945%
19	13.869	1999	2003	2014	rVV	1073440	1156977	27.71%	3.413%
20	13.974	2017	2021	2028	rVB4	31478	45117	1.08%	0.133%
21	14.045	2029	2033	2038	rVB	277116	274919	6.58%	0.811%
22	14.345	2078	2084	2088	rBV	535565	467799	11.20%	1.380%
23	14.639	2130	2134	2139	rBV	751719	718600	17.21%	2.120%
24	14.710	2142	2146	2150	rBV	51109	49858	1.19%	0.147%
25	14.957	2183	2188	2194	rBV	820041	860202	20.60%	2.537%
26	15.280	2238	2243	2245	rBV	422423	537607	12.88%	1.586%
27	15.316	2245	2249	2256	rVB	710371	927817	22.22%	2.737%
28	15.715	2311	2317	2327	rVB	499834	733755	17.58%	2.164%
29	16.186	2391	2397	2408	rBV2	260117	454962	10.90%	1.342%
30	16.727	2483	2489	2496	rVB	97618	191077	4.58%	0.564%
31	17.374	2594	2599	2606	rVB3	37739	83324	2.00%	0.246%
32	18.145	2727	2730	2737	rVB7	26607	44919	1.08%	0.132%

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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

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

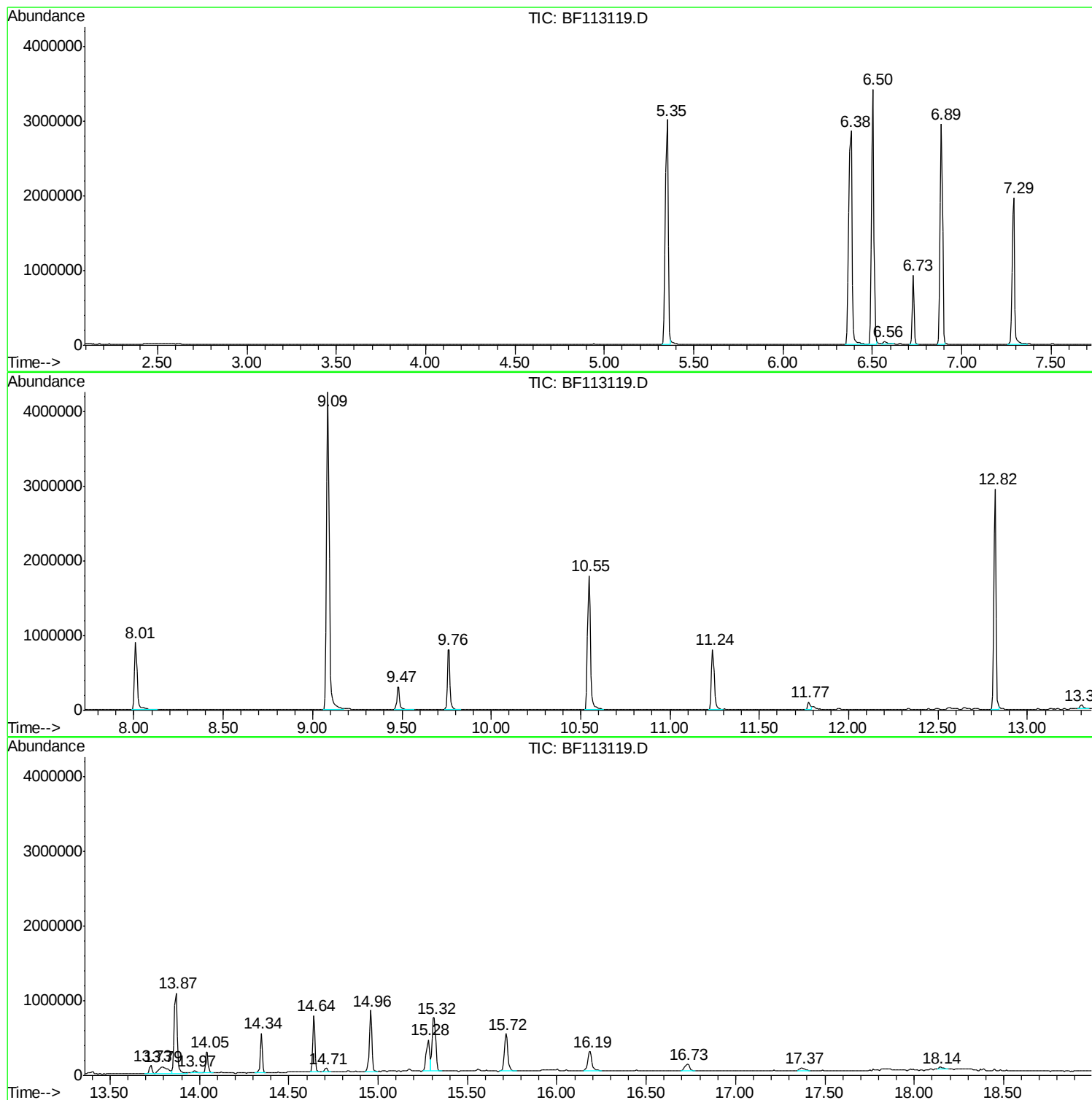
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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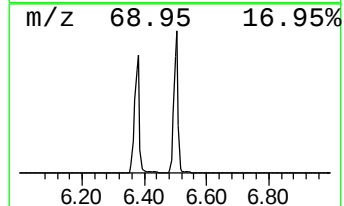
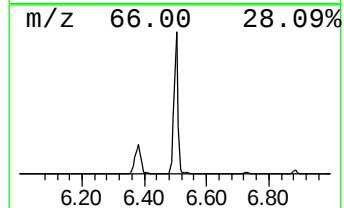
