

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
 Data File : BF121726.D
 Acq On : 29 Sep 2020 12:29
 Operator : JU/CG
 Sample : L4158-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-1

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-BF091020.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	5.404	560	564	567	rBV	2500348	2307884	33.04%	6.306%
2	6.416	732	736	745	rBV	2383100	2414904	34.57%	6.599%
3	6.781	795	798	802	rBV	1009739	777732	11.13%	2.125%
4	7.345	889	894	897	rBV	1822420	1643163	23.52%	4.490%
5	8.063	1012	1016	1020	rBV	1201792	1015588	14.54%	2.775%
6	9.139	1194	1199	1203	rBV	2887370	2695387	38.59%	7.365%
7	9.533	1262	1266	1270	rBV	277005	223317	3.20%	0.610%
8	9.822	1310	1315	1318	rBV	1181534	1131024	16.19%	3.091%
9	10.604	1444	1448	1458	rBV	1336523	1200182	17.18%	3.280%
10	11.304	1563	1567	1570	rBV	1297355	1127912	16.15%	3.082%
11	11.845	1652	1659	1681	rBV	1213109	2147337	30.74%	5.868%
12	12.157	1708	1712	1717	rVB2	82201	96010	1.37%	0.262%
13	12.486	1737	1768	1786	rBV2	1031135	6984994	100.00%	19.087%
14	12.627	1786	1792	1803	rVB	1270606	1688458	24.17%	4.614%
15	12.886	1832	1836	1840	rVB	2744987	2597948	37.19%	7.099%
16	13.804	1988	1992	2005	rVV	275552	510686	7.31%	1.395%
17	13.939	2006	2015	2028	rVB2	1890584	3617666	51.79%	9.885%
18	14.410	2092	2095	2097	rBV	96931	83838	1.20%	0.229%
19	14.498	2097	2110	2118	rVV10	140289	732629	10.49%	2.002%
20	14.710	2142	2146	2148	rBV	143401	139867	2.00%	0.382%
21	14.757	2148	2154	2167	rVB2	412999	945551	13.54%	2.584%
22	15.039	2198	2202	2209	rVB	161013	181711	2.60%	0.497%
23	15.380	2255	2260	2263	rBV	688499	831948	11.91%	2.273%
24	15.521	2273	2284	2292	rBV5	110013	414016	5.93%	1.131%
25	15.604	2294	2298	2311	rVB3	127203	350136	5.01%	0.957%
