

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
 Data File : BF113115.D
 Acq On : 19 Mar 2019 3:13
 Operator : JU/SJ
 Sample : K1947-04
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-025-B032-031319

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	3582956	3563131	90.85%	10.875%
2	6.381	724	730	733	rBV	3613494	3888433	99.15%	11.868%
3	6.504	746	751	754	rBV	4099284	3921862	100.00%	11.970%
4	6.569	759	762	771	rVB	33382	54763	1.40%	0.167%
5	6.728	786	789	793	rBV	1121942	902524	23.01%	2.755%
6	6.886	812	816	819	rBV	3563206	3141825	80.11%	9.589%
7	7.292	880	885	888	rBV	2348918	2311417	58.94%	7.055%
8	8.010	1003	1007	1021	rBV	864351	843765	21.51%	2.575%
9	9.086	1185	1190	1204	rBV	3435797	3404454	86.81%	10.391%
10	9.480	1253	1257	1267	rBV	200963	217466	5.54%	0.664%
11	9.763	1301	1305	1323	rVB	805265	842196	21.47%	2.570%
12	10.545	1434	1438	1454	rBV	1822100	2009151	51.23%	6.132%
13	11.239	1552	1556	1571	rVB	801893	811788	20.70%	2.478%
14	11.774	1644	1647	1657	rBV2	98469	139139	3.55%	0.425%
15	12.368	1737	1748	1761	rBV7	30156	122432	3.12%	0.374%
16	12.821	1820	1825	1828	rBV	3275839	3069275	78.26%	9.368%
17	13.786	1982	1989	1999	rBV3	103105	384079	9.79%	1.172%
18	13.868	1999	2003	2012	rVB	906869	903795	23.05%	2.758%
