

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
 Data File : BF109106.D
 Acq On : 18 Sep 2018 20:02
 Operator : JU/SJ
 Sample : J4952-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2015-161-20-RB36584RT-RB47184R

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-BF091418.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	4.907	434	437	447	rVB	62903	74951	3.49%	0.334%
2	5.331	504	509	512	rBV	2026512	1783541	83.15%	7.948%
3	6.354	679	683	689	rBV	1873088	1967191	91.72%	8.767%
4	6.490	702	706	709	rBV	2228810	1884665	87.87%	8.399%
5	6.719	742	745	749	rBV	908458	769372	35.87%	3.429%
6	6.878	768	772	775	rBV	1963774	1534798	71.56%	6.840%
7	7.278	836	840	843	rBV	1339247	1159899	54.08%	5.169%
8	8.001	959	963	967	rBV	1176646	926414	43.19%	4.128%
9	9.078	1142	1146	1149	rBV	2686489	2144882	100.00%	9.558%
10	9.472	1209	1213	1216	rBV	307904	254444	11.86%	1.134%
11	9.754	1257	1261	1264	rBV	1041020	931574	43.43%	4.151%
12	10.536	1390	1394	1398	rBV	1172466	1102293	51.39%	4.912%
13	11.230	1508	1512	1514	rBV	961867	829804	38.69%	3.698%
14	11.248	1514	1515	1518	rVB	49835	35975	1.68%	0.160%
15	11.766	1600	1603	1607	rBV2	81706	91243	4.25%	0.407%
16	12.436	1714	1717	1720	rVB	103717	96210	4.49%	0.429%
17	12.660	1753	1755	1758	rVB	100278	80198	3.74%	0.357%
18	12.813	1777	1781	1784	rBV	2108810	1846744	86.10%	8.230%