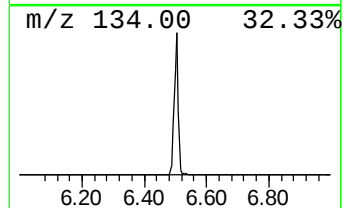
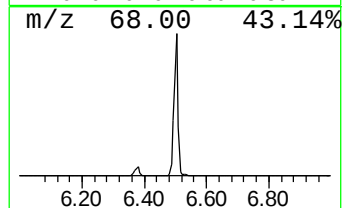
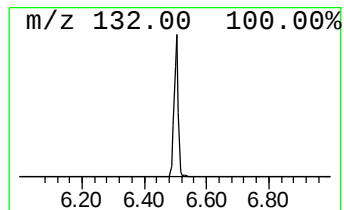
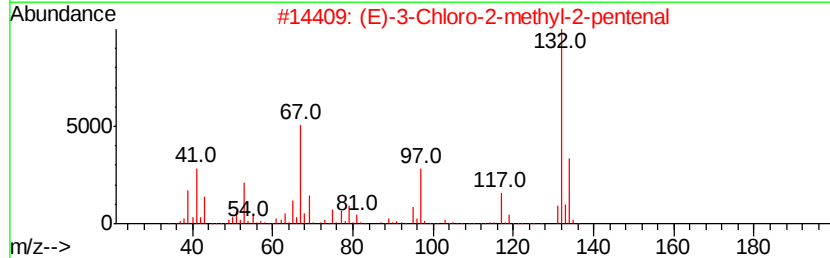
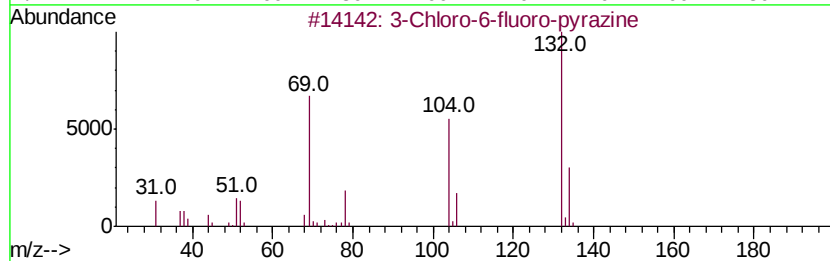
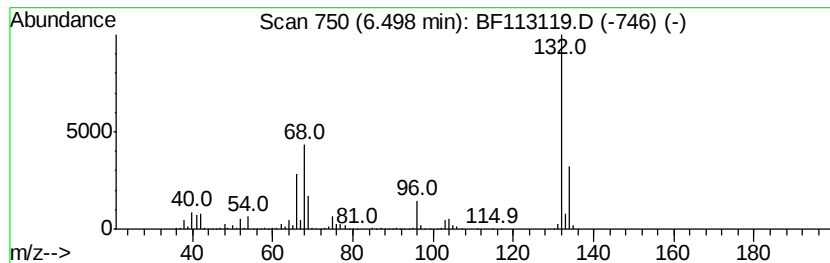
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	86.58 ng	3214000	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	12
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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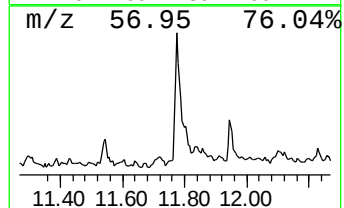
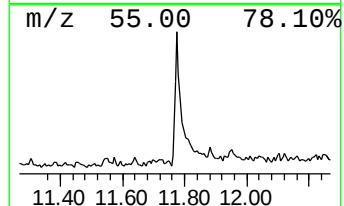
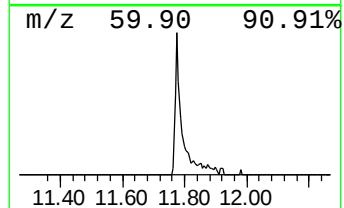
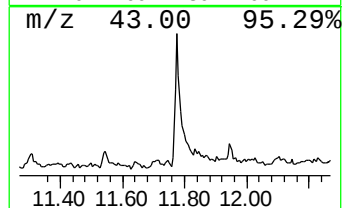
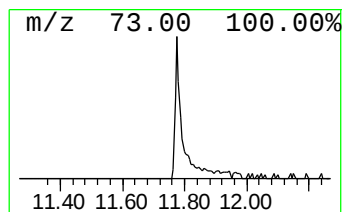
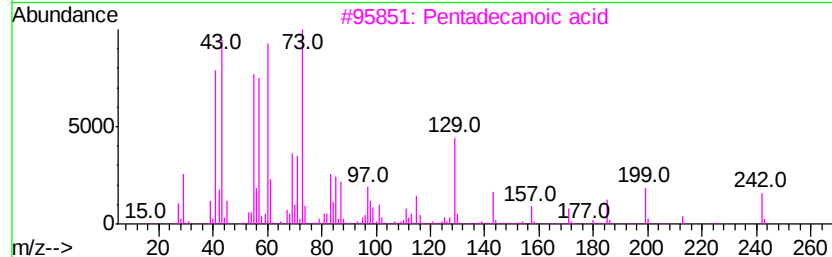
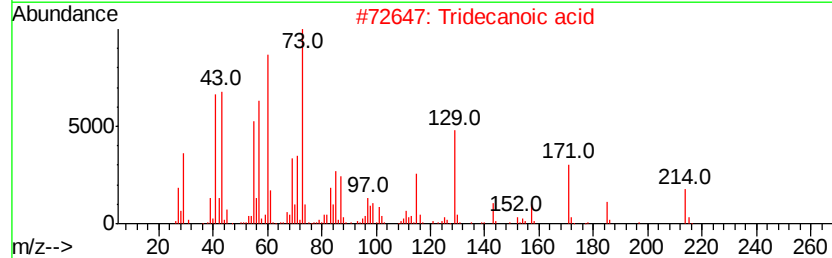
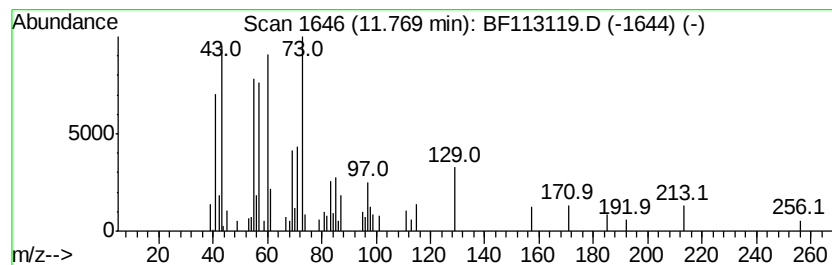
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	2.83 ng	115145	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53



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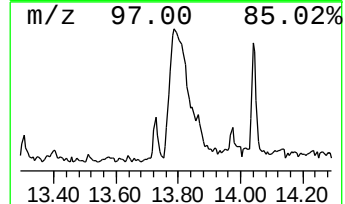
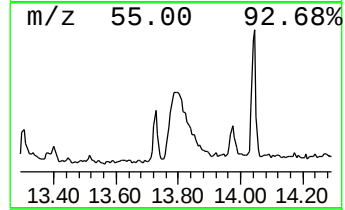
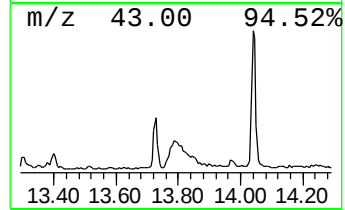
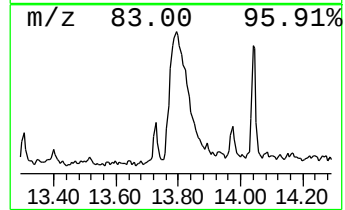
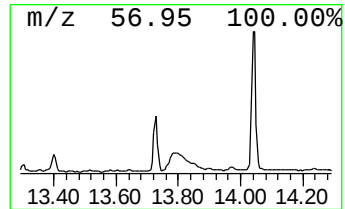