26	15.827	2331	2336	2341	rBV	96315	137107	1.96%	0.375%
27	16.598	2462	2467	2478	rVB3	52095	147480	2.11%	0.403%
28	17.650	2638	2646	2656	rBV4	74337	258900	3.71%	0.707%
29	18.268	2743	2751	2760	rVB3	64212	192896	2.76%	0.527%

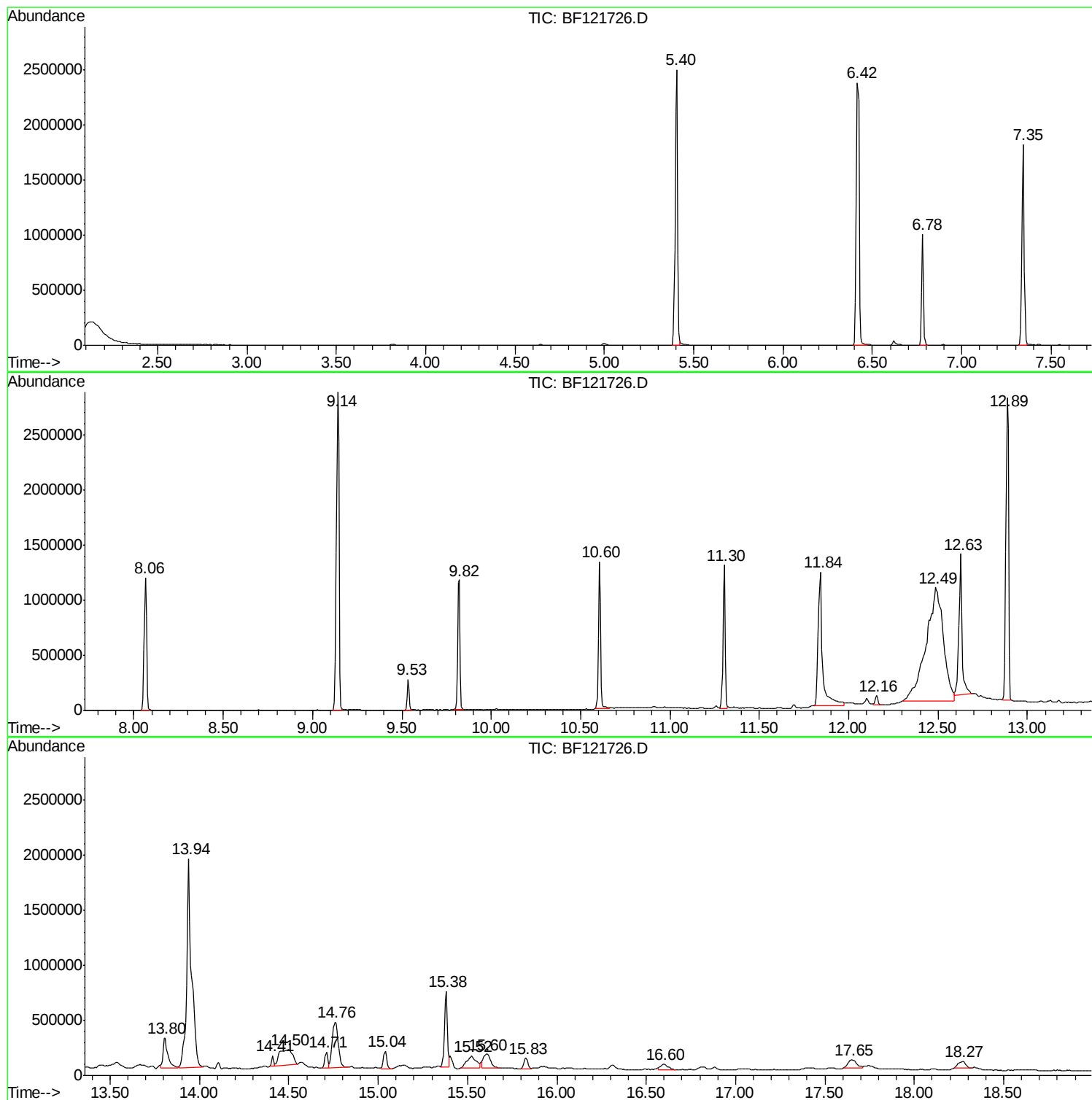
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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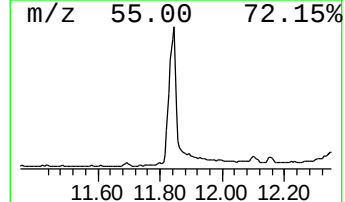
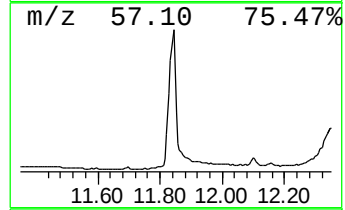
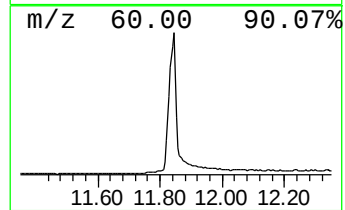
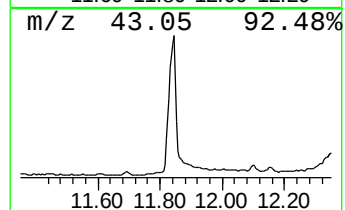
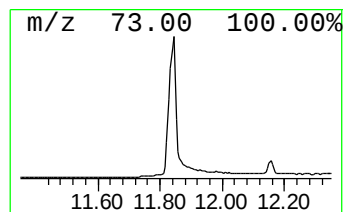
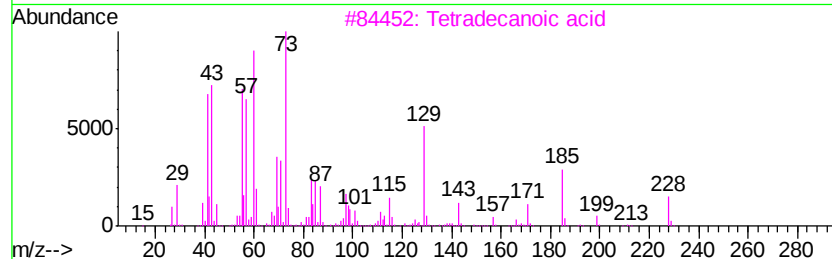
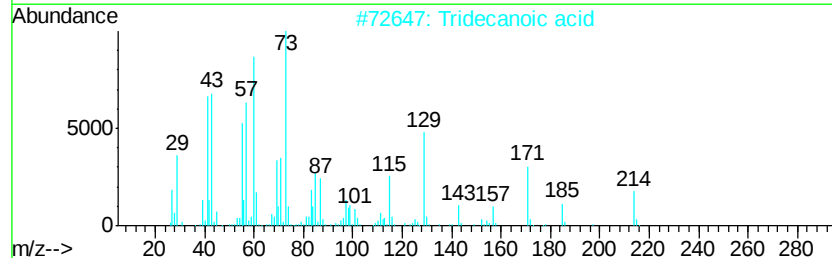
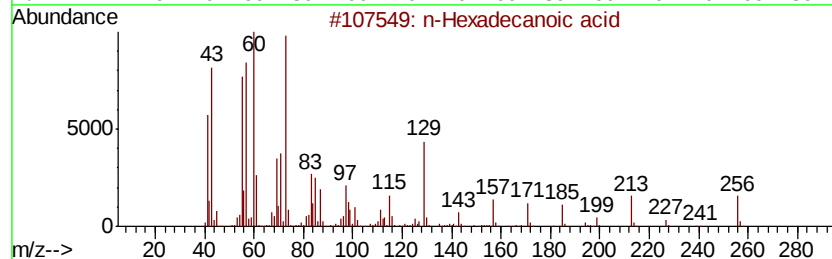
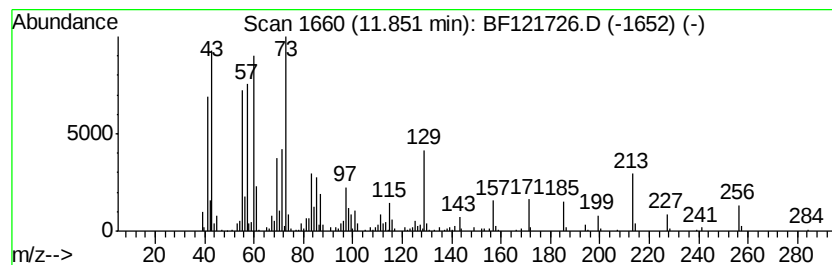
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	38.08 ng	2147340	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	25



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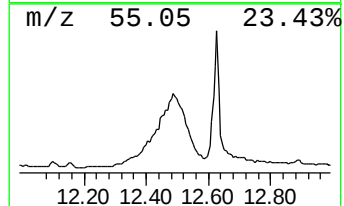
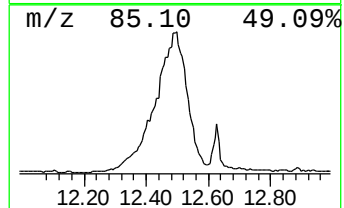
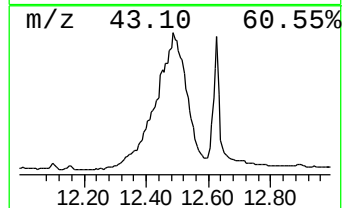
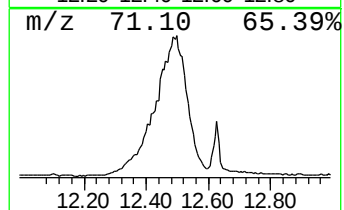
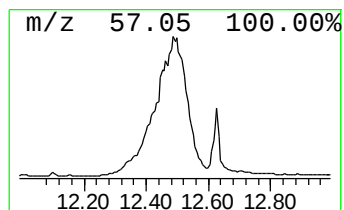
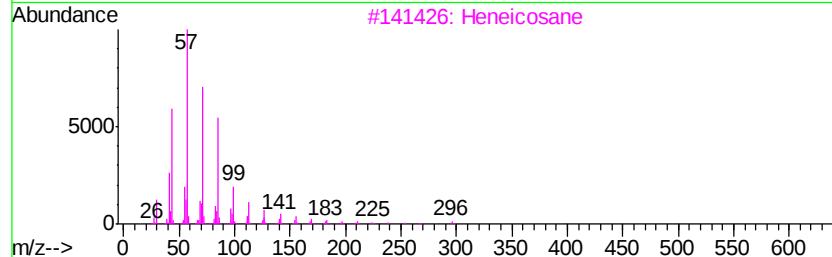
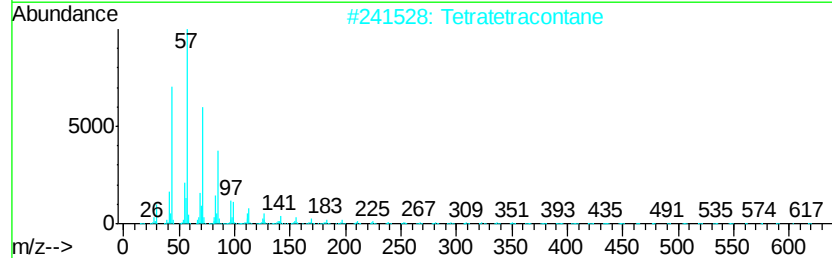
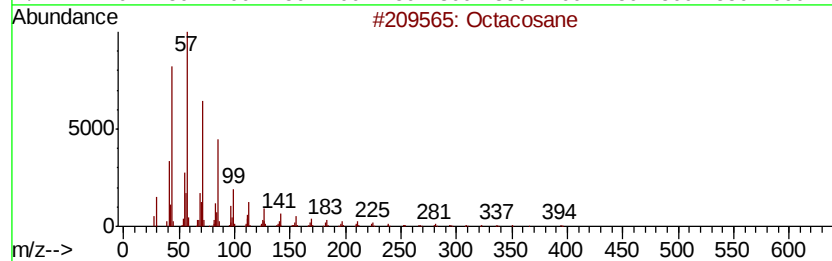
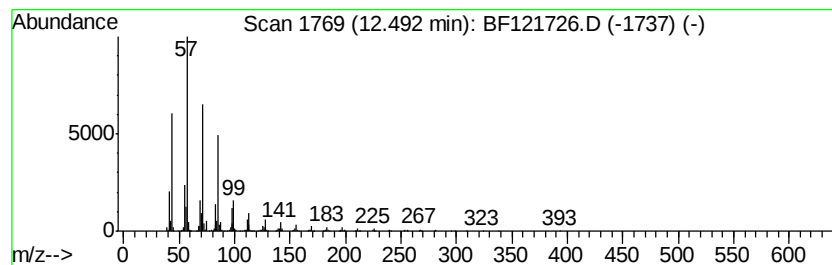
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Peak Number 2 Octacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	123.86 ng	6984990	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Tetratetracontane		619	C44H90	007098-22-8	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91



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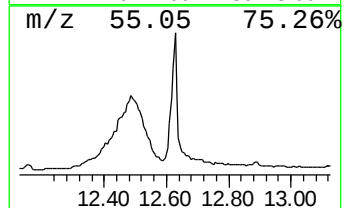