19	13.060	1820	1823	1825	rVB	38685	32325	1.51%	0.144%
20	13.242	1852	1854	1856	rBV	32114	28887	1.35%	0.129%
21	13.719	1931	1935	1943	rBV2	258709	356211	16.61%	1.587%
22	13.854	1953	1958	1961	rBV	1397536	1322098	61.64%	5.892%
23	13.877	1961	1962	1965	rVB	113550	64326	3.00%	0.287%
24	14.042	1987	1990	1994	rBV	86415	81221	3.79%	0.362%
25	14.348	2039	2042	2047	rBV	240790	260132	12.13%	1.159%
26	14.642	2089	2092	2101	rVB	140920	180423	8.41%	0.804%
27	14.771	2111	2114	2118	rBV	115181	112685	5.25%	0.502%
28	14.860	2126	2129	2132	rBV	174960	236487	11.03%	1.054%
29	14.960	2142	2146	2148	rBV2	265919	289649	13.50%	1.291%
30	15.142	2174	2177	2182	rVB	126836	144963	6.76%	0.646%
31	15.201	2183	2187	2190	rVB	151035	173623	8.09%	0.774%
32	15.260	2193	2197	2201	rVV	730261	914670	42.64%	4.076%
33	15.313	2203	2206	2213	rVB	142801	179641	8.38%	0.801%
34	15.495	2234	2237	2241	rBV2	83459	99423	4.64%	0.443%

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Misc :
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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 >
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35	15.718	2271	2275	2279	rBV	234796	305101	14.22%	1.360%
36	16.607	2423	2426	2434	rVB3	85180	143764	6.70%	0.641%

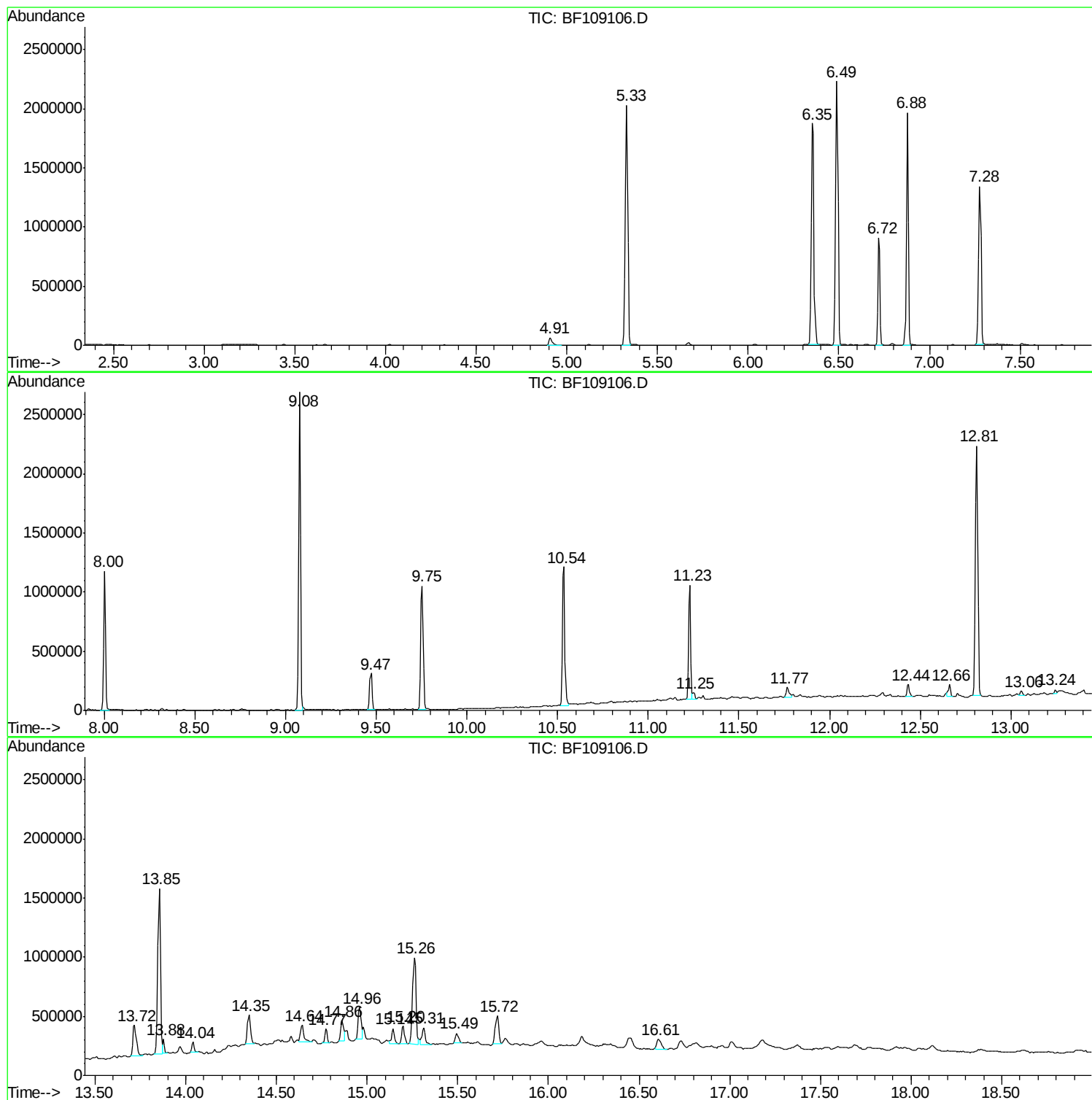