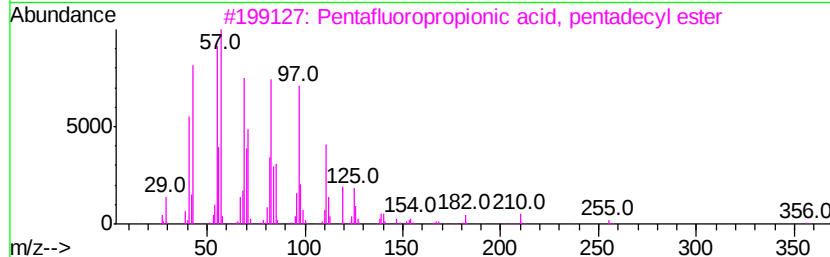
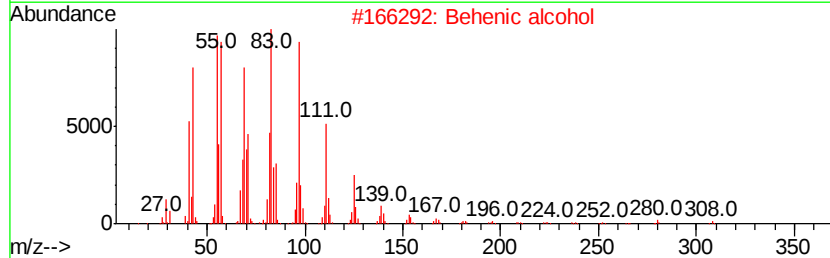
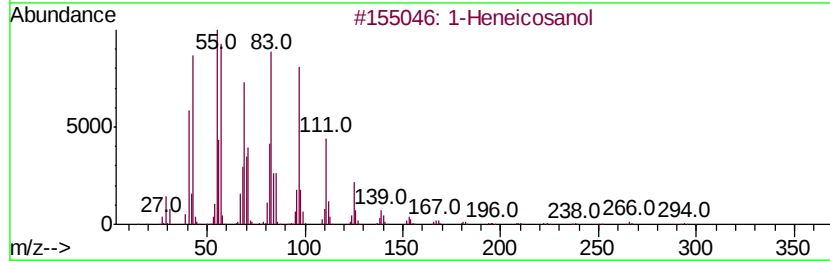
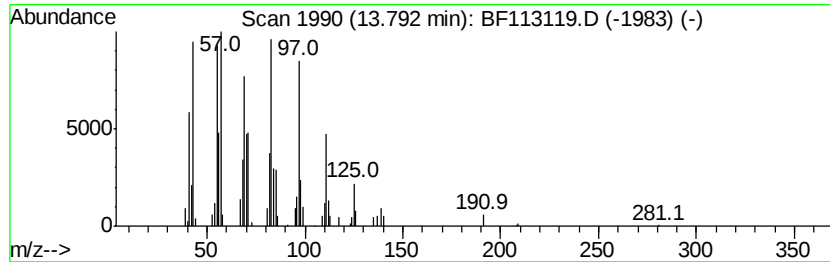
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	5.54 ng	320227	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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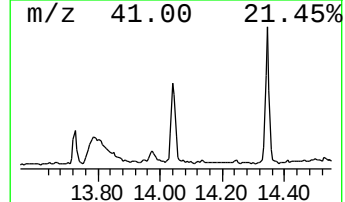
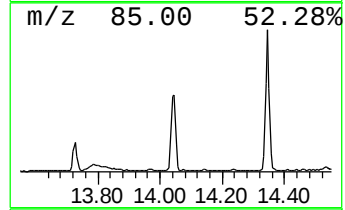
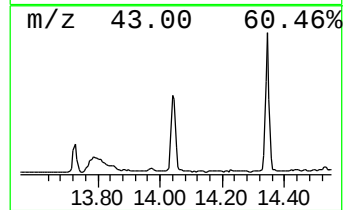
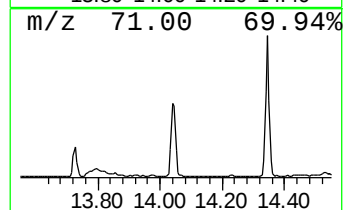
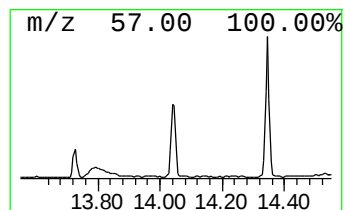
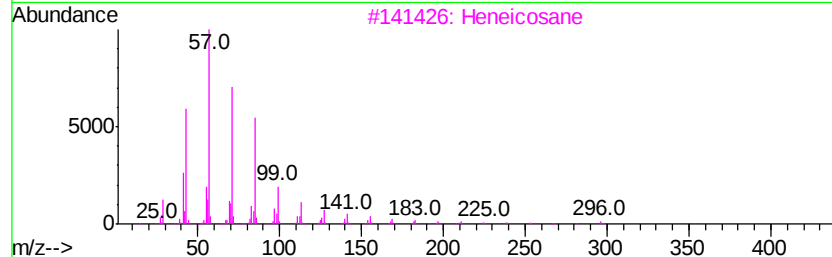
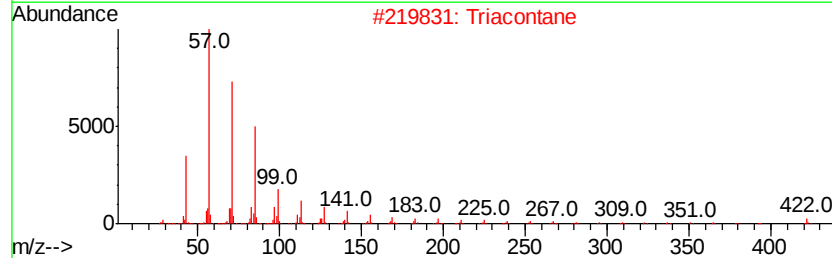
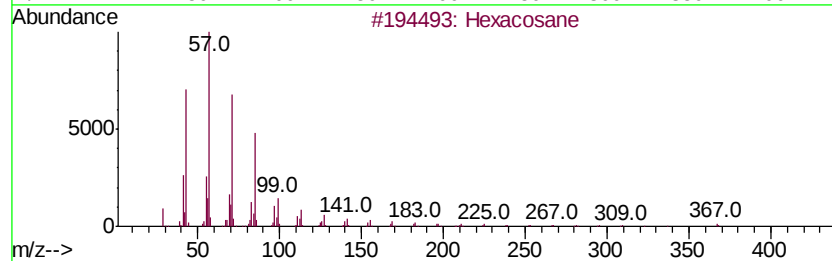
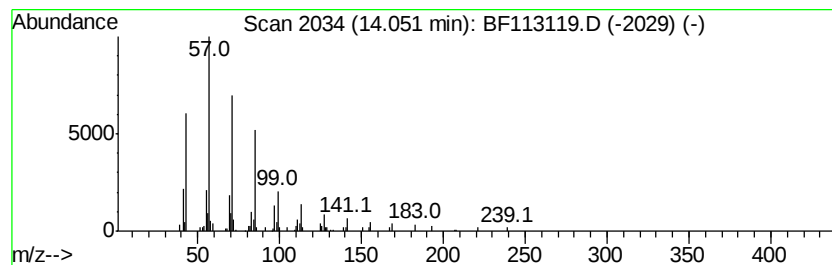
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.05	4.75 ng	274919	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	triacontane	422	C30H62	000638-68-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Octadecane	254	C18H38	000593-45-3	90



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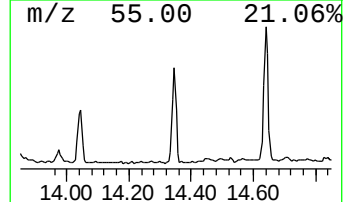
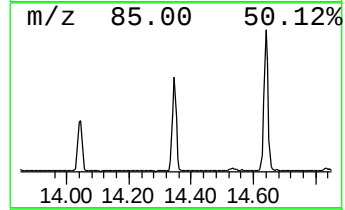
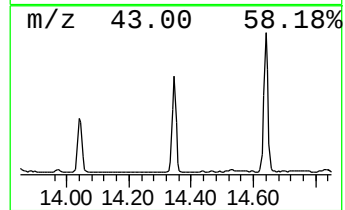
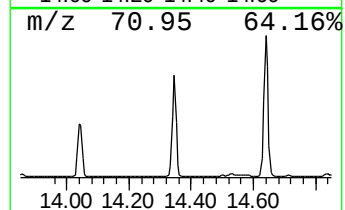
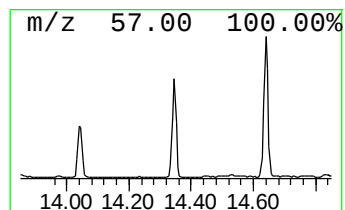