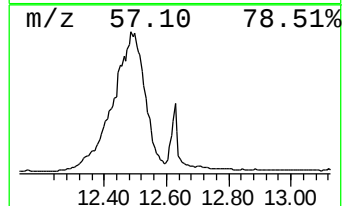
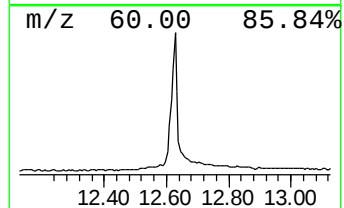
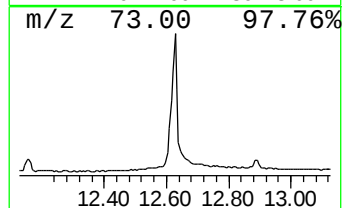
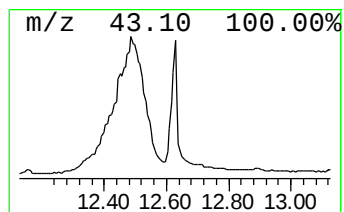
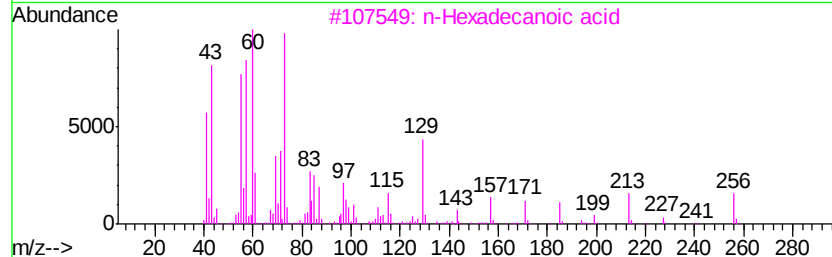
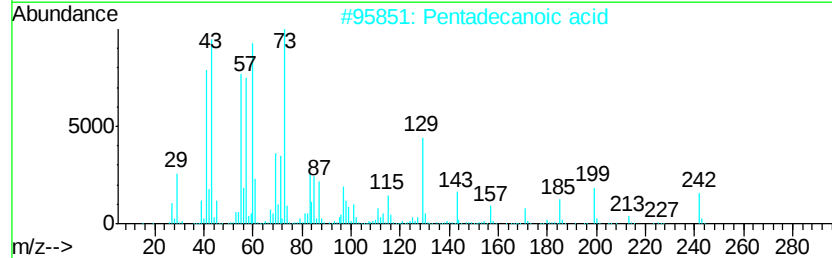
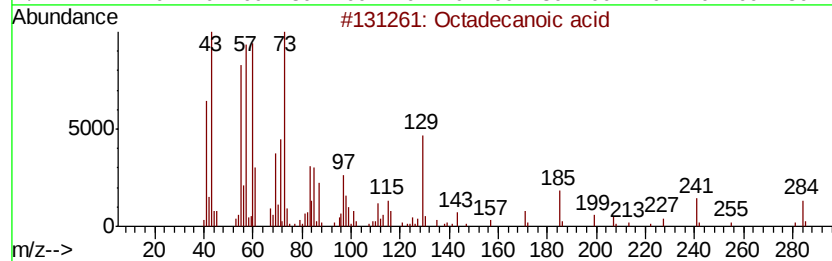
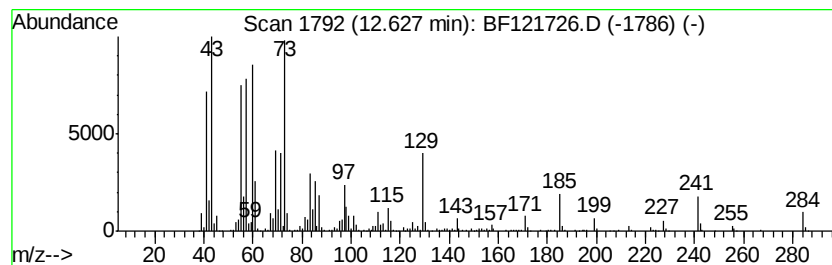
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 Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.63	9.33 ng	1688460	Chrysene-d12		13.94	
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		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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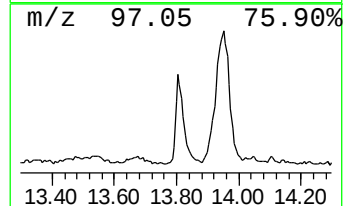
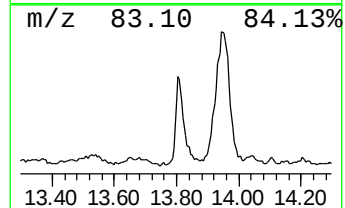
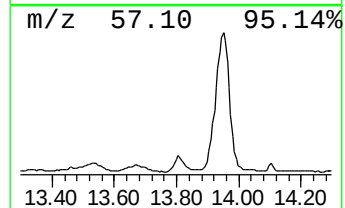
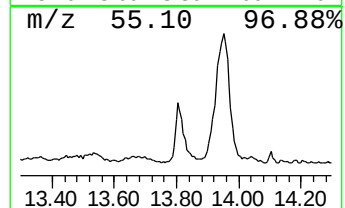
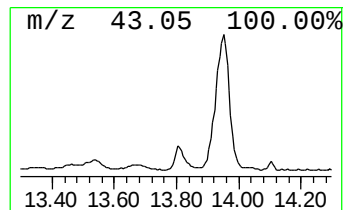
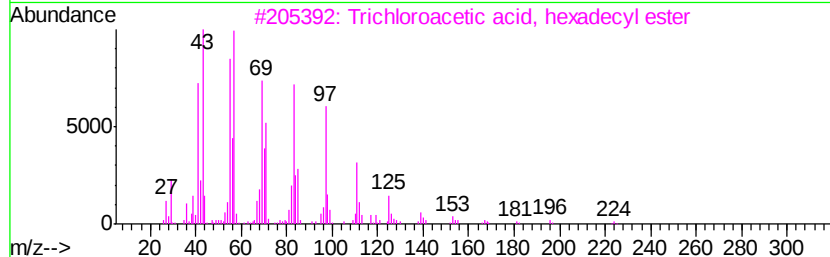
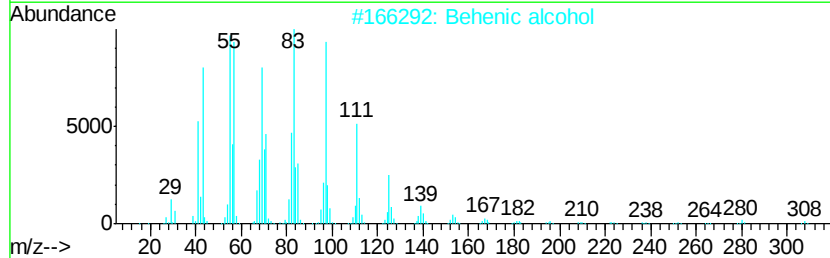
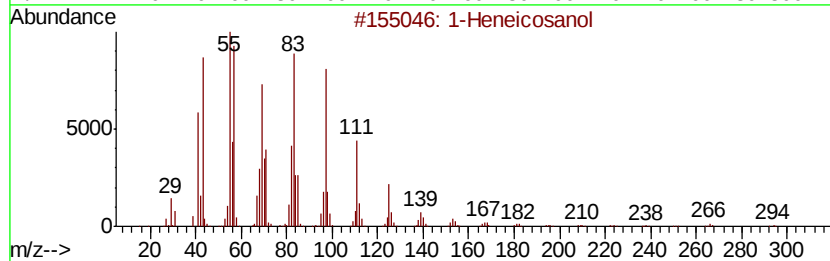
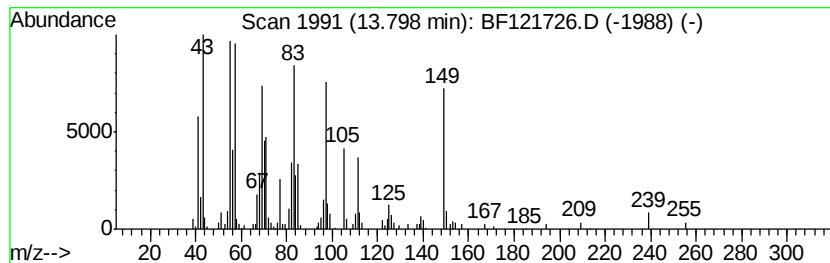
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Peak Number 4 1-Heneicosanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.82 ng	510686	Chrysene-d12	13.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	93
2	Behenic alcohol	326 C22H46O	000661-19-8	93
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	91
4	1-Docosene	308 C22H44	001599-67-3	89
5	n-Tetracosanol-1	354 C24H50O	000506-51-4	89



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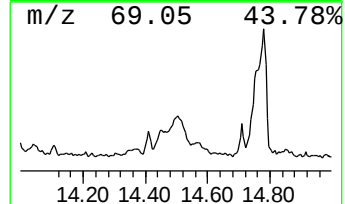
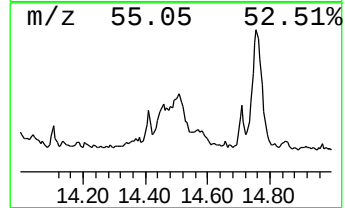
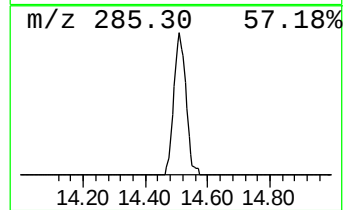
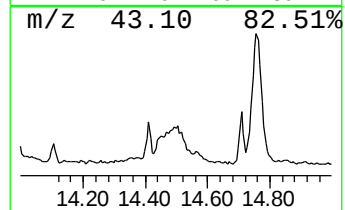
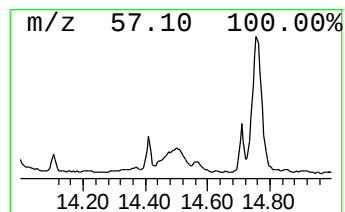
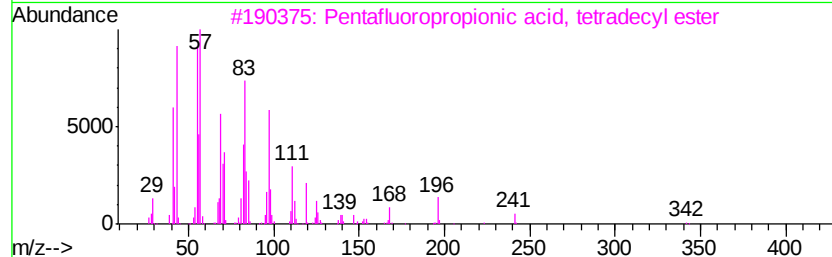
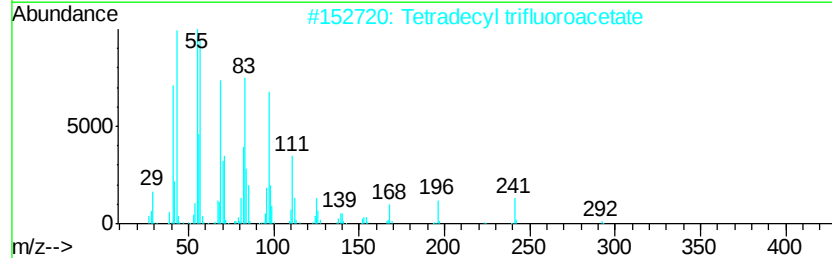