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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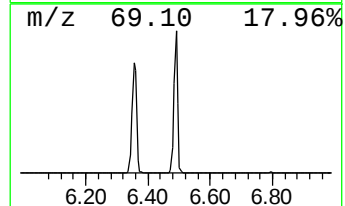
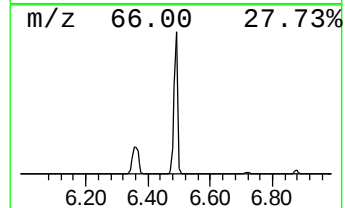
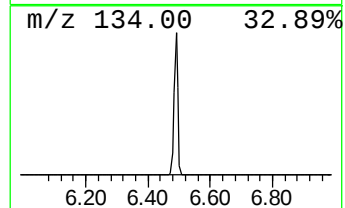
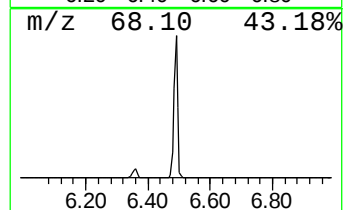
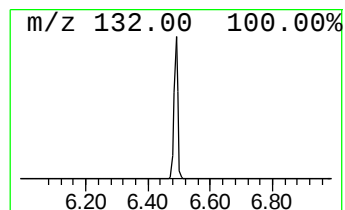
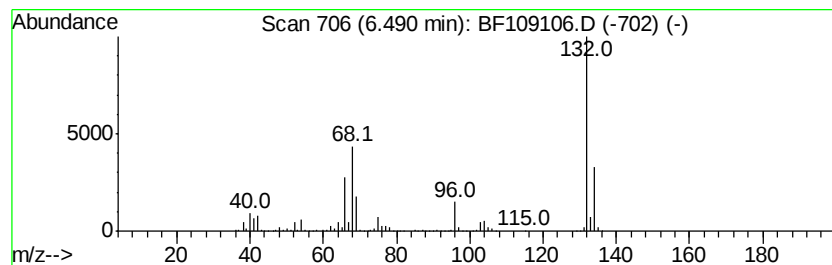
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	48.99 ng	1884670	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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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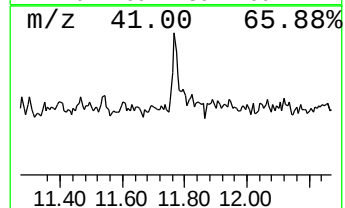
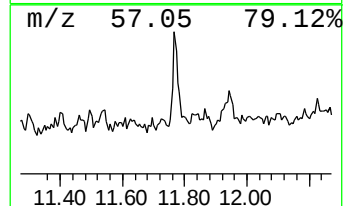
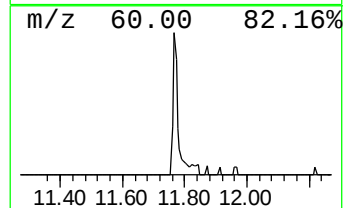
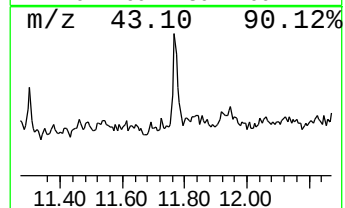
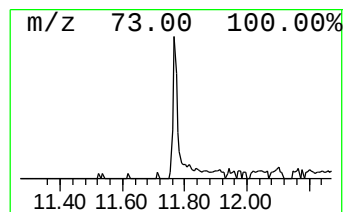
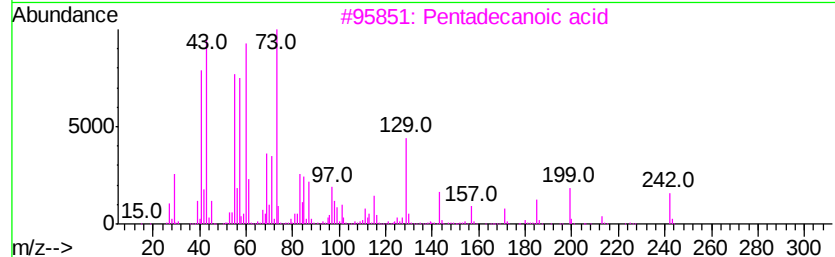
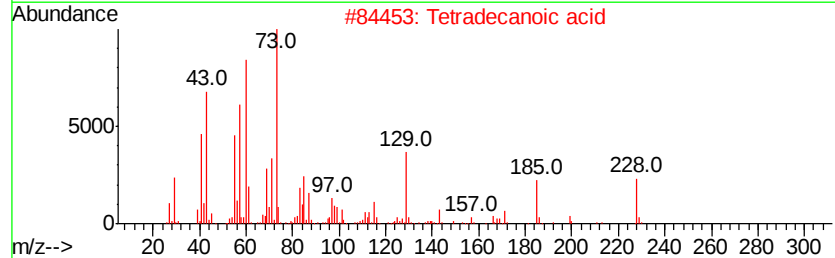
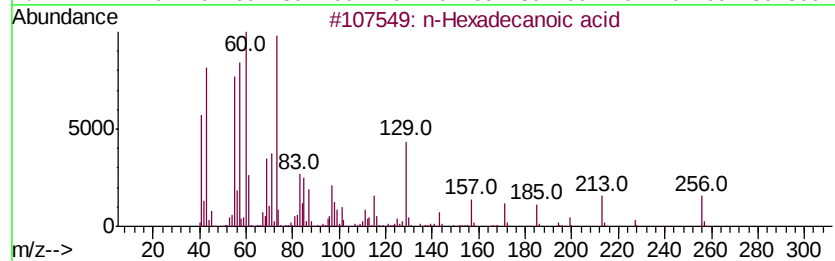
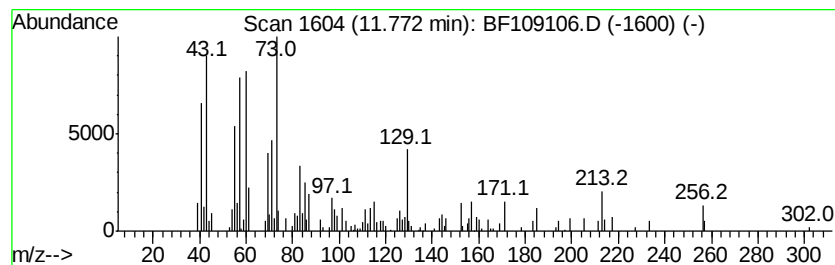
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	2.20 ng	91243	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	18
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	18



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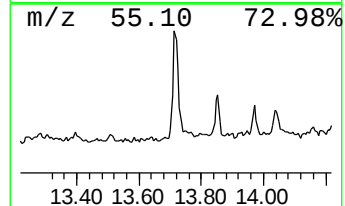
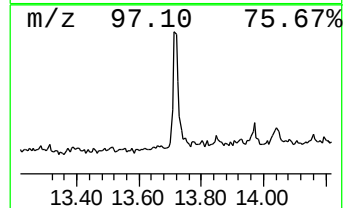
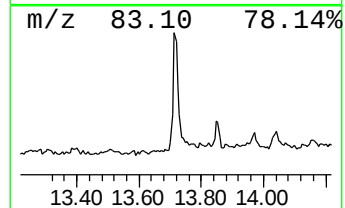
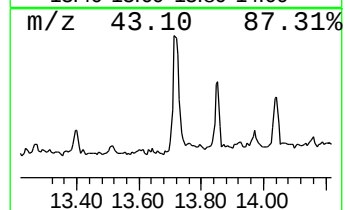