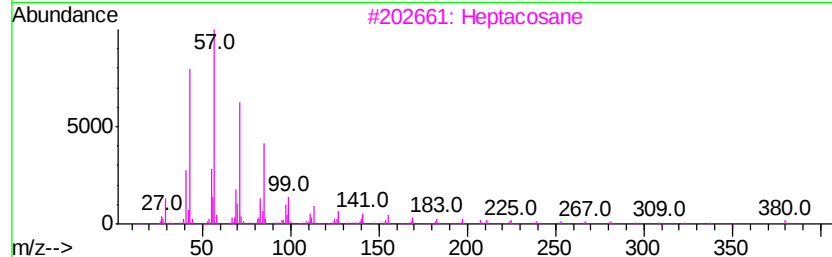
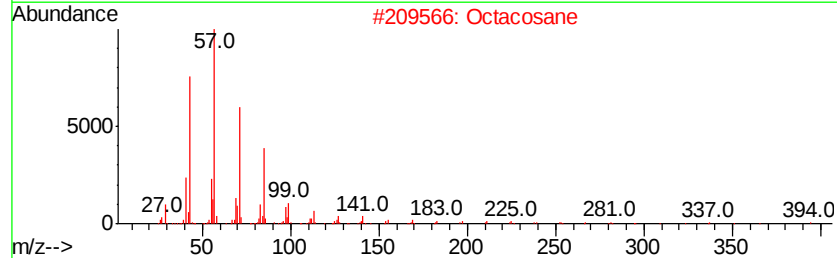
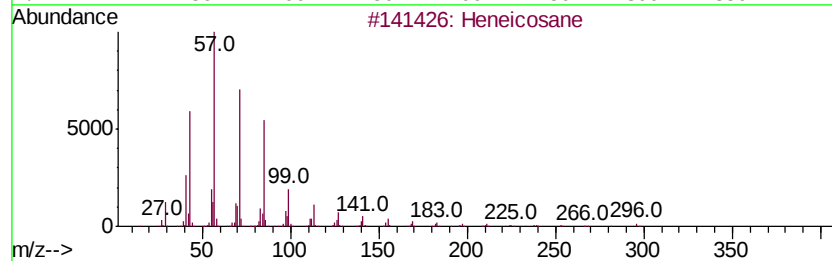
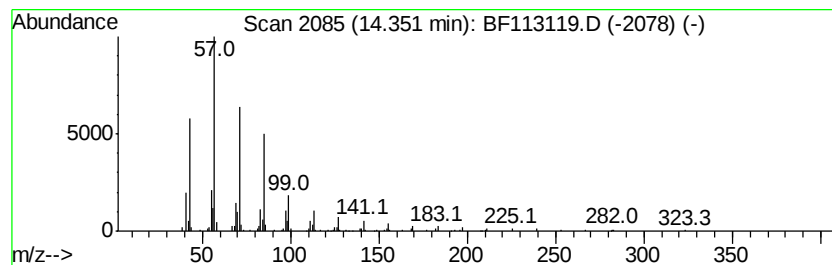
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	8.09 ng	467799	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Triacontane		422	C30H62	000638-68-6	91



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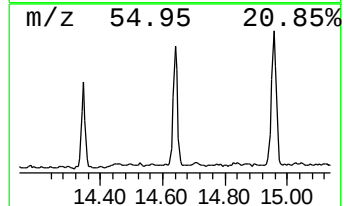
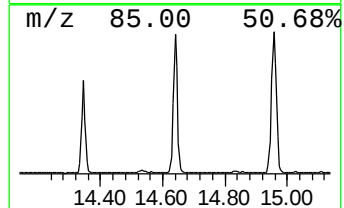
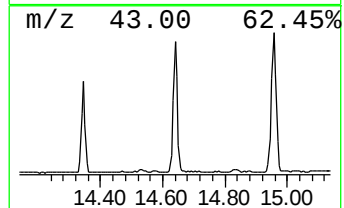
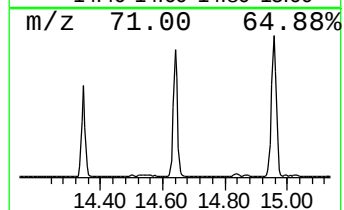
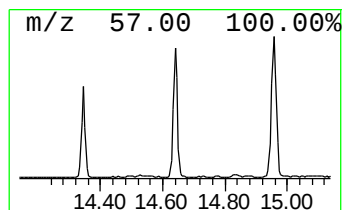
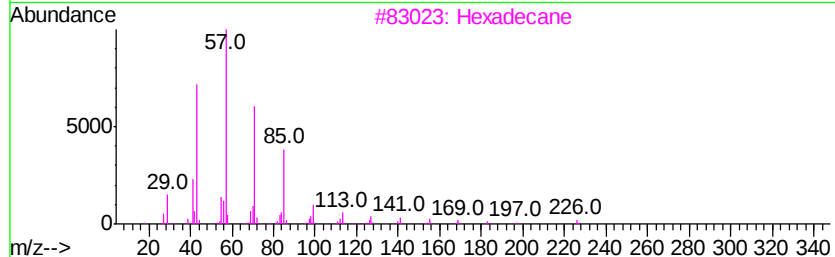
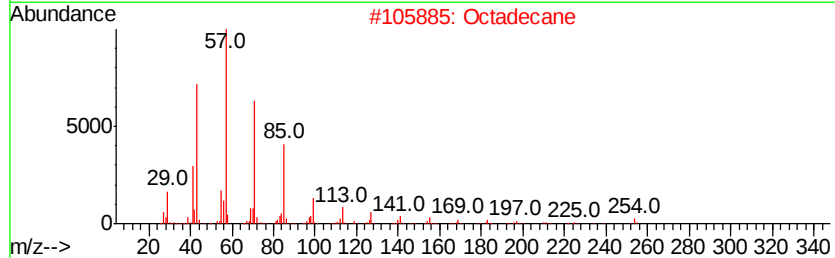
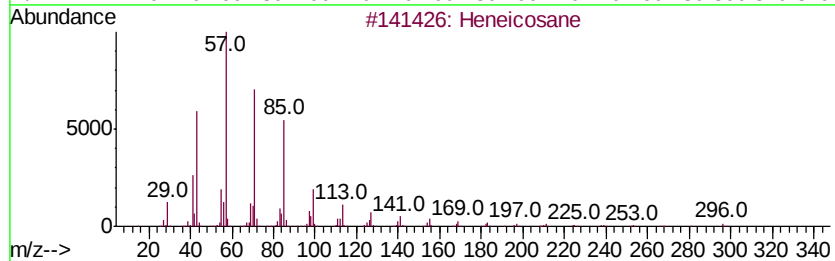
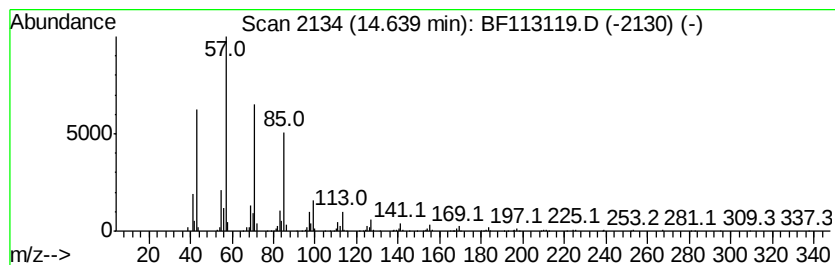
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	26.73 ng	718600	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octadecane	254	C18H38	000593-45-3	87
3		Hexadecane	226	C16H34	000544-76-3	87
4		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113119.D
Acq On : 19 Mar 2019 5:02
Operator : JU/SJ
Sample : K1947-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

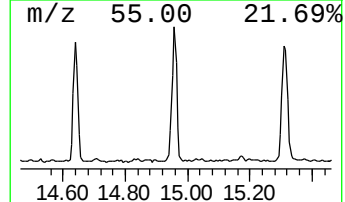
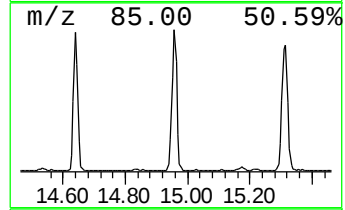