19	14.039	2029	2032	2036	rBV	77633	78000	1.99%	0.238%
20	14.345	2081	2084	2087	rVB	152790	131635	3.36%	0.402%
21	14.445	2096	2101	2107	rBV9	19777	55099	1.40%	0.168%
22	14.498	2107	2110	2114	rVV	92671	84851	2.16%	0.259%
23	14.639	2130	2134	2138	rVB	247787	222498	5.67%	0.679%
24	14.957	2184	2188	2192	rBV	249711	259649	6.62%	0.792%
25	15.280	2238	2243	2246	rBV	394292	557291	14.21%	1.701%
26	15.309	2246	2248	2254	rVB	247632	284692	7.26%	0.869%
27	15.715	2312	2317	2329	rVB	170083	248538	6.34%	0.759%
28	16.186	2392	2397	2411	rVB2	103216	231922	5.91%	0.708%
29	16.727	2486	2489	2496	rVB	41799	79029	2.02%	0.241%

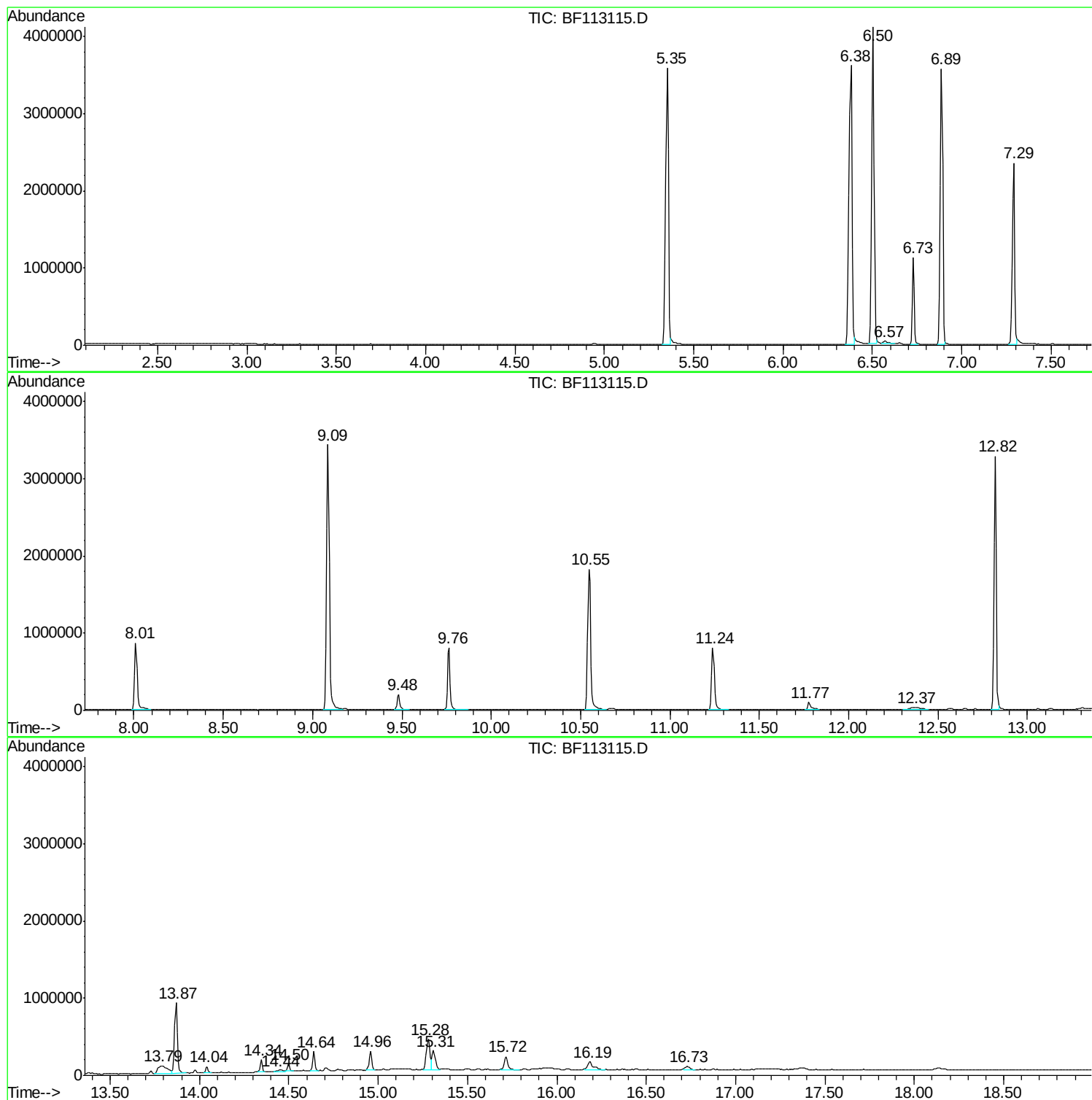
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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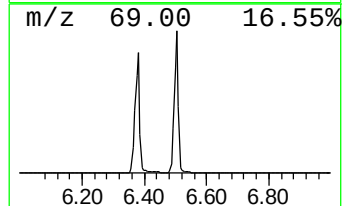
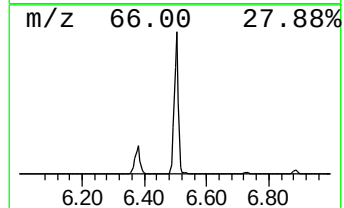
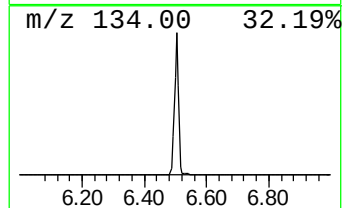
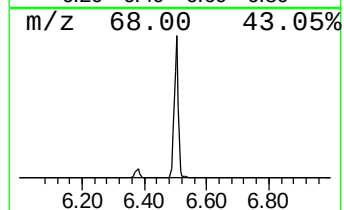
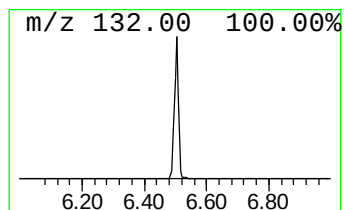
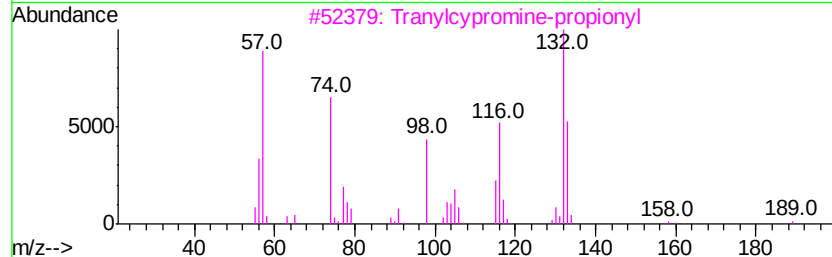
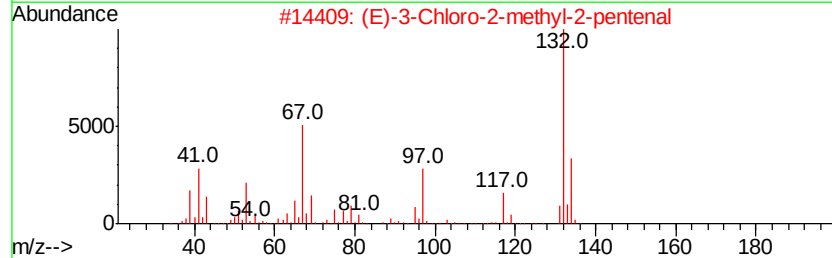
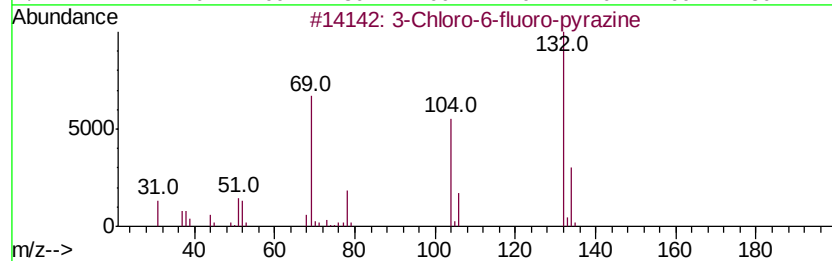
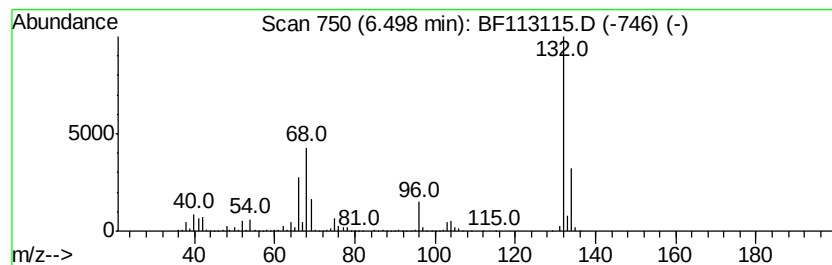