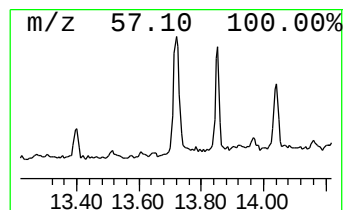
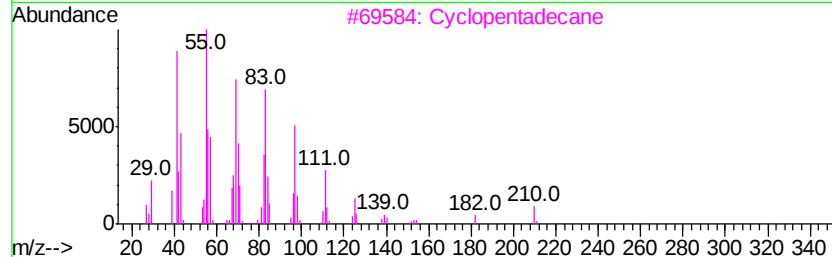
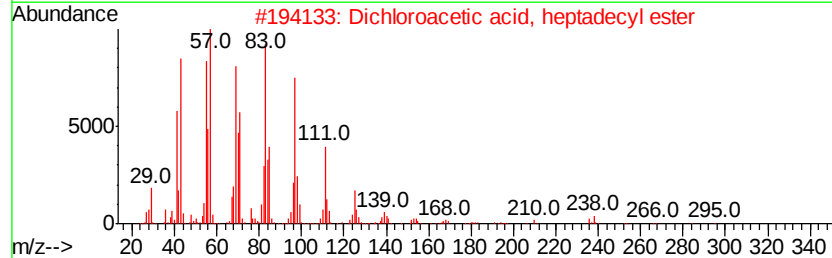
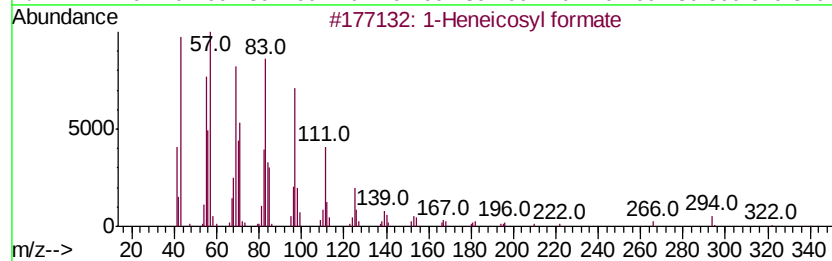
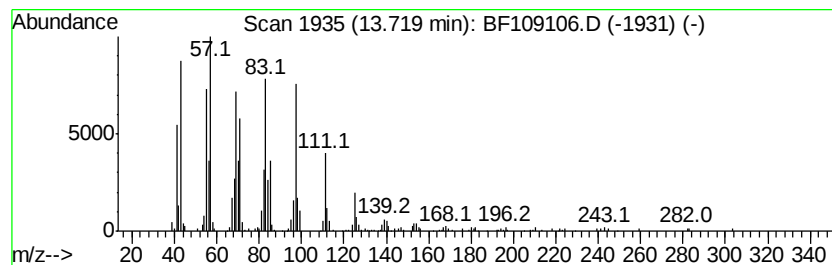
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	5.39 ng	356211	Chrysene-d12	13.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Cyclopentadecane	210	C15H30	000295-48-7	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94



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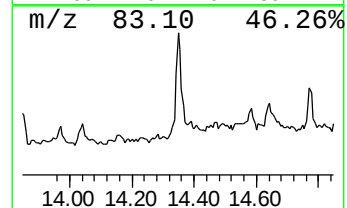
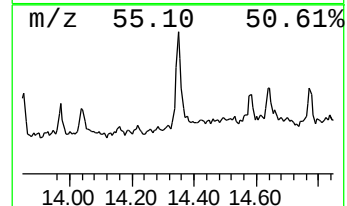
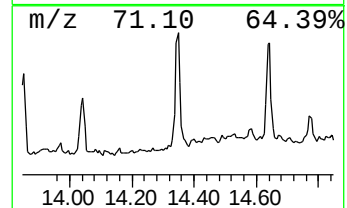
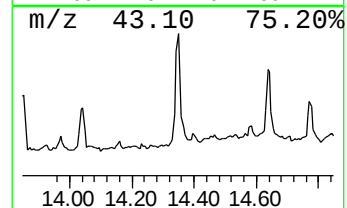
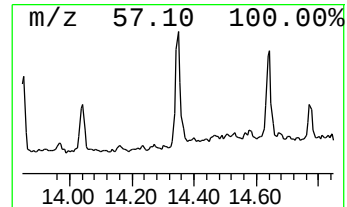
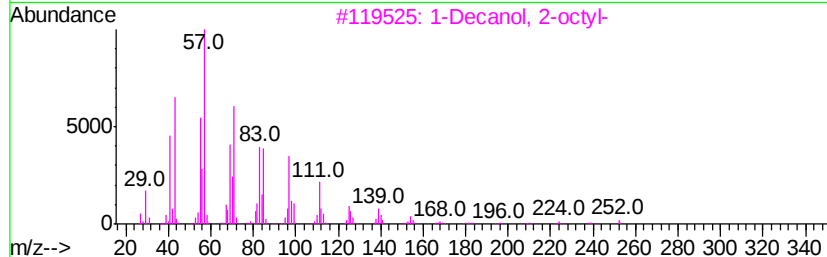
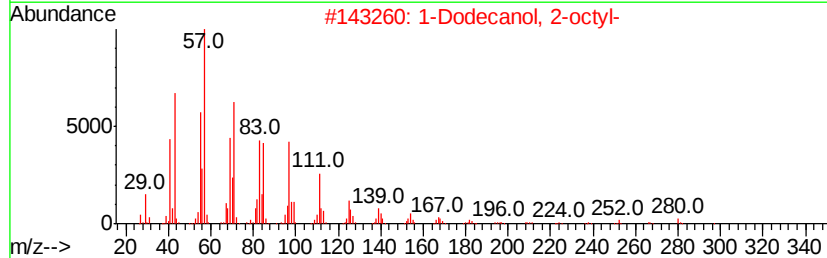
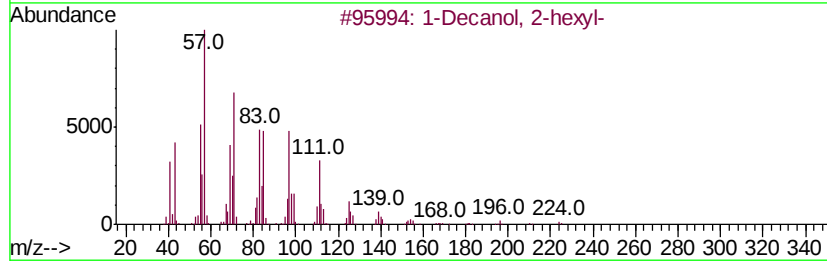
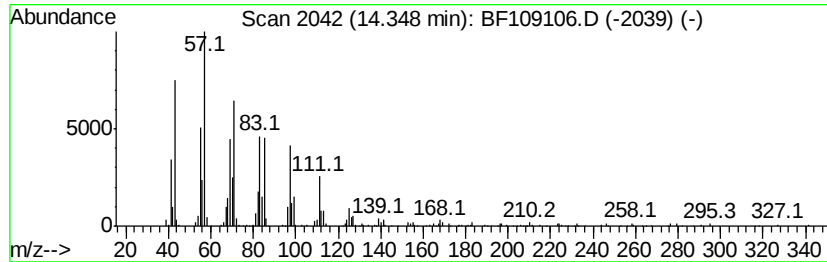
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.35	3.94 ng	260132	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	91
2	1-Dodecanol, 2-octyl-		298	C20H42O	005333-42-6	91
3	1-Decanol, 2-octyl-		270	C18H38O	045235-48-1	91
4	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	90
5	Dotriacontyl pentafluoropropionate		612	C35H65F5O2	1000351-81-4	87



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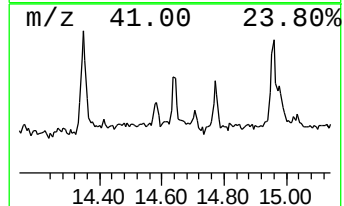