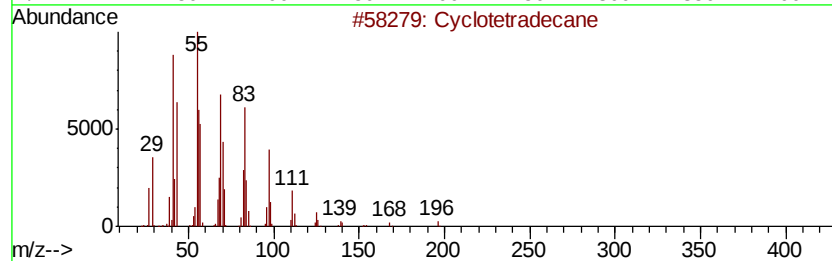
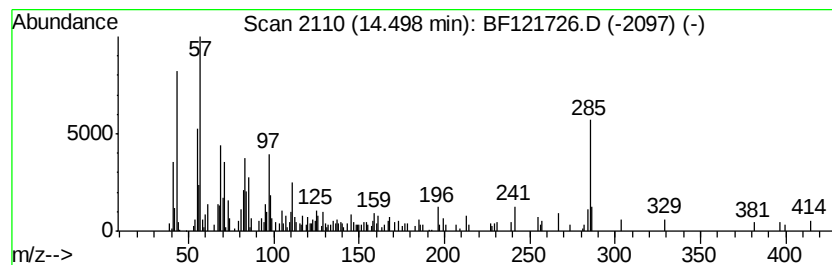
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Cyclotetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	4.05 ng	732629	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetradecane	196	C14H28	000295-17-0	72
2		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	55
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	50
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	50
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	46



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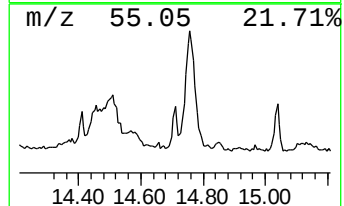
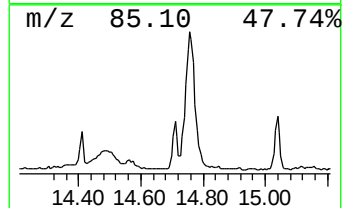
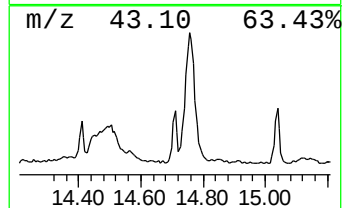
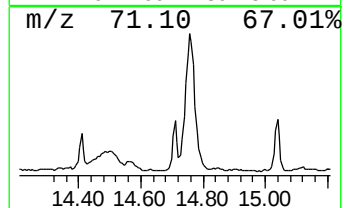
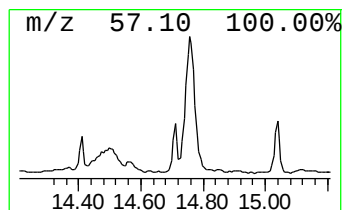
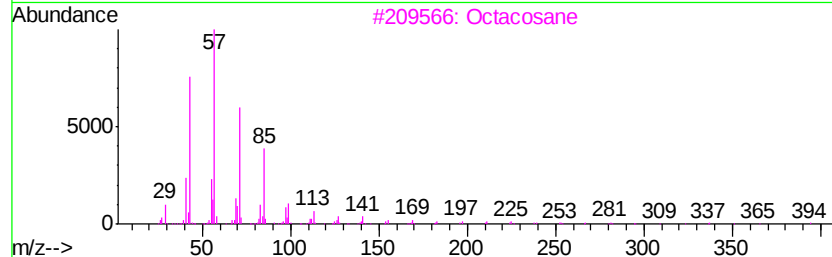
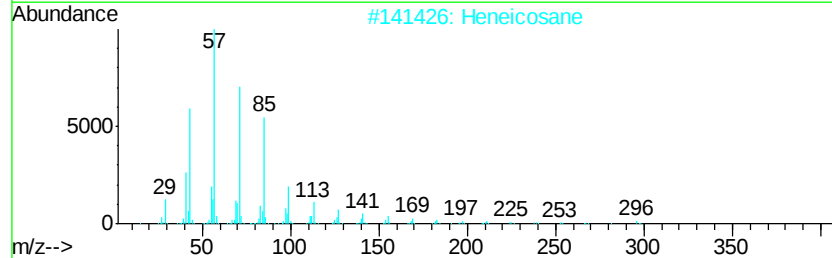
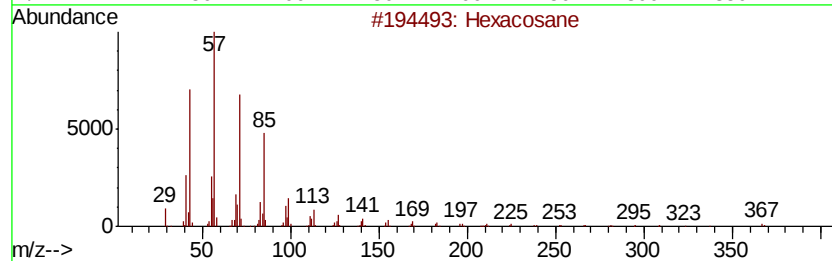
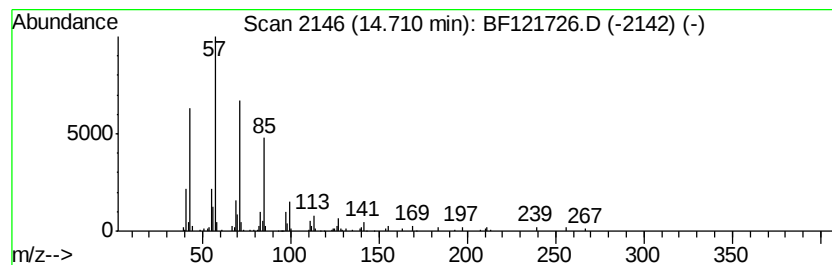
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.36 ng	139867	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
Data File : BF121726.D
Acq On : 29 Sep 2020 12:29
Operator : JU/CG
Sample : L4158-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-1-1

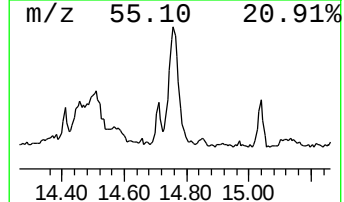
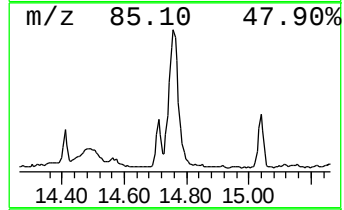
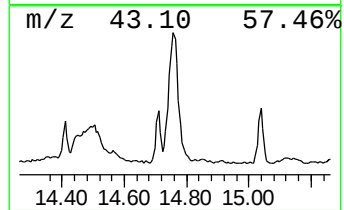
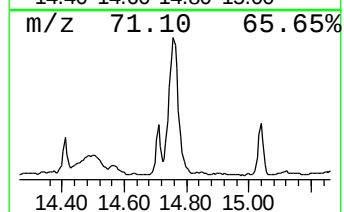
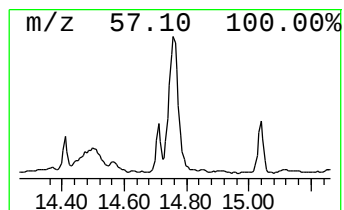
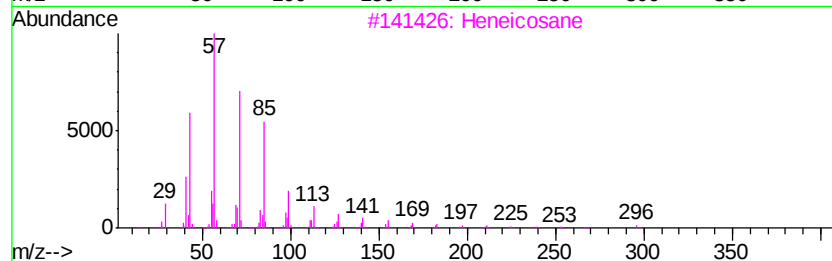
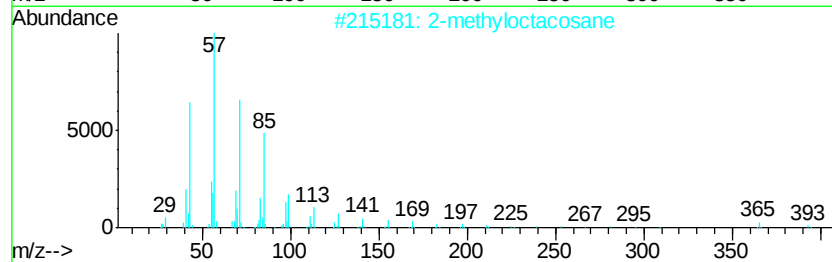
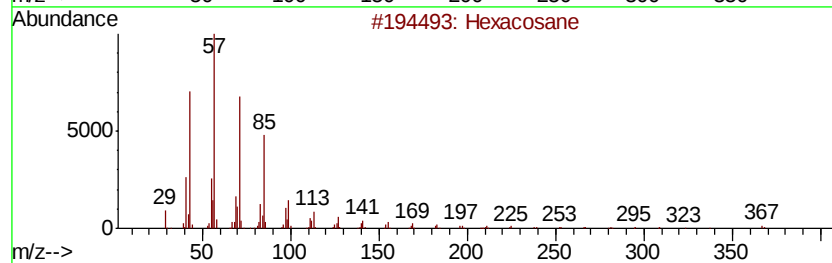
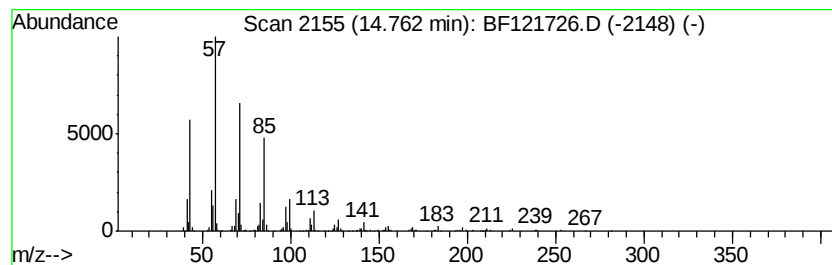
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	22.73 ng	945551	Perylene-d12	15.38