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	86.91 ng	3921860	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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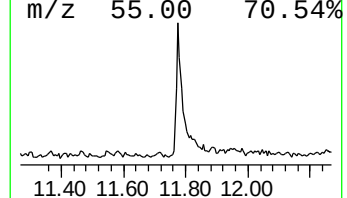
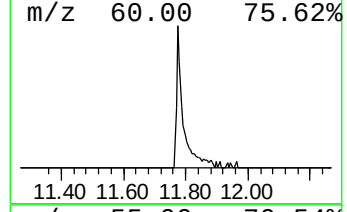
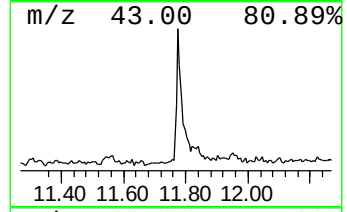
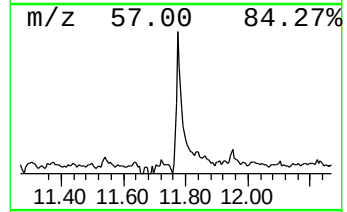
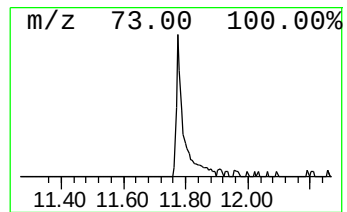
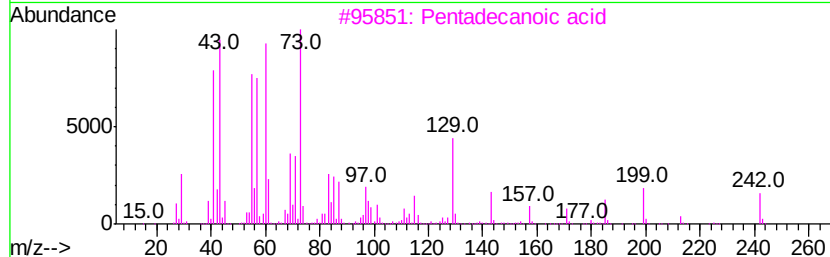
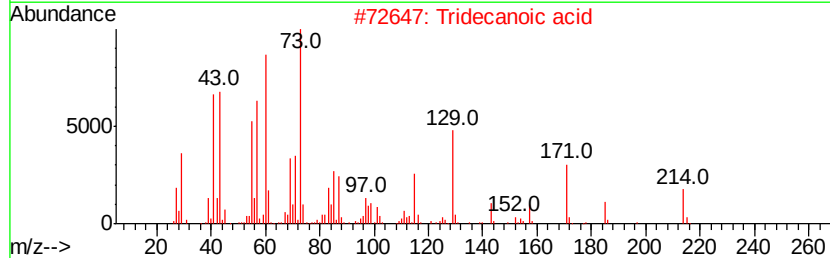
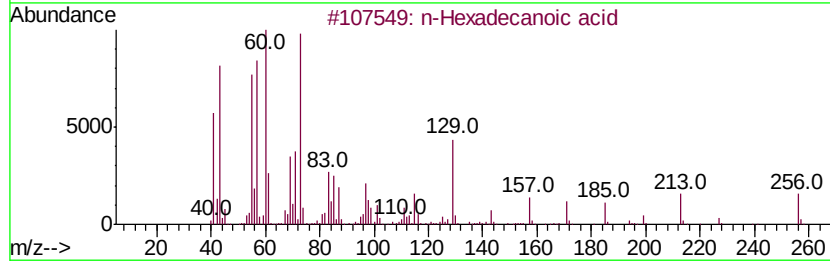
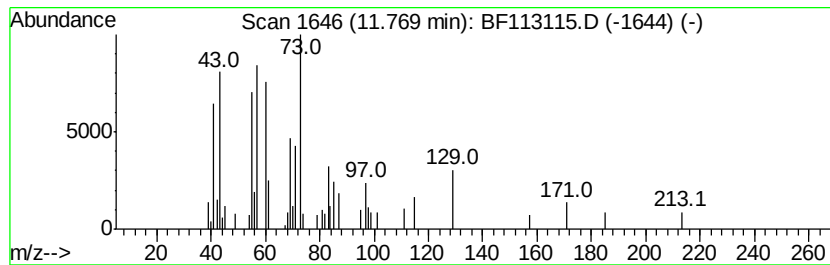
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	3.43 ng	139139	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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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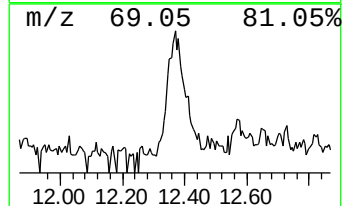
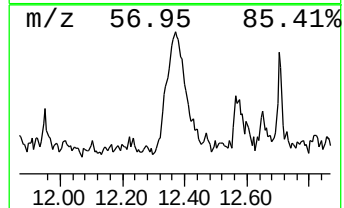
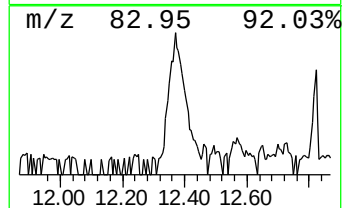
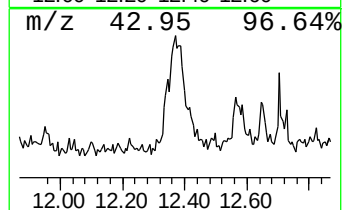
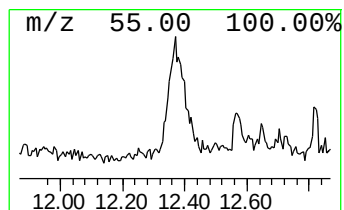
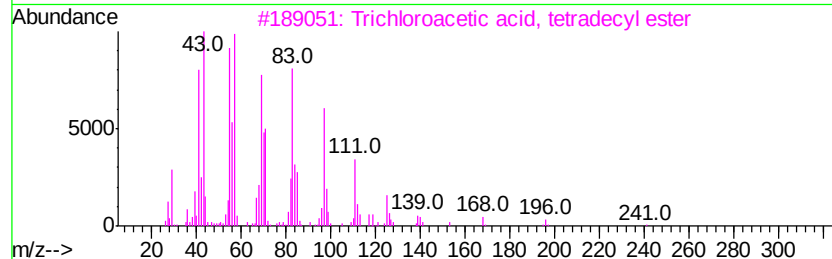
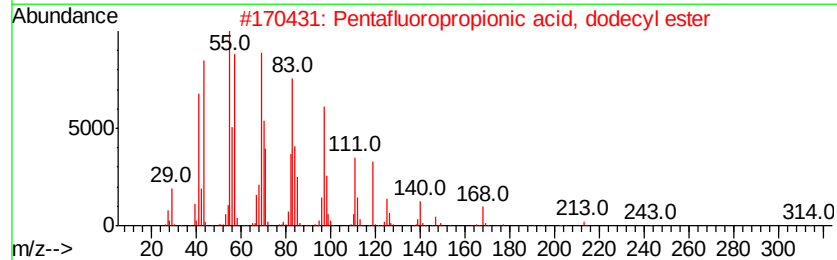
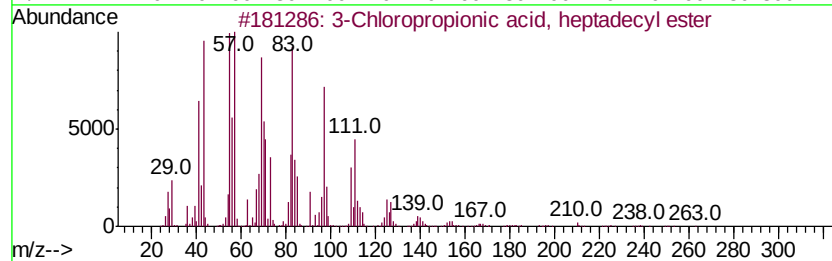
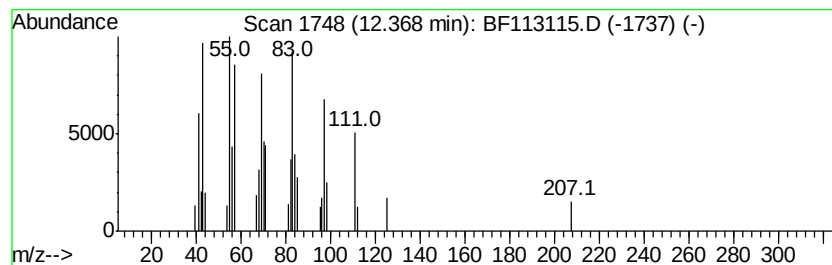
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Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.37	3.02 ng	122432	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	91