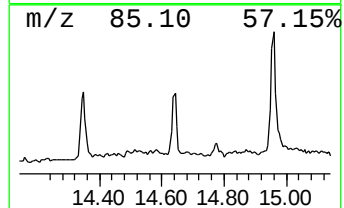
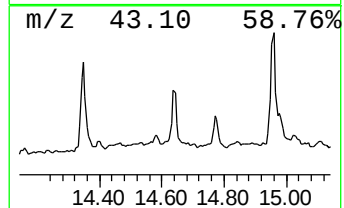
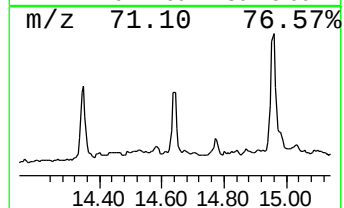
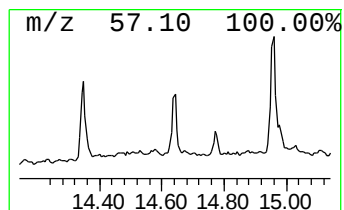
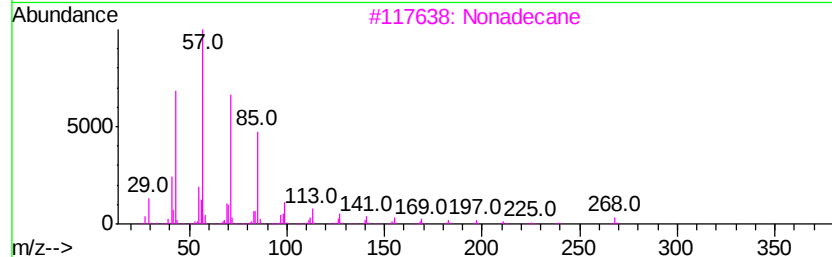
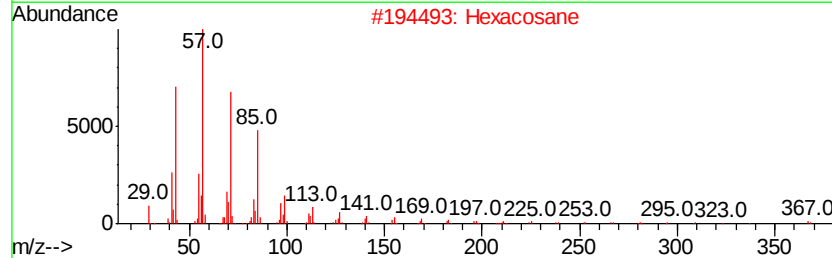
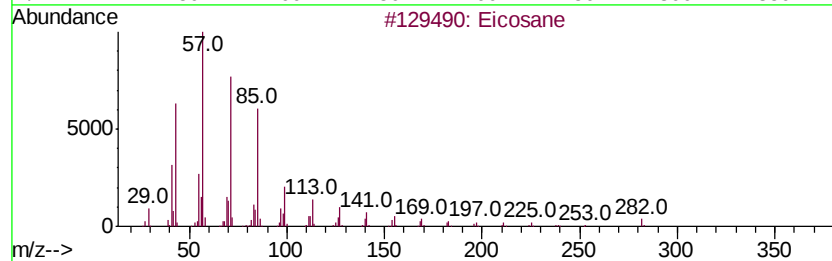
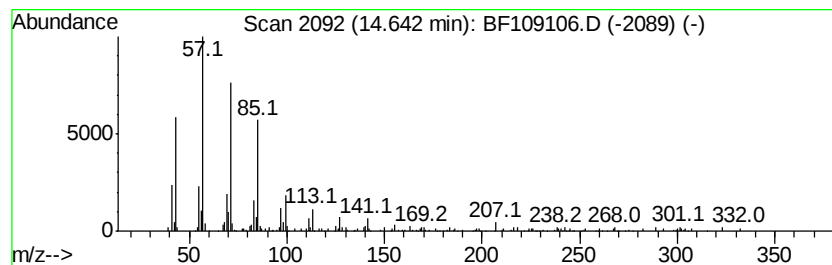
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Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.95 ng	180423	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	94
2	Hexacosane	366 C26H54	000630-01-3	91
3	Nonadecane	268 C19H40	000629-92-5	90
4	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	90
5	Nonadecane, 2,3-dimethyl-	296 C21H44	075163-99-4	90



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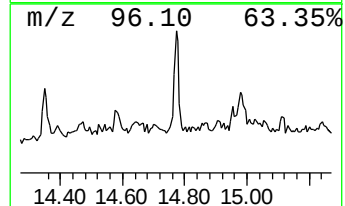
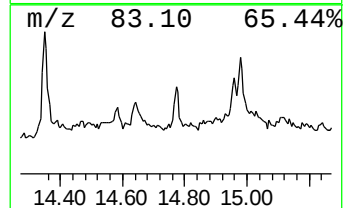
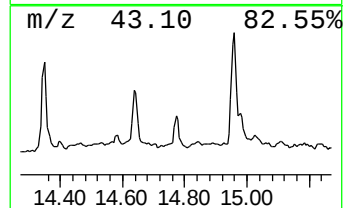
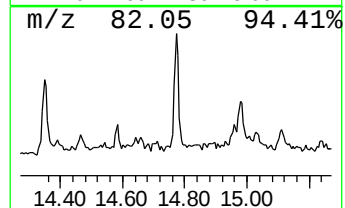
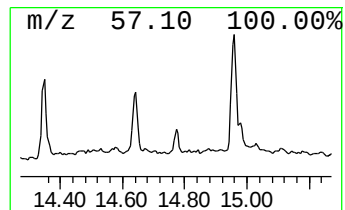
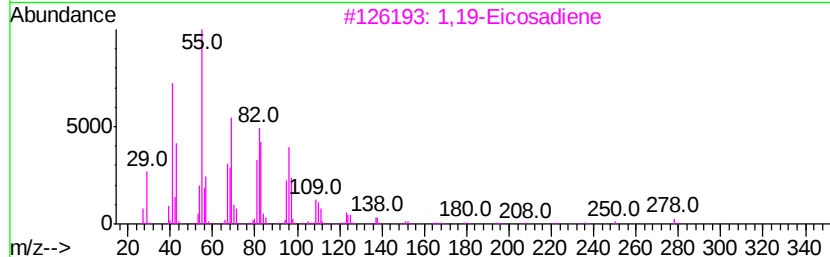
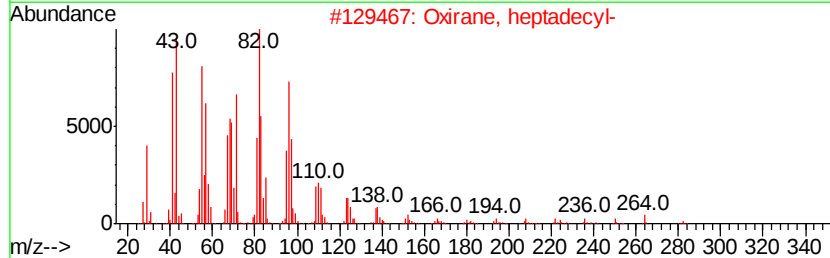
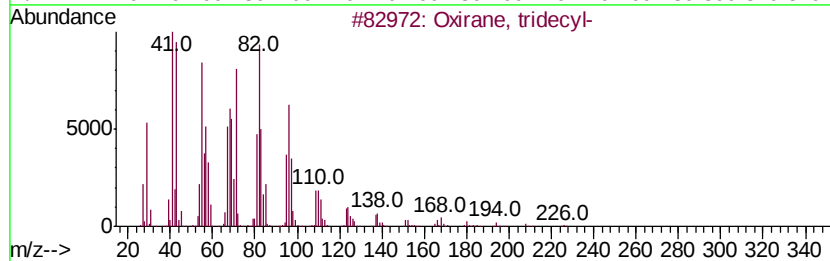
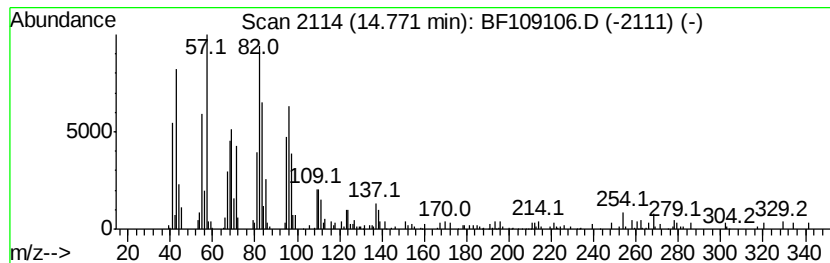
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, tridecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.46 ng	112685	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, tridecyl-	226	C15H30O	018633-25-5	95