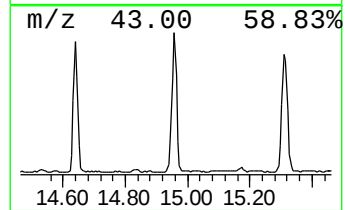
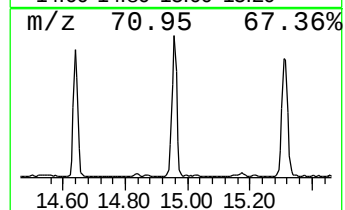
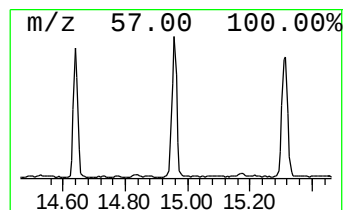
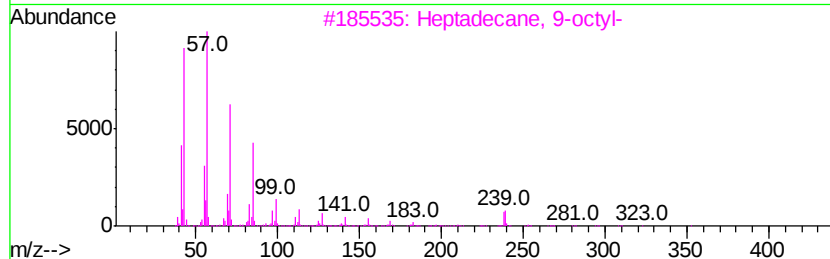
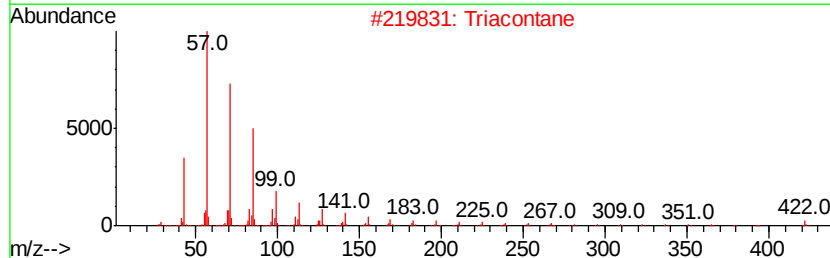
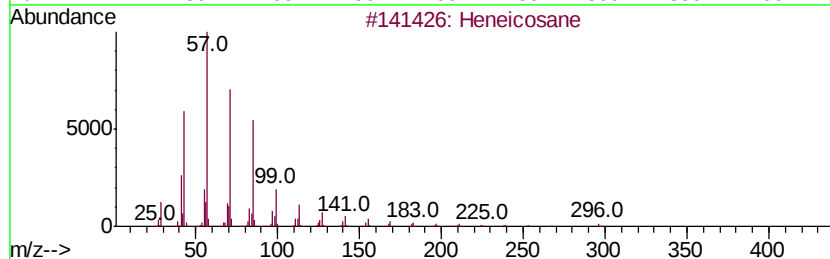
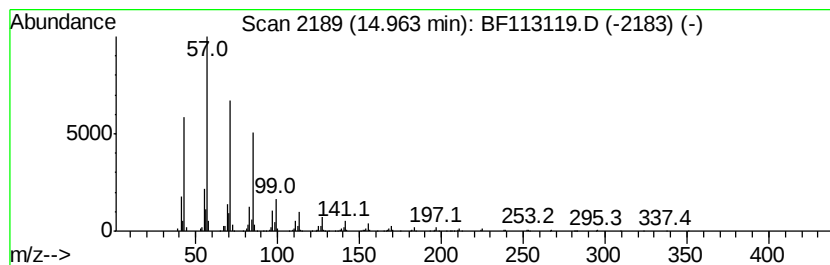
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	32.00 ng	860202	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heneicosane	296 C21H44	000629-94-7 91
2		Triacontane	422 C30H62	000638-68-6 91
3		Heptadecane, 9-octyl-	352 C25H52	007225-64-1 91
4		Eicosane, 7-hexyl-	366 C26H54	055333-99-8 90
5		Eicosane	282 C20H42	000112-95-8 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
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Sample : K1947-08
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Instrument :
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ClientSampleId :
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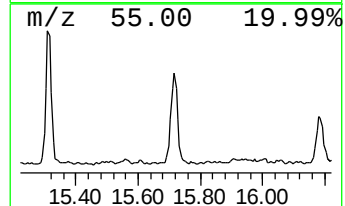
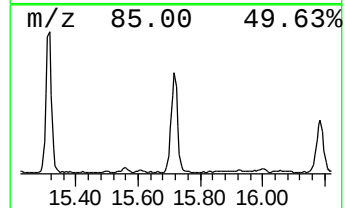
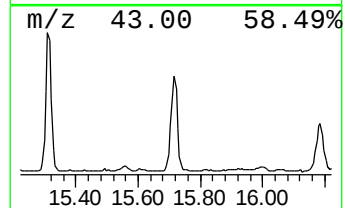
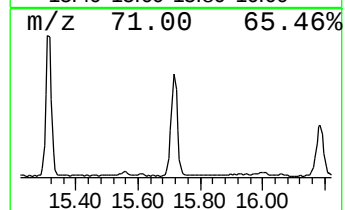
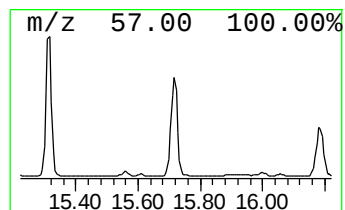
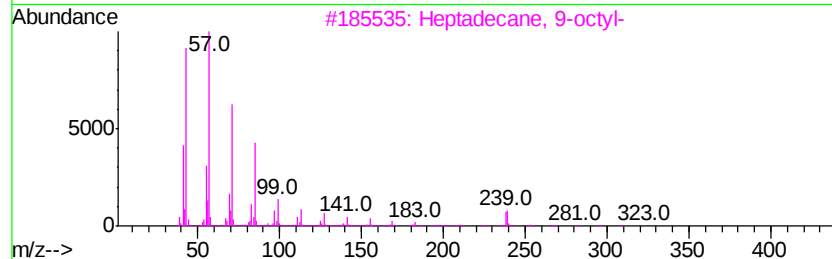