5		11-Tricosene	322	C23H46	052078-56-5	91



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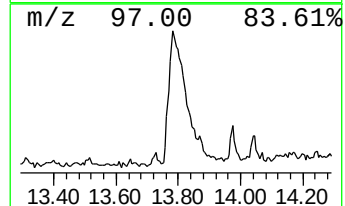
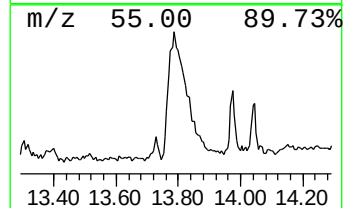
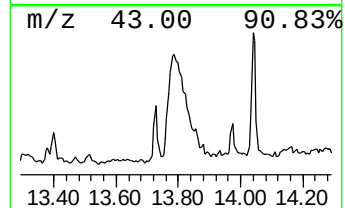
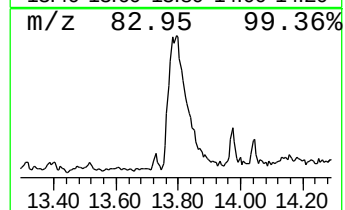
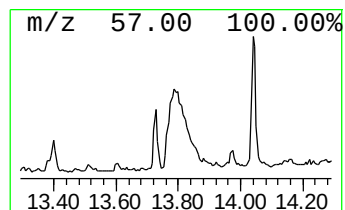
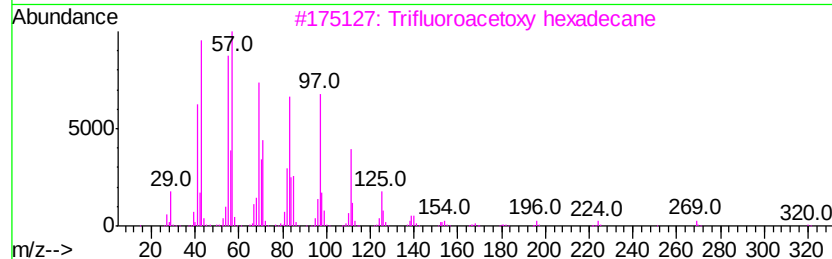
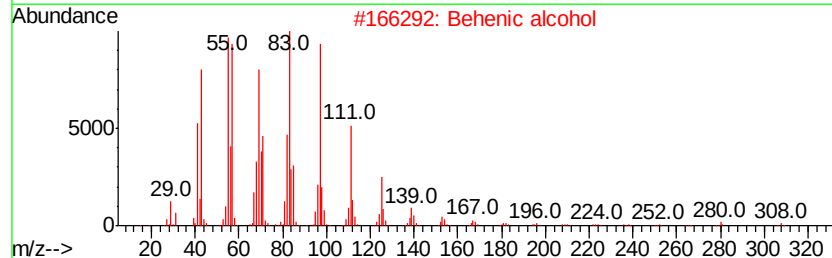
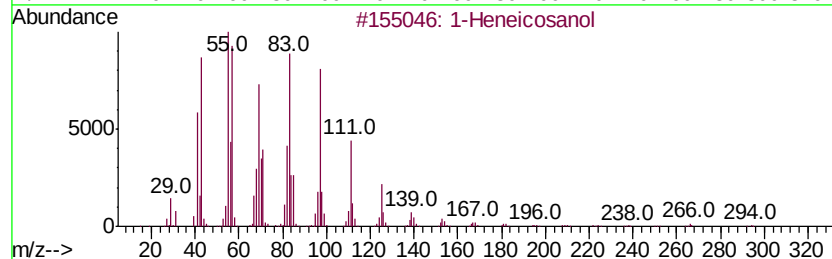
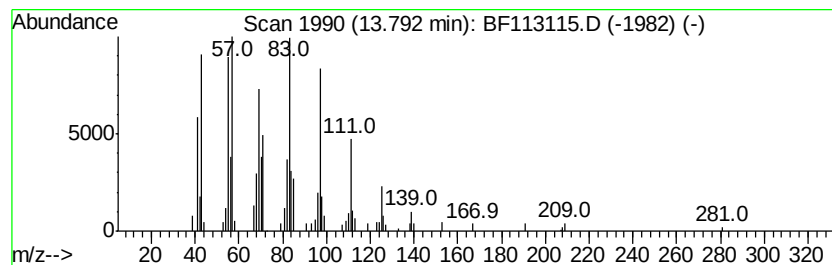
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	8.50 ng	384079	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	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92
5	1-Nonadecene	266	C19H38	018435-45-5	91



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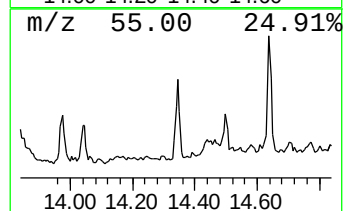
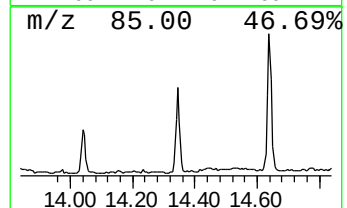
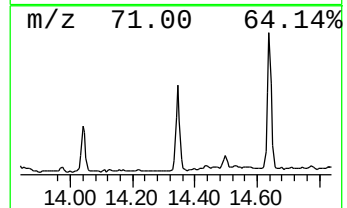
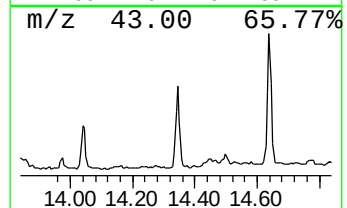
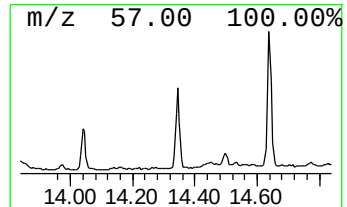
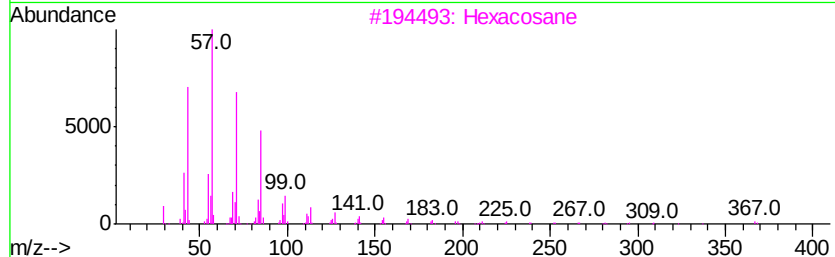
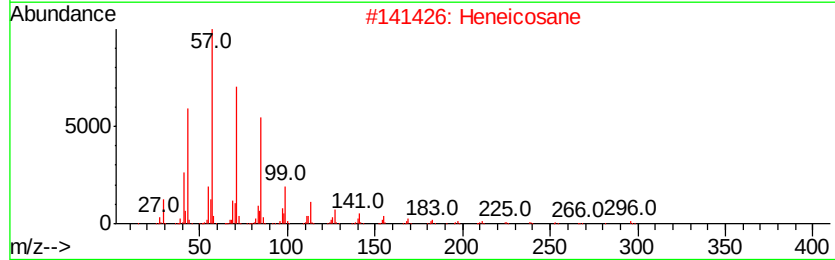
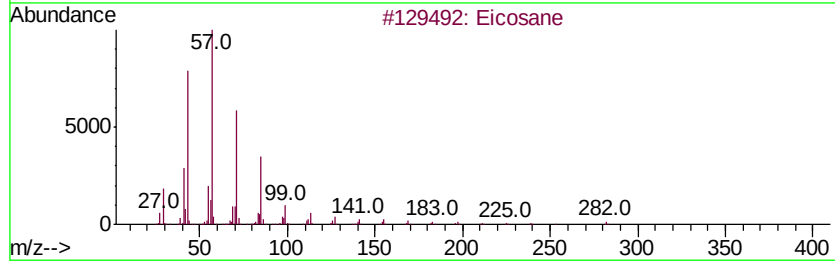
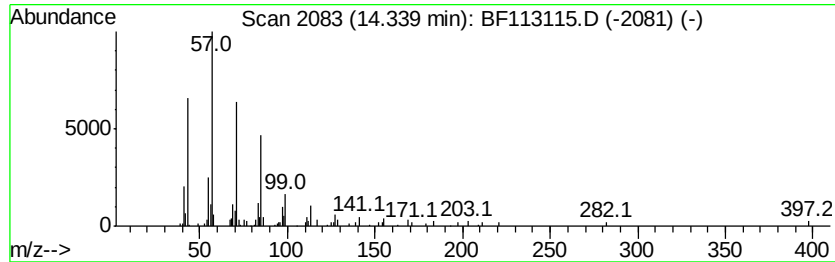
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.91 ng	131635	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		Triacontane	422	C30H62	000638-68-6	87