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
3		1,19-Eicosadiene	278	C20H38	014811-95-1	91
4		Octadecanal	268	C18H36O	000638-66-4	91
5		17-Octadecenal	266	C18H34O	056554-86-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109106.D
Acq On : 18 Sep 2018 20:02
Operator : JU/SJ
Sample : J4952-01
Misc :
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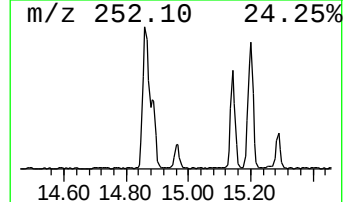
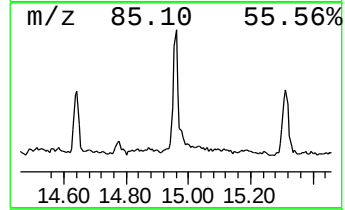
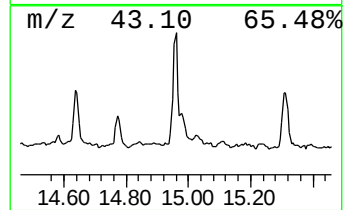
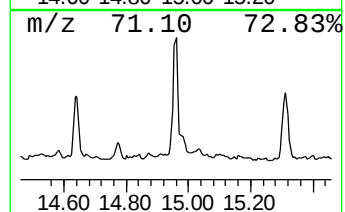
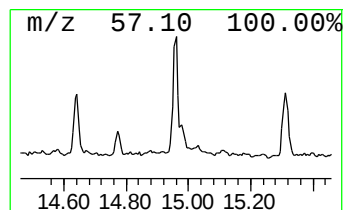
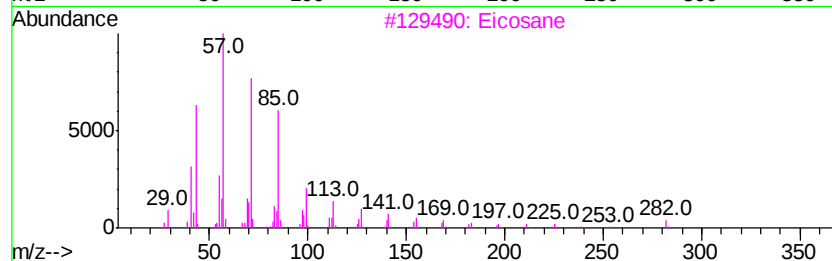
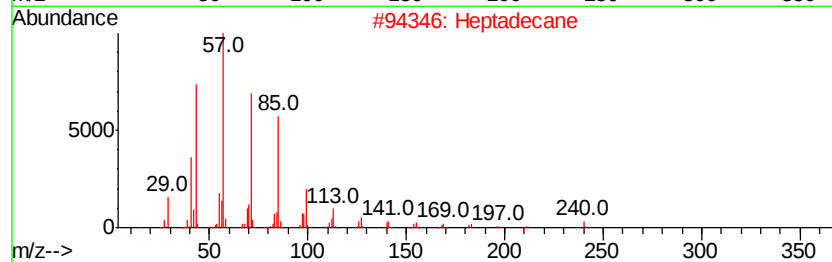
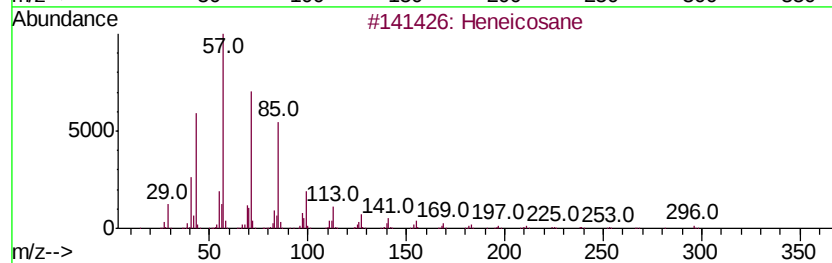
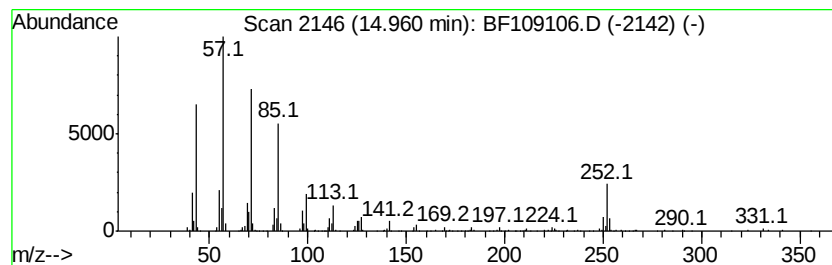
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ClientSampleId :
2015-161-20-RB36584RT-RB47184R

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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 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.96	6.33 ng	289649	Perylene-d12		15.26
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	81
2	Heptadecane	240	C17H36	000629-78-7	81
3	Eicosane	282	C20H42	000112-95-8	74
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109106.D
Acq On : 18 Sep 2018 20:02
Operator : JU/SJ