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		Tetratetracontane	619	C44H90	007098-22-8	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
Data File : BF121726.D
Acq On : 29 Sep 2020 12:29
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ALS Vial : 5 Sample Multiplier: 1

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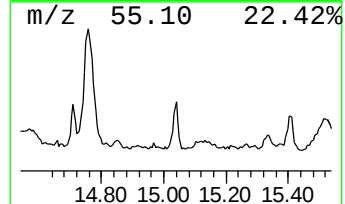
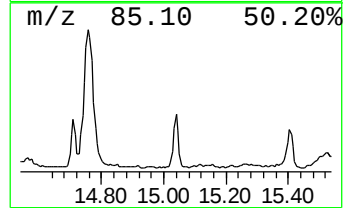
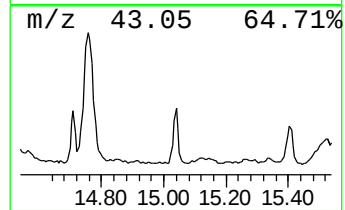
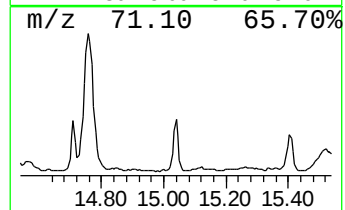
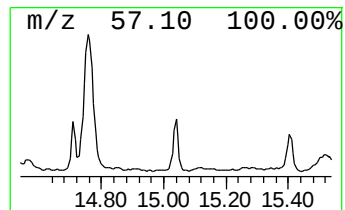
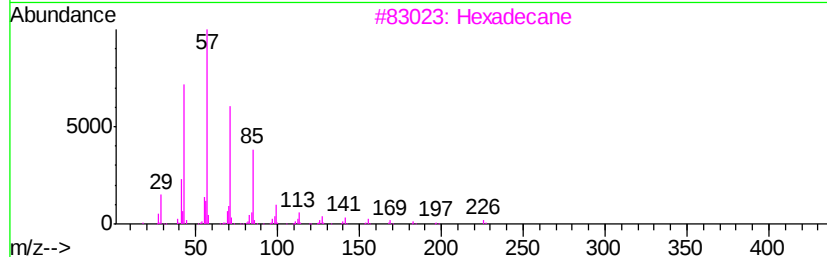
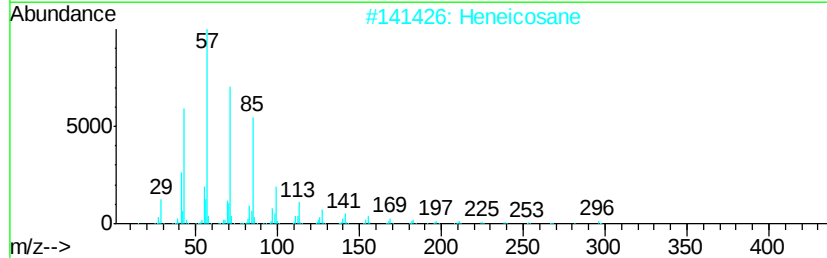
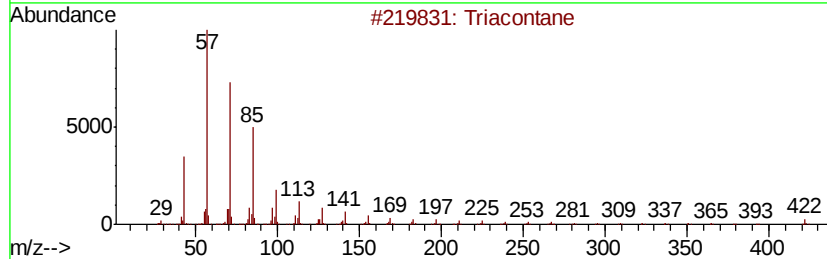
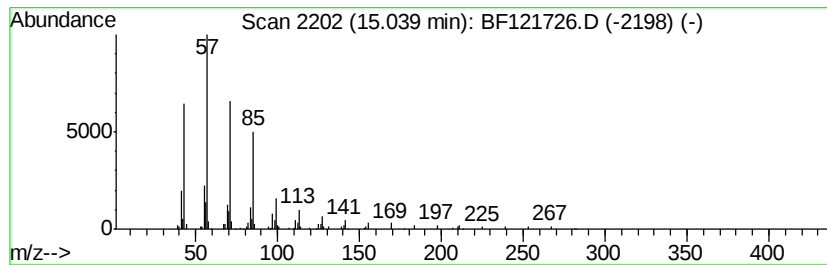
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.37 ng	181711	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
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Sample : L4158-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

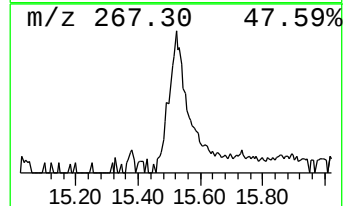
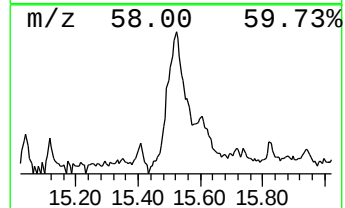
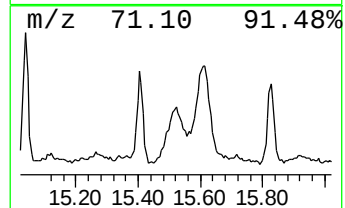
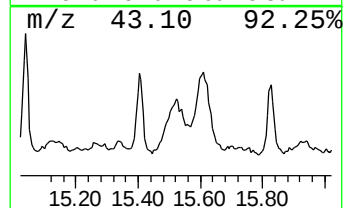
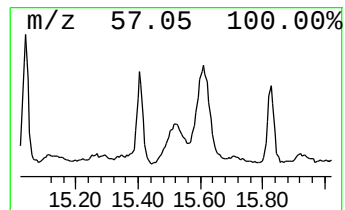
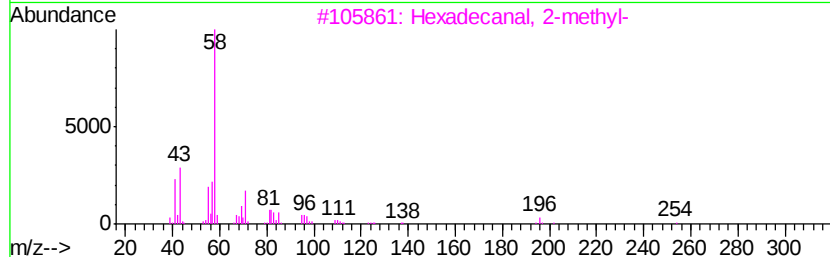
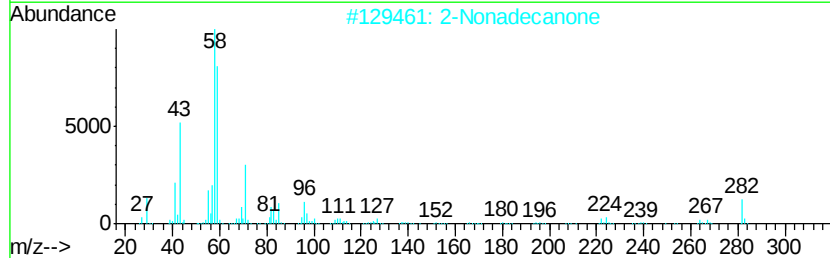
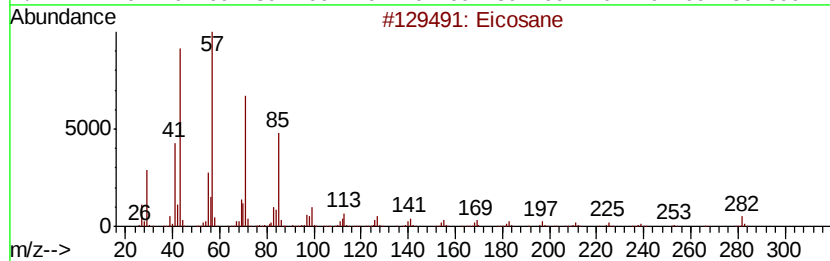
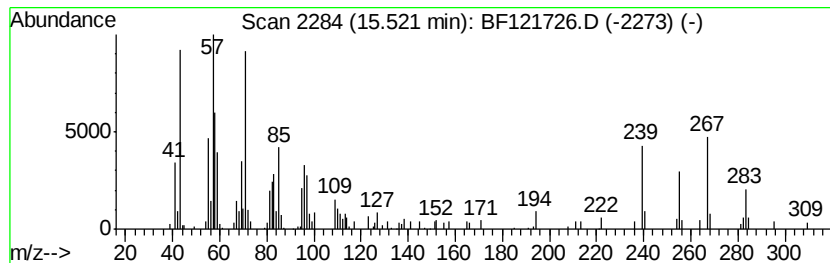
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.52	9.95 ng	414016	Perylene-d12	15.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	46
2	2-Nonadecanone	282	C19H38O	000629-66-3	38
3	Hexadecanal, 2-methyl-	254	C17H34O	055019-46-0	30
4	Tritetracontane	605	C43H88	007098-21-7	27
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
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Misc :