5		Tetracosane	338	C24H50	000646-31-1	81



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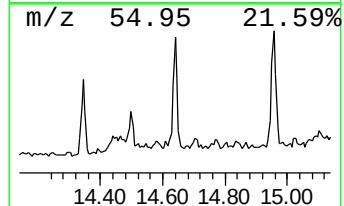
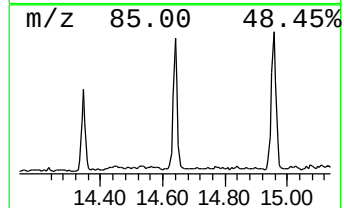
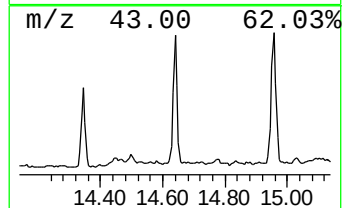
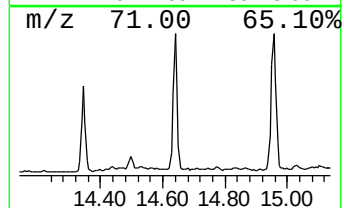
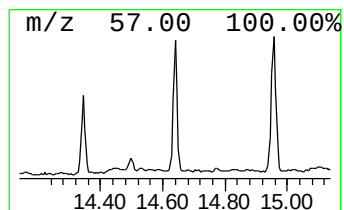
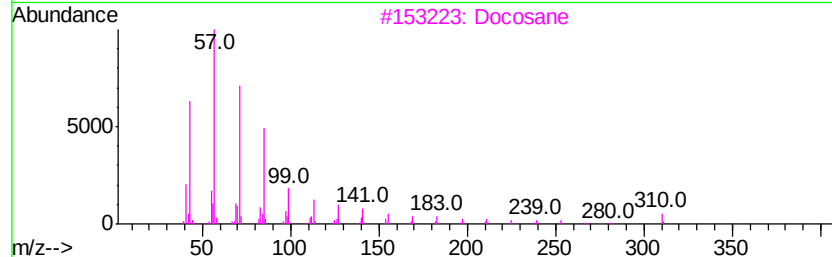
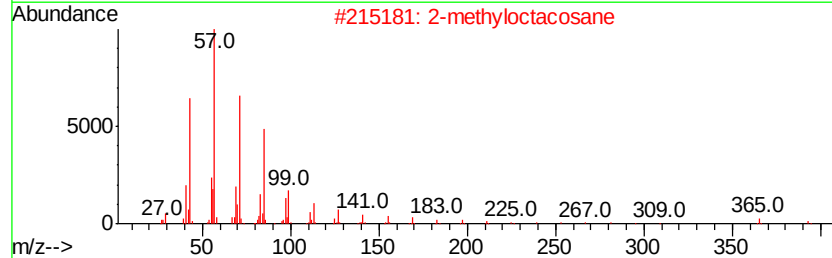
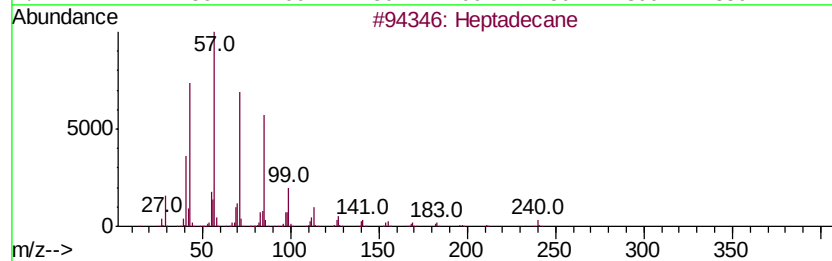
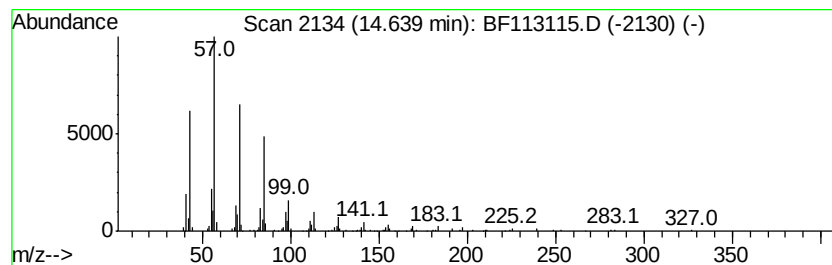
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	7.98 ng	222498	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Docosane	310	C22H46	000629-97-0	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\BF031819\
Data File : BF113115.D
Acq On : 19 Mar 2019 3:13
Operator : JU/SJ
Sample : K1947-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

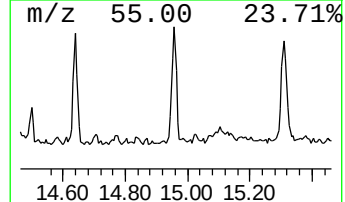
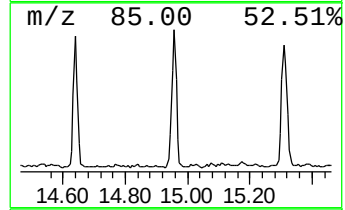
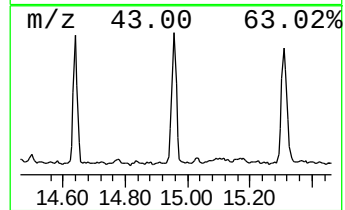
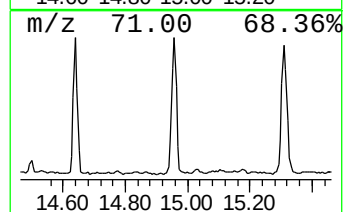
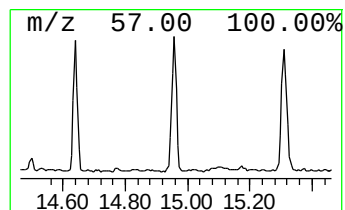
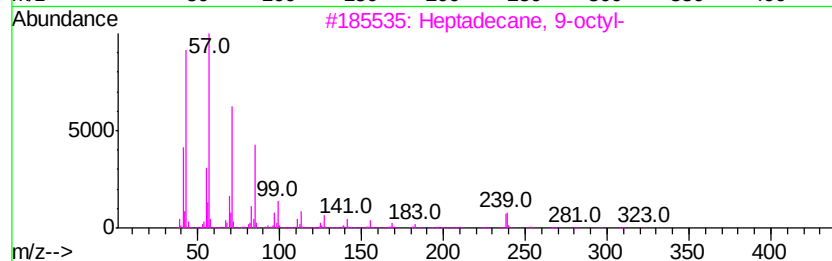
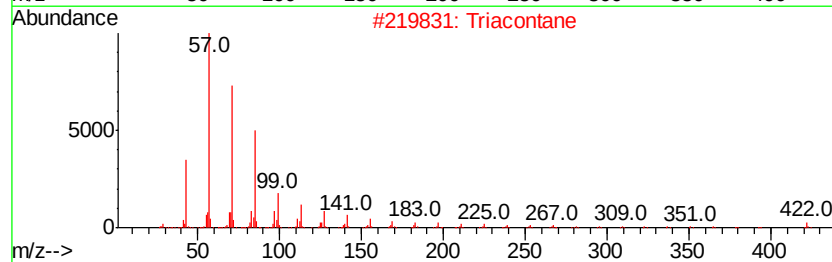
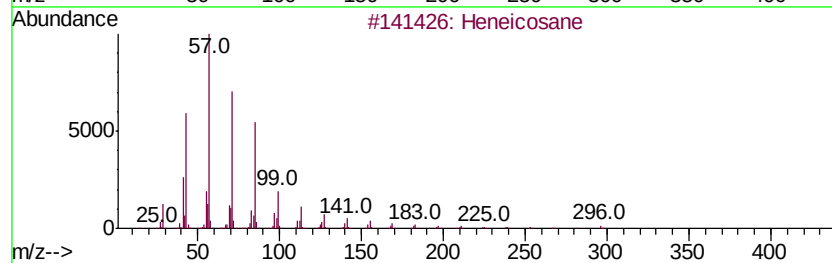
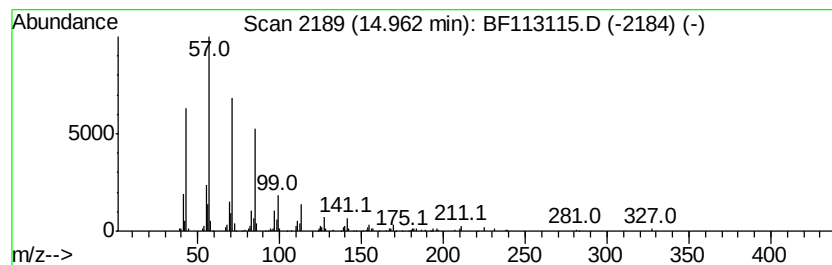
Instrument :