Sample : J4952-01
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Instrument :
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ClientSampleId :
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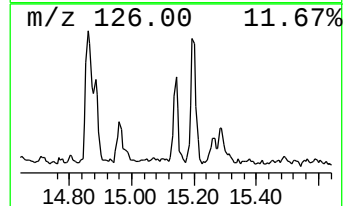
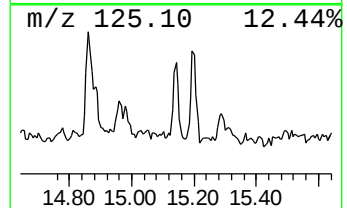
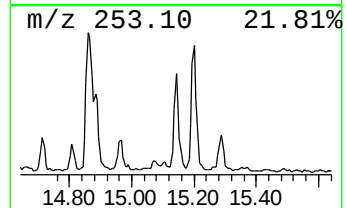
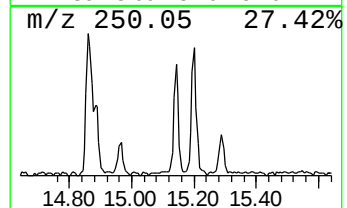
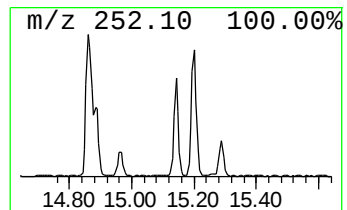
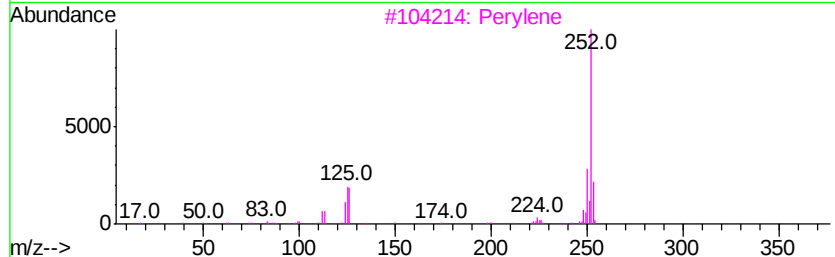
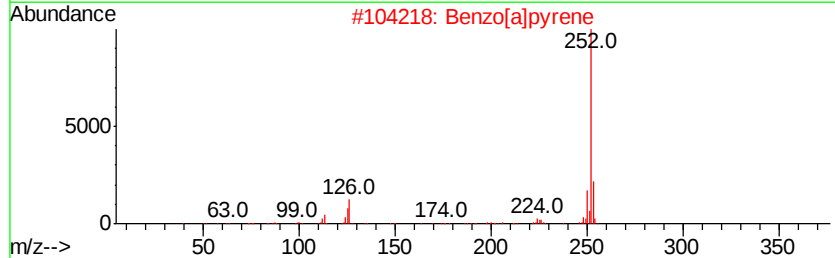
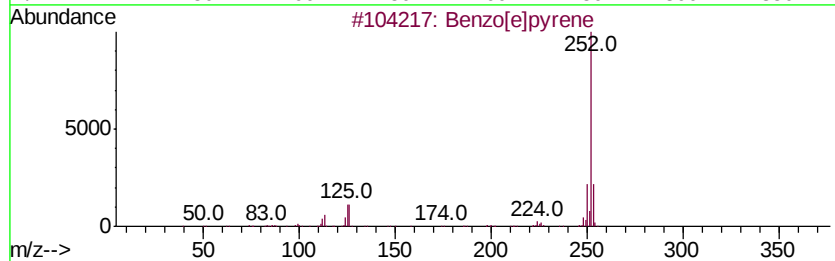
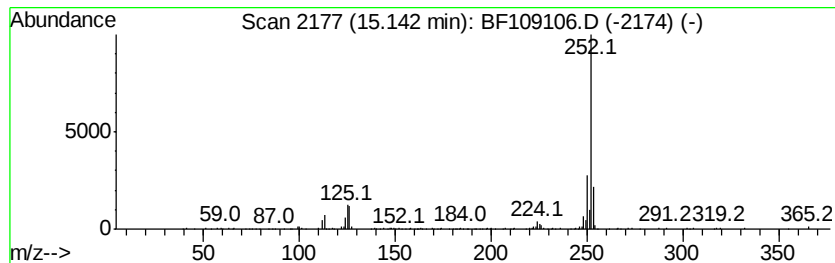
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	3.17 ng	144963	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[a]pyrene	252	C20H12	000050-32-8	97
3		Perylene	252	C20H12	000198-55-0	96
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109106.D
Acq On : 18 Sep 2018 20:02
Operator : JU/SJ
Sample : J4952-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

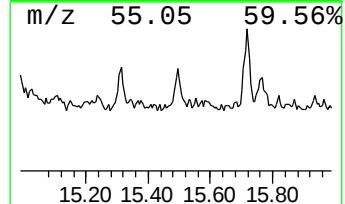
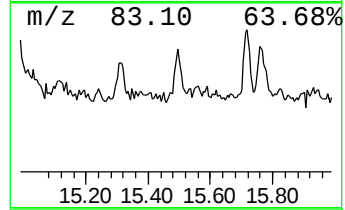
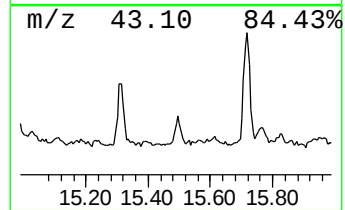
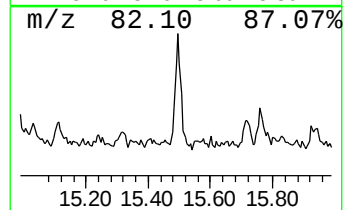
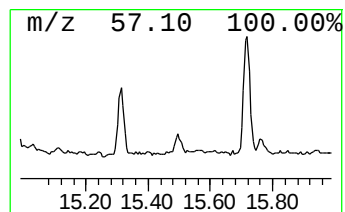
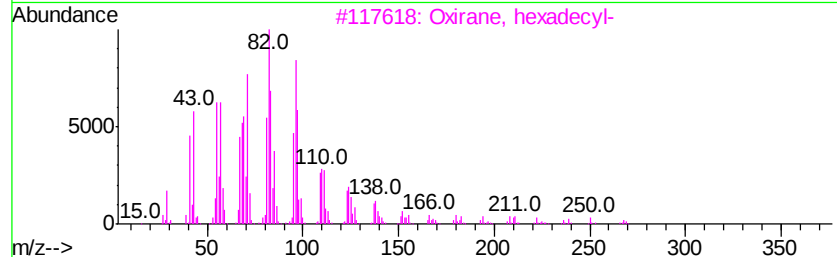
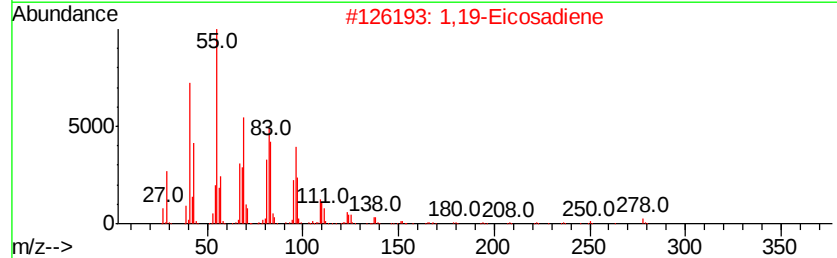
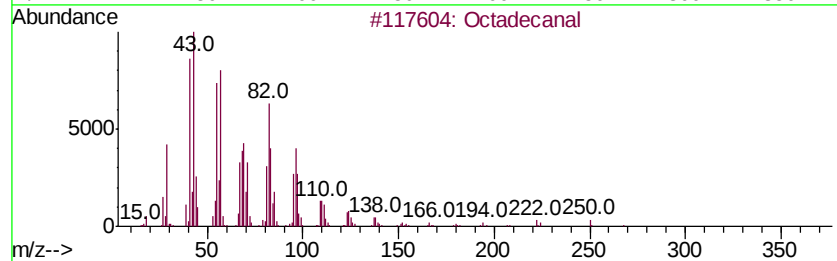
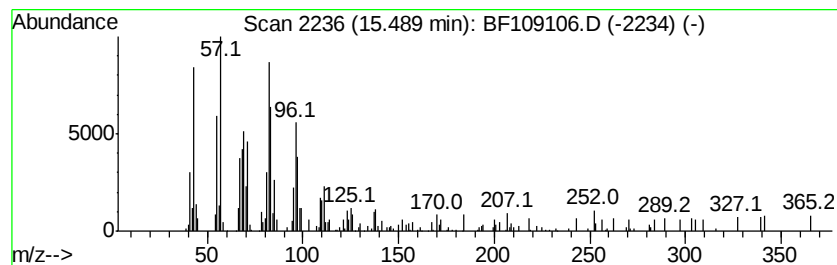