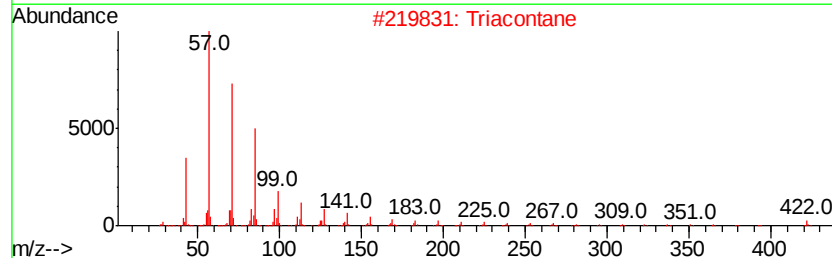
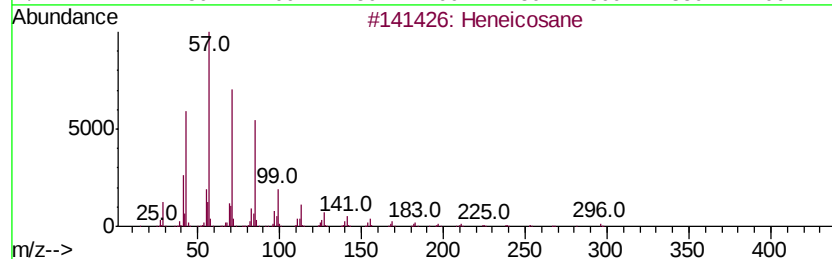
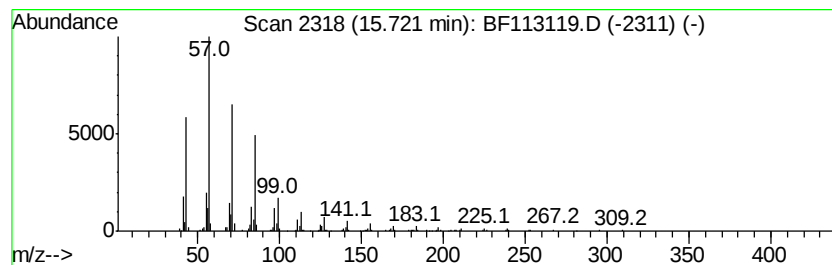
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	27.30 ng	733755	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		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
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 Acq On : 19 Mar 2019 5:02
 Operator : JU/SJ
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 ALS Vial : 39 Sample Multiplier: 1

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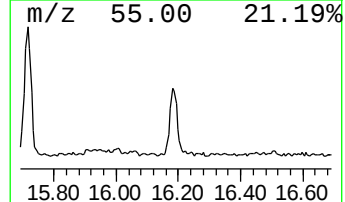
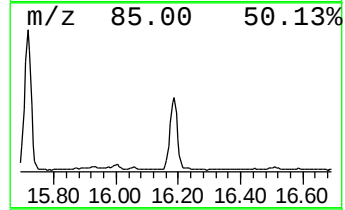
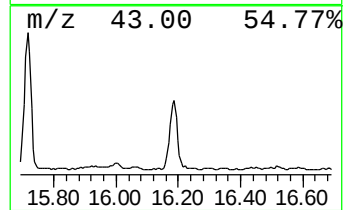
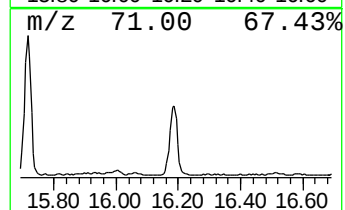
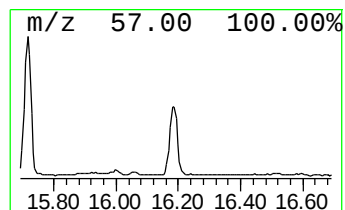
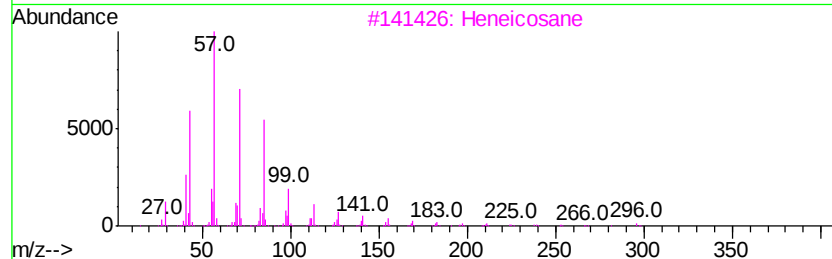
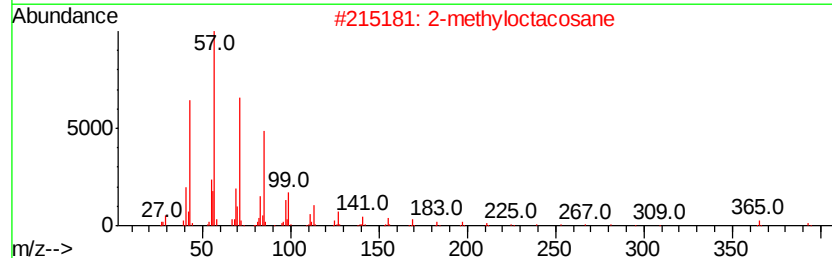
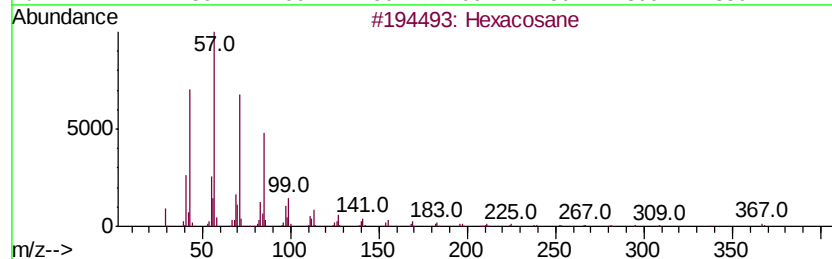
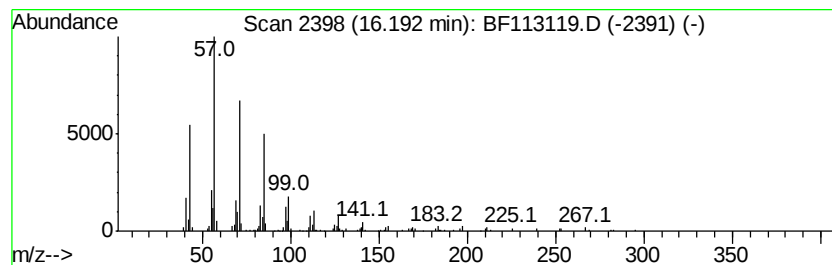
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	16.93 ng	454962	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113119.D
Acq On : 19 Mar 2019 5:02
Operator : JU/SJ
Sample : K1947-08
Misc :
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Instrument :