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ClientSampleId :
PST-025-B032-031319

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	9.32 ng	259649	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	Docosane	310 C22H46	000629-97-0	90
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
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Acq On : 19 Mar 2019 3:13
Operator : JU/SJ
Sample : K1947-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

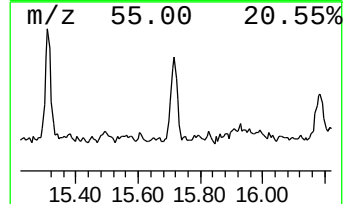
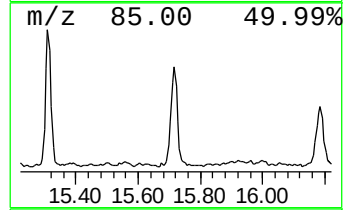
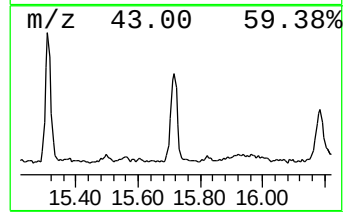
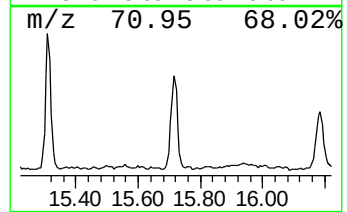
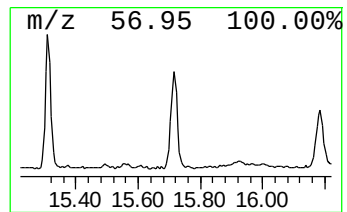
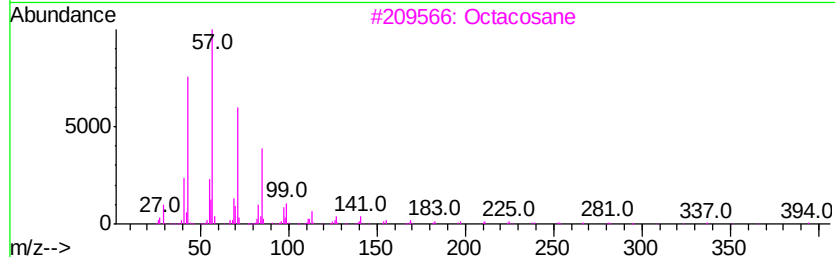
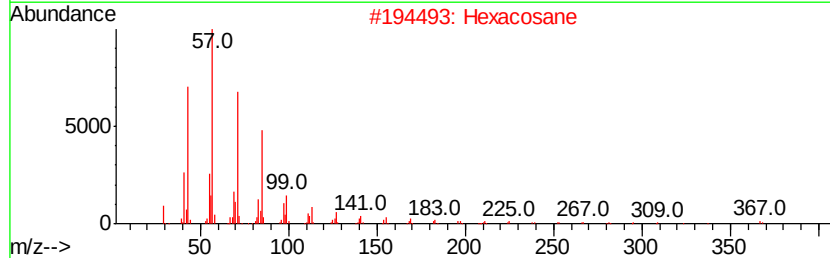
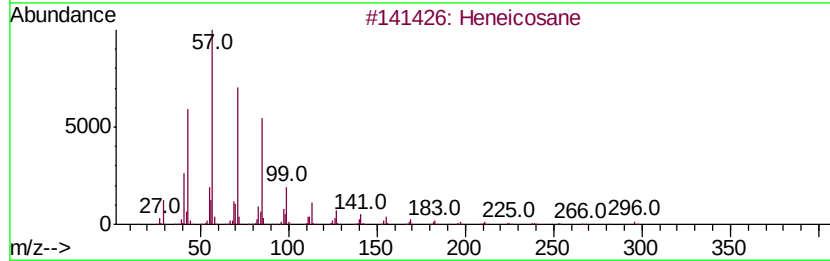
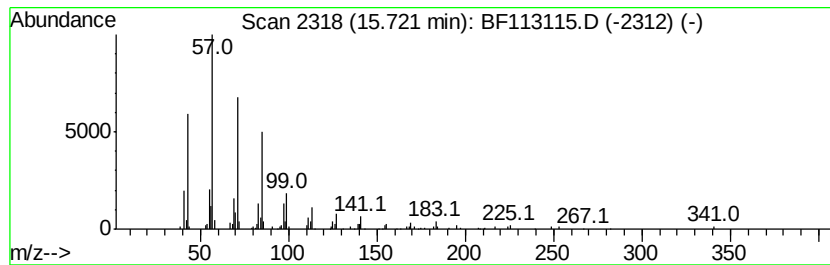
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ClientSampleId :
PST-025-B032-031319

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

Peak Number 9 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	8.92 ng	248538	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Hexacosane	366 C26H54	000630-01-3	91
3	Octacosane	394 C28H58	000630-02-4	91
4	Tetratetracontane	619 C44H90	007098-22-8	91