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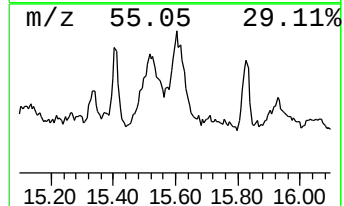
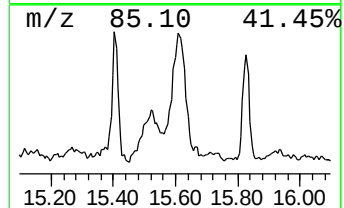
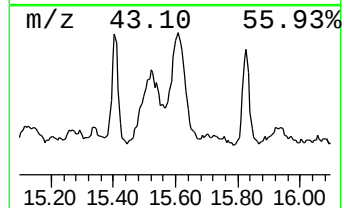
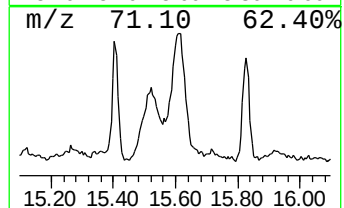
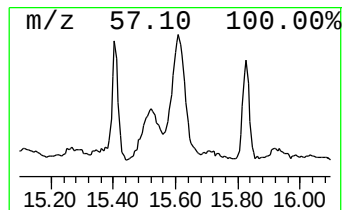
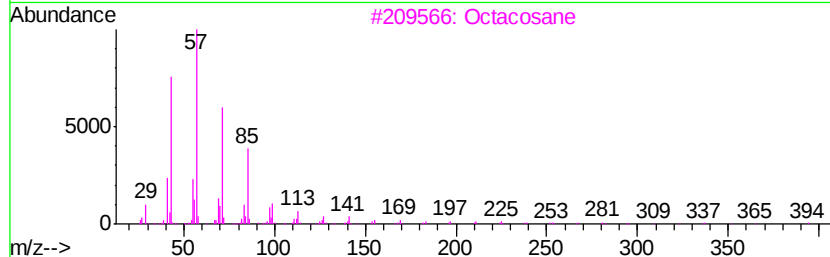
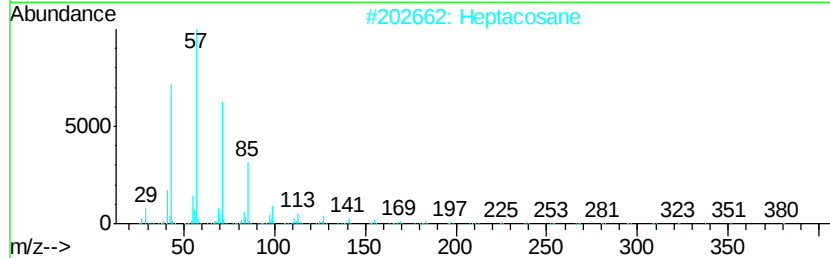
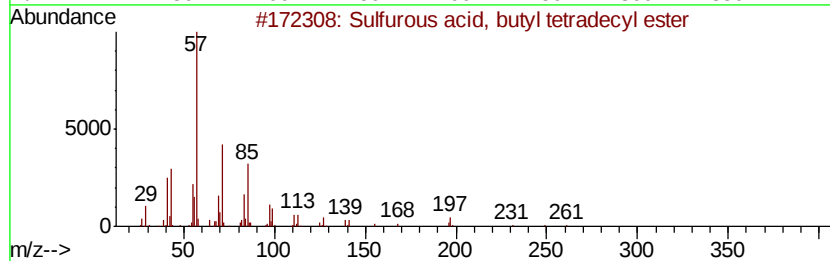
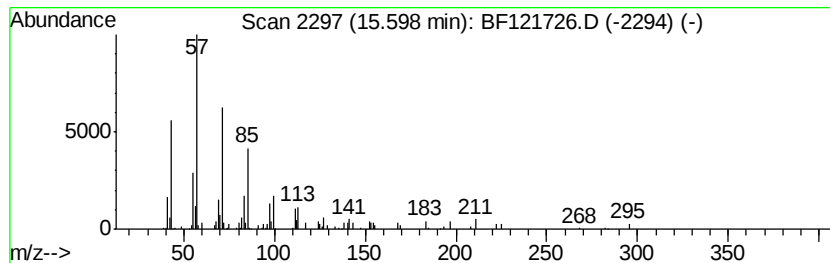
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, butyl tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	8.42 ng	350136	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
2		Heptacosane	380	C27H56	000593-49-7	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Docosane	310	C22H46	000629-97-0	86
5		Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
Data File : BF121726.D
Acq On : 29 Sep 2020 12:29
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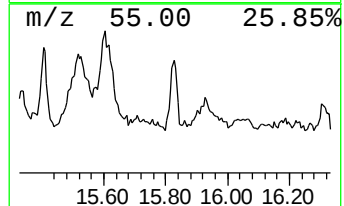
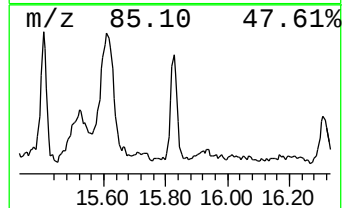
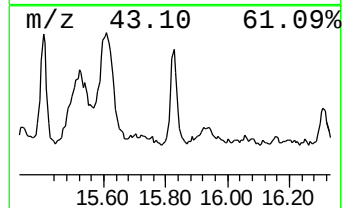
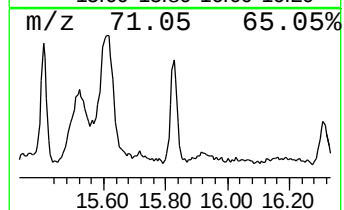
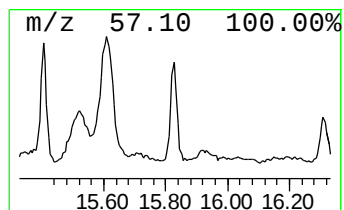
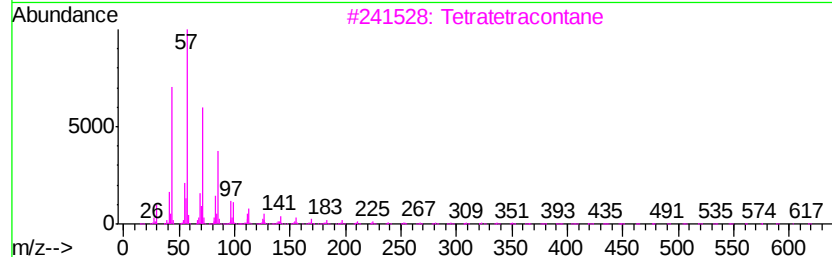
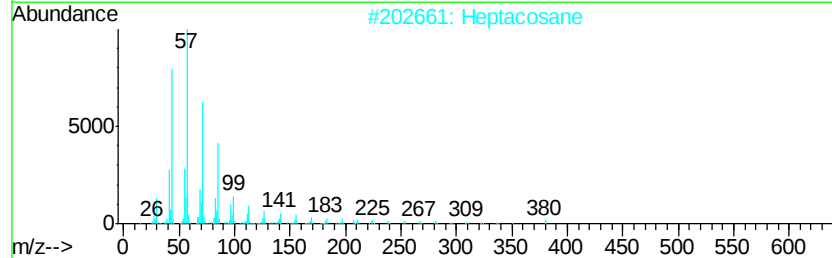
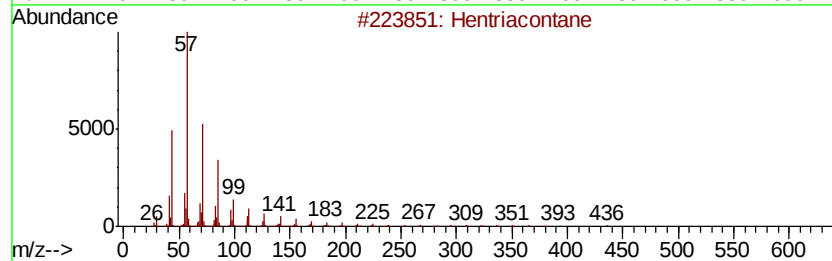
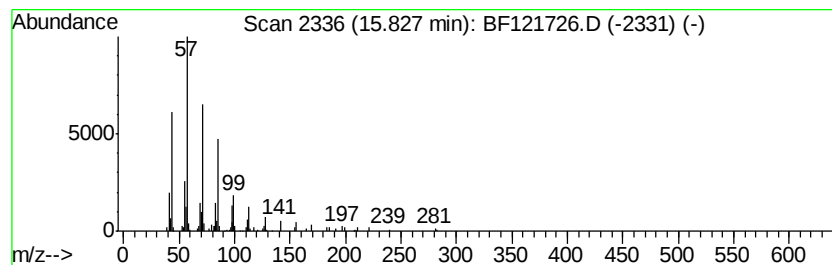
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.30 ng	137107	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Octacosane	394	C28H58	000630-02-4	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



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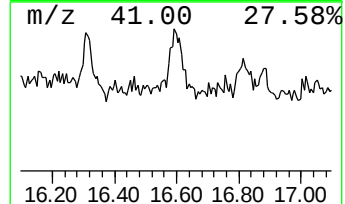
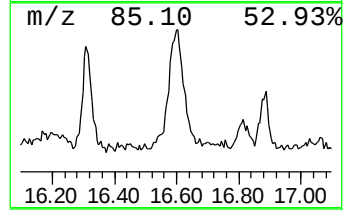
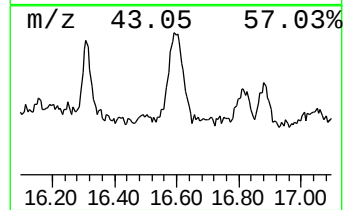
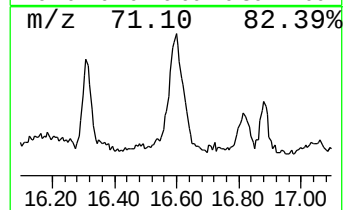
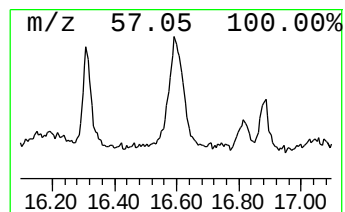