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ClientSampleId :
PST-025-B128-031319

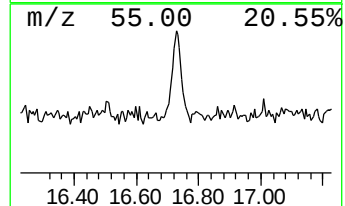
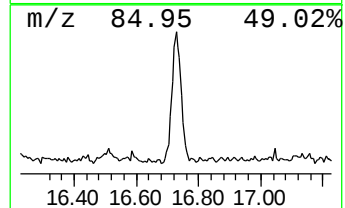
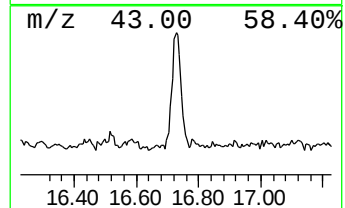
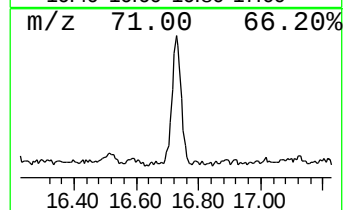
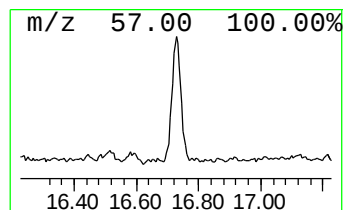
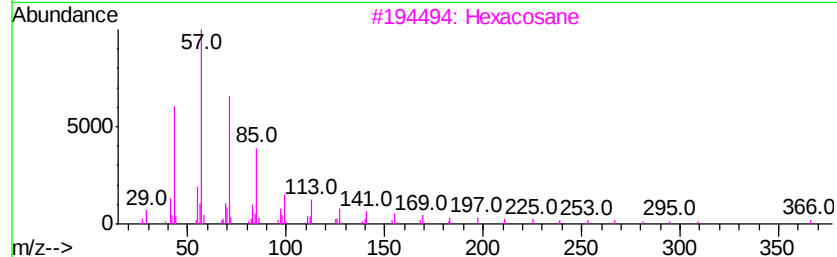
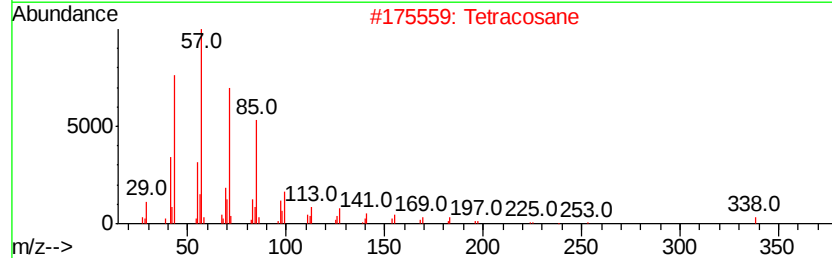
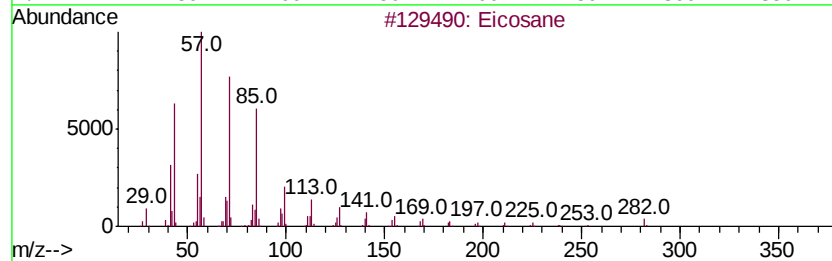
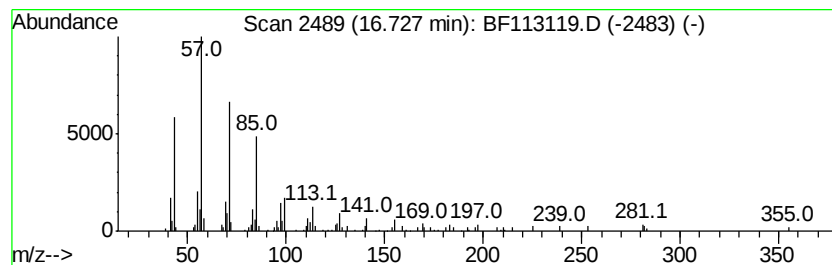
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	7.11 ng	191077	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Tetracosane	338	C24H50	000646-31-1	93
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octacosane	394	C28H58	000630-02-4	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113119.D
Acq On : 19 Mar 2019 5:02
Operator : JU/SJ
Sample : K1947-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

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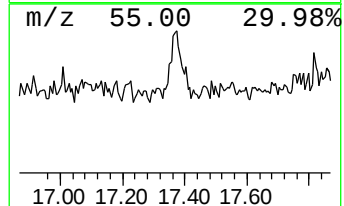
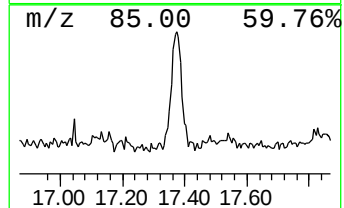
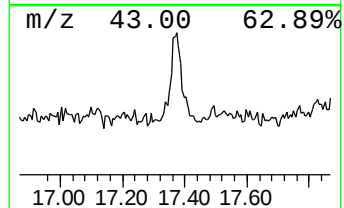
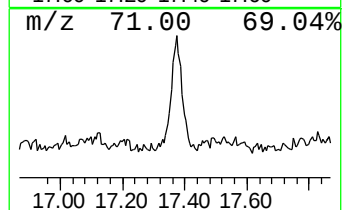
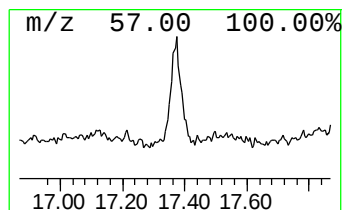
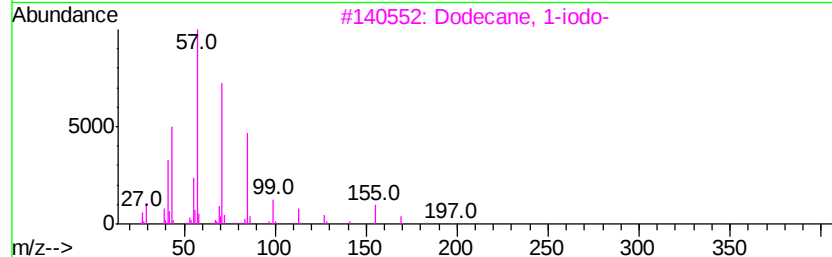
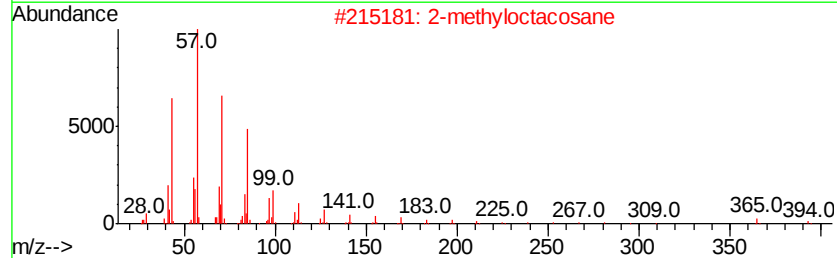