5	Hentriacontane	437 C31H64	000630-04-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113115.D
Acq On : 19 Mar 2019 3:13
Operator : JU/SJ
Sample : K1947-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

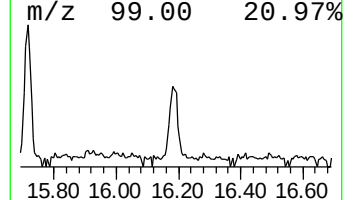
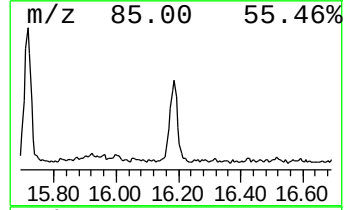
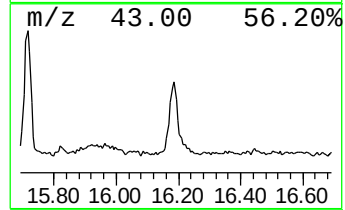
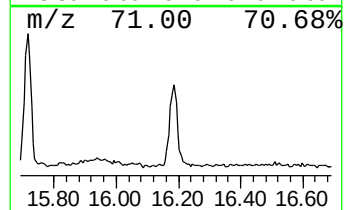
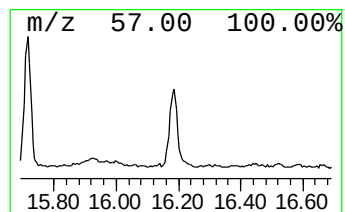
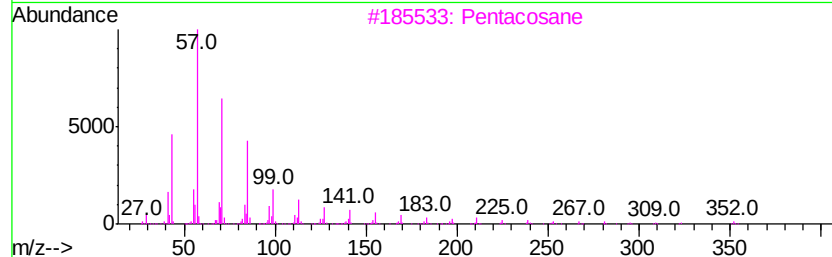
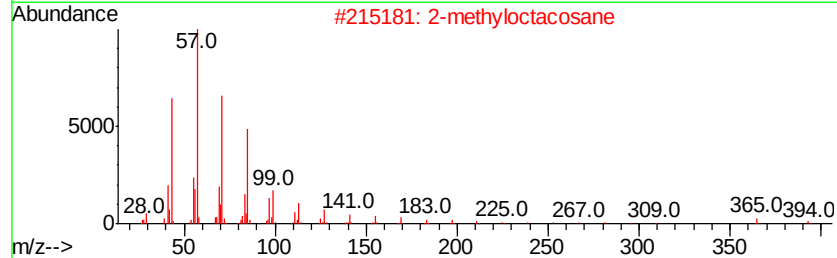
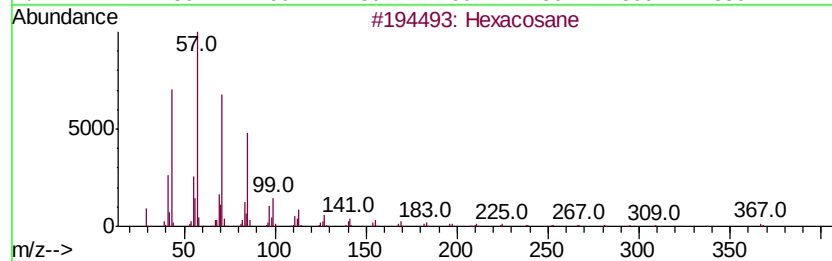
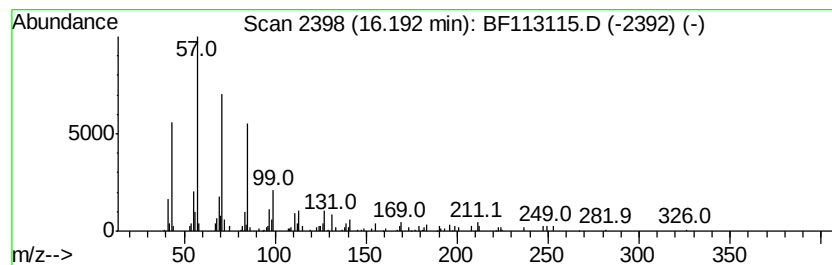
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	8.32 ng	231922	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	91
2	2-methyloctacosane	408 C29H60	1000376-72-8	91
3	Pentacosane	352 C25H52	000629-99-2	91
4	Tetracosane	338 C24H50	000646-31-1	91
5	Heptadecane	240 C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
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Acq On : 19 Mar 2019 3:13
Operator : JU/SJ
Sample : K1947-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

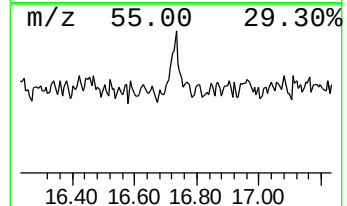
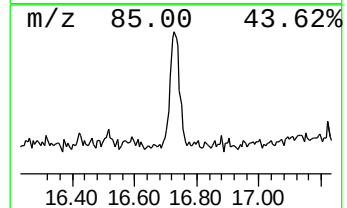
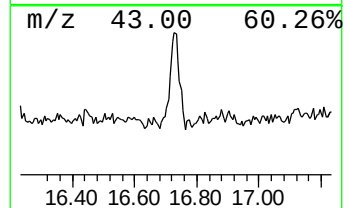
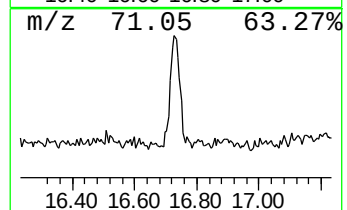