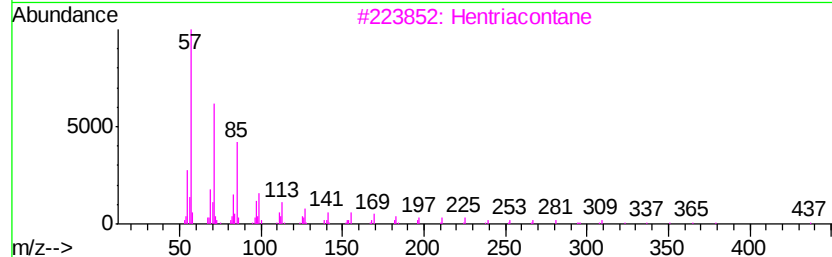
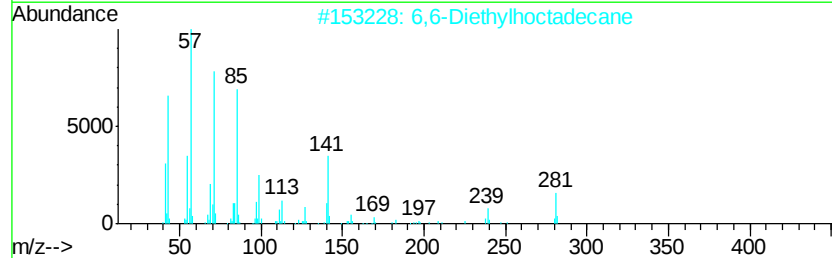
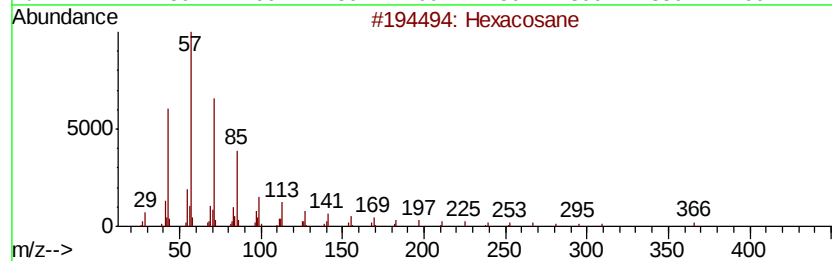
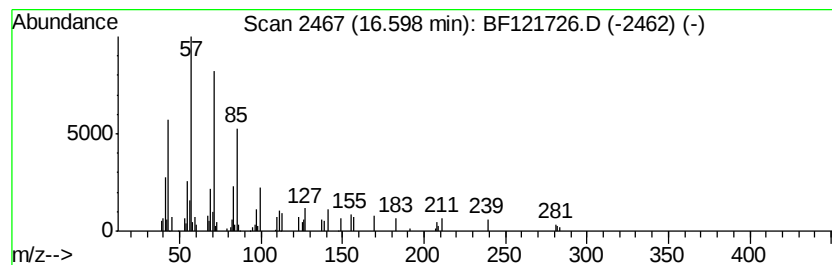
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 6,6-Diethylhooctadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.55 ng	147480	Perylene-d12	15.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	86
2	6,6-Diethylhooctadecane	310 C22H46	1000360-41-8	86
3	Hentriacontane	437 C31H64	000630-04-6	80
4	Tetracosane	338 C24H50	000646-31-1	72
5	Tetratriacontane	479 C34H70	014167-59-0	72



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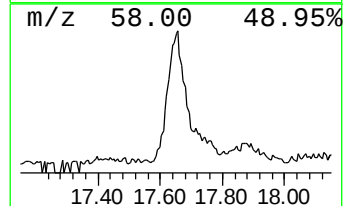
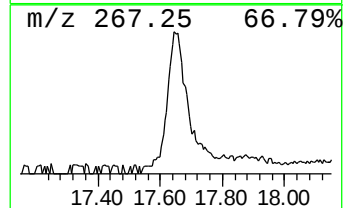
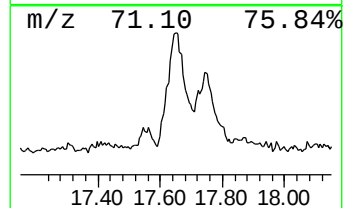
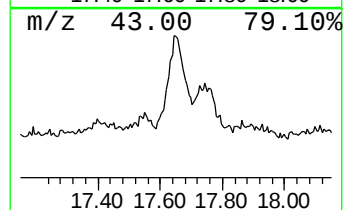
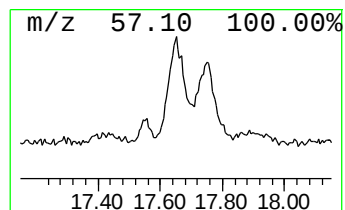
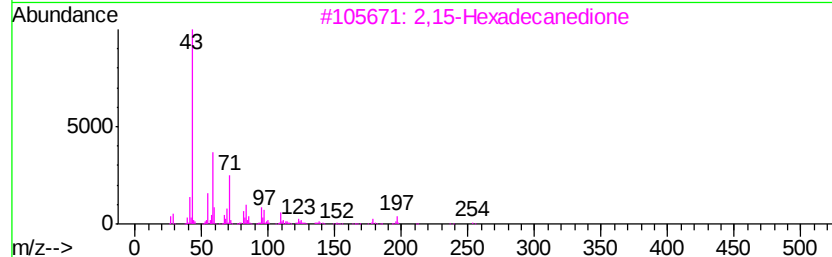
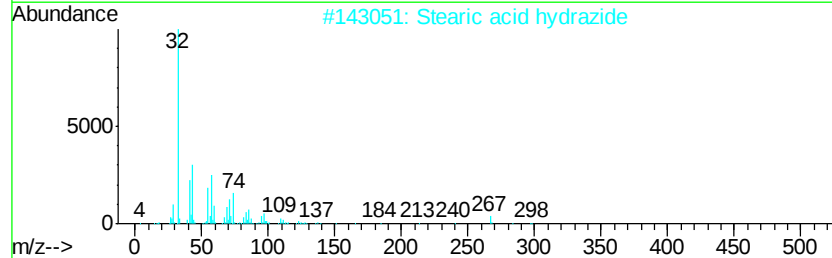
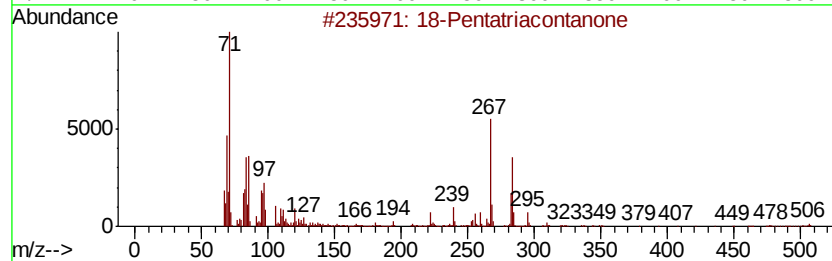
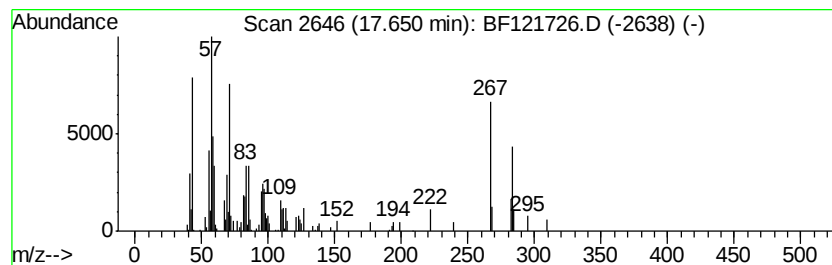
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 18-Pentatriacontanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	6.22 ng	258900	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	18-Pentatriacontanone	507	C35H70O	000504-53-0	91
2		Stearic acid hydrazide	298	C18H38N2O	004130-54-5	38
3		2,15-Hexadecanedione	254	C16H30O2	018650-13-0	35
4		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	22
5		1-Methylcycloheptanol	128	C8H16O	003761-94-2	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092920\
Data File : BF121726.D
Acq On : 29 Sep 2020 12:29
Operator : JU/CG
Sample : L4158-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-1

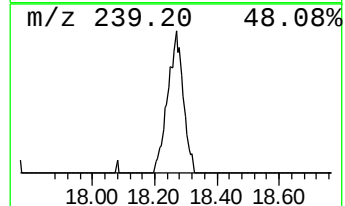
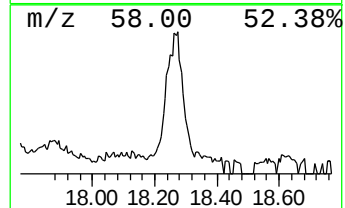