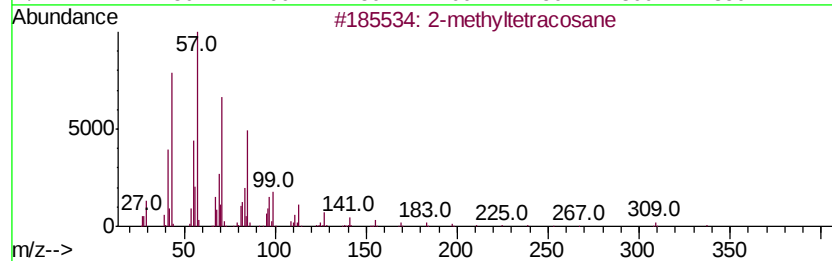
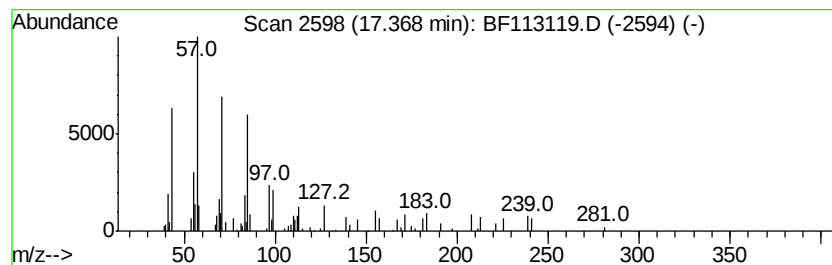
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyltetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	3.10 ng	83324	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyltetracosane	352	C25H52	1000376-72-6	86
2			2-methyloctacosane	408	C29H60	1000376-72-8	86
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4			Hexacosane	366	C26H54	000630-01-3	80
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
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Acq On : 19 Mar 2019 5:02
Operator : JU/SJ
Sample : K1947-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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1-Heneicosanol	13.79	5.5	ng	320227	5	13.87	1156980	20.0
Hexacosane	14.05	4.8	ng	274919	5	13.87	1156980	20.0
Heneicosane	14.35	8.1	ng	467799	5	13.87	1156980	20.0
Octadecane	14.64	26.7	ng	718600	6	15.28	537607	20.0
Heptadecane, 9-oc...	14.96	32.0	ng	860202	6	15.28	537607	20.0
Triacontane	15.72	27.3	ng	733755	6	15.28	537607	20.0
2-methyloctacosane	16.19	16.9	ng	454962	6	15.28	537607	20.0
Eicosane	16.73	7.1	ng	191077	6	15.28	537607	20.0
2-methyltetracosane	17.37	3.1	ng	83324	6	15.28	537607	20.0