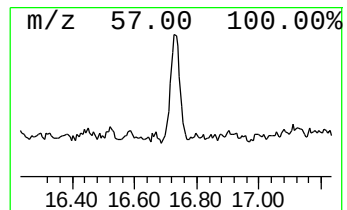
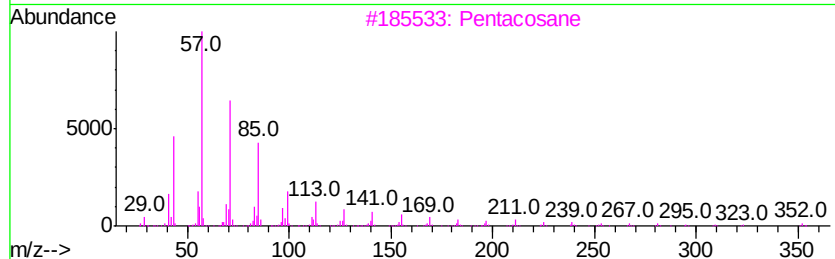
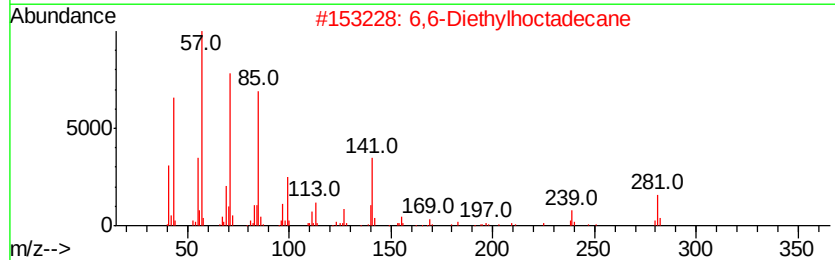
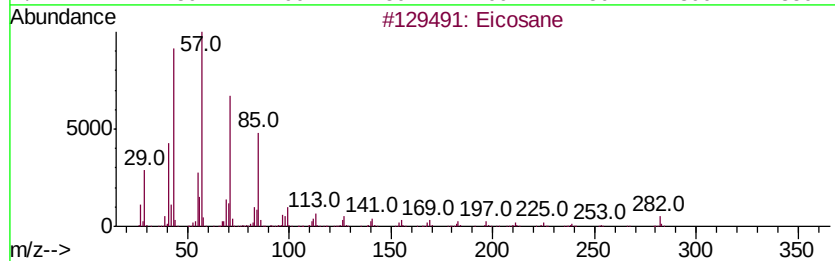
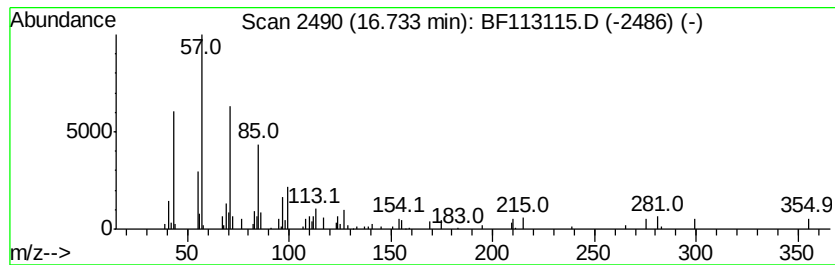
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.73	2.84 ng	79029	Perylene-d12		15.28		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	80
3			Pentacosane	352	C25H52	000629-99-2	74
4			Heptadecane	240	C17H36	000629-78-7	74
5			Octacosane	394	C28H58	000630-02-4	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
Data File : BF113115.D
Acq On : 19 Mar 2019 3:13
Operator : JU/SJ
Sample : K1947-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-025-B032-031319

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	86.9	ng	3921860	1	6.73	902524	20.0
n-Hexadecanoic acid	11.77	3.4	ng	139139	4	11.24	811788	20.0
3-Chloropropionic...	12.37	3.0	ng	122432	4	11.24	811788	20.0
1-Heneicosanol	13.79	8.5	ng	384079	5	13.87	903795	20.0
Eicosane	14.34	2.9	ng	131635	5	13.87	903795	20.0
Heptadecane	14.64	8.0	ng	222498	6	15.28	557291	20.0
Heneicosane	14.96	9.3	ng	259649	6	15.28	557291	20.0
Hexacosane	15.72	8.9	ng	248538	6	15.28	557291	20.0
Pentacosane	16.19	8.3	ng	231922	6	15.28	557291	20.0
Octacosane	16.73	2.8	ng	79029	6	15.28	557291	20.0