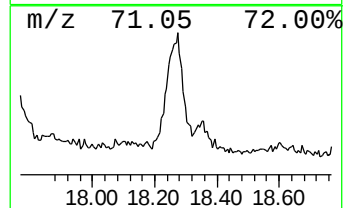
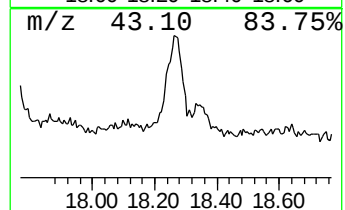
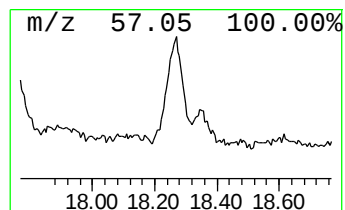
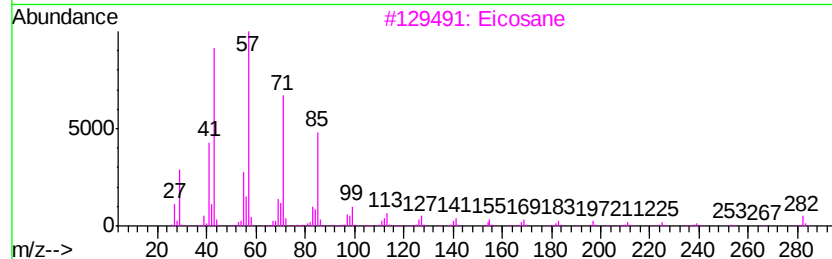
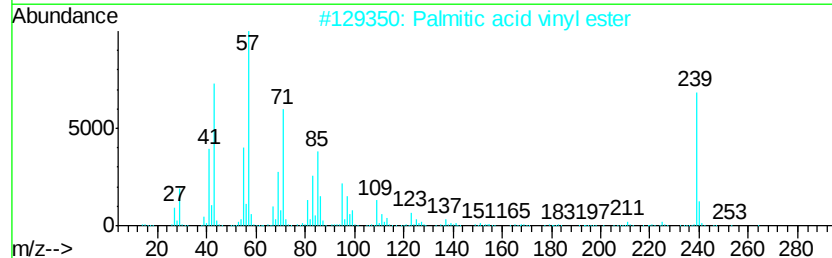
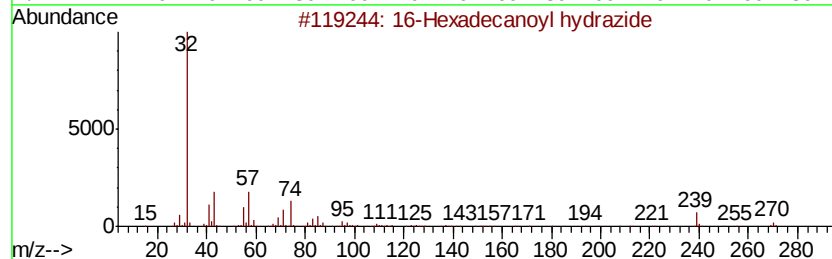
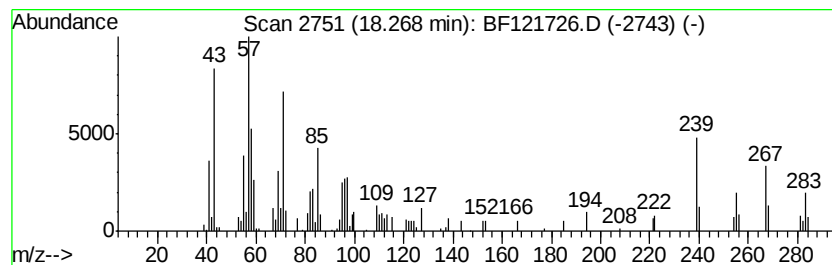
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.27 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	4.64 ng	192896	Perylene-d12	15.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Hexadecanoyl	hydrazide	270	C16H34N2O	002619-88-7	38	
2	Palmitic acid	vinyl ester	282	C18H34O2	000693-38-9	22	
3	Eicosane		282	C20H42	000112-95-8	11	
4	2-methyltetra	cocosane	352	C25H52	1000376-72-6	11	
5	Octadecane		254	C18H38	000593-45-3	11	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092920\
 Data File : BF121726.D
 Acq On : 29 Sep 2020 12:29
 Operator : JU/CG
 Sample : L4158-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
n-Hexadecanoic acid	11.85	38.1 ng		2147340	4	11.30	1127910	20.0
Octacosane	12.49	123.9 ng		6984990	4	11.30	1127910	20.0
Octadecanoic acid	12.63	9.3 ng		1688460	5	13.94	3617670	20.0
1-Heneicosanol	13.80	2.8 ng		510686	5	13.94	3617670	20.0
Cyclotetradecane	14.50	4.0 ng		732629	5	13.94	3617670	20.0
Heneicosane	14.71	3.4 ng		139867	6	15.38	831948	20.0
Hexacosane	14.76	22.7 ng		945551	6	15.38	831948	20.0
triacontane	15.04	4.4 ng		181711	6	15.38	831948	20.0
unknown15.52	15.52	9.9 ng		414016	6	15.38	831948	20.0
Sulfurous acid, b...	15.60	8.4 ng		350136	6	15.38	831948	20.0
Hentriacontane	15.83	3.3 ng		137107	6	15.38	831948	20.0
6,6-Diethylhooctad...	16.60	3.5 ng		147480	6	15.38	831948	20.0
18-Pentatriaconta...	17.65	6.2 ng		258900	6	15.38	831948	20.0
unknown18.27	18.27	4.6 ng		192896	6	15.38	831948	20.0