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.49	2.17 ng	99423	Perylene-d12		15.26
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	93
2	1,19-Eicosadiene	278	C20H38	014811-95-1	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
4	Tetracosanal	352	C24H48O	057866-08-7	87
5	9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
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Acq On : 18 Sep 2018 20:02
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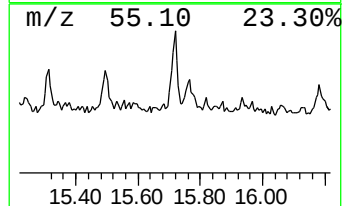
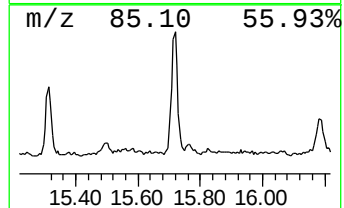
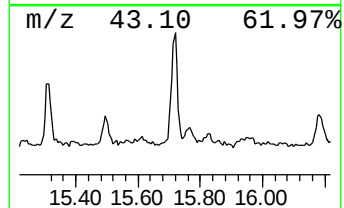
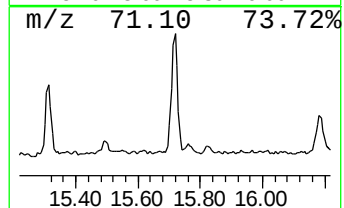
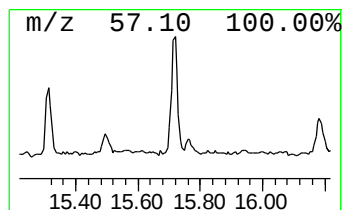
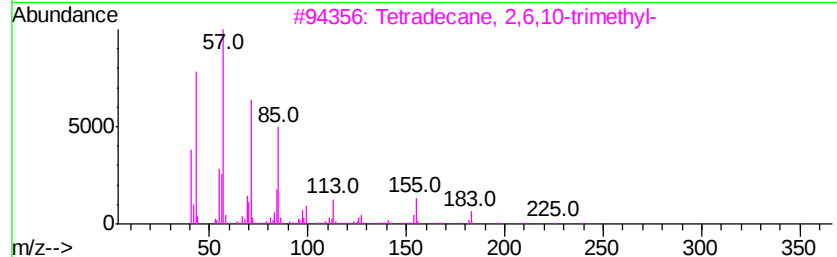
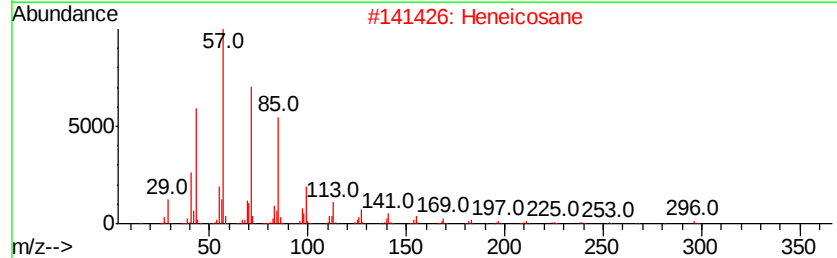
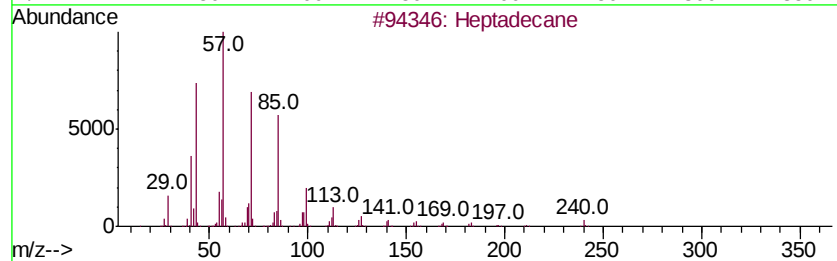
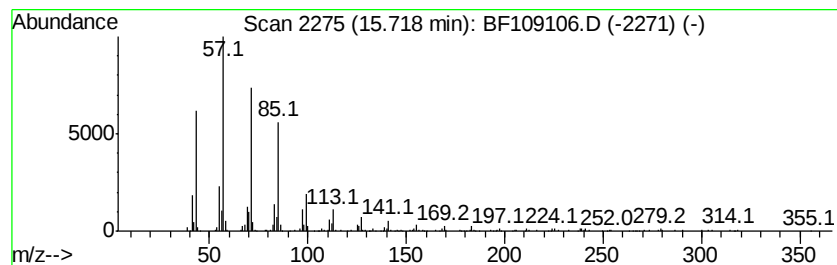
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.72	6.67 ng	305101	Perylene-d12		15.26
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091818\
Data File : BF109106.D
Acq On : 18 Sep 2018 20:02
Operator : JU/SJ
Sample : J4952-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
2015-161-20-RB36584RT-RB47184R

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
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n-Hexadecanoic acid	11.77	2.2	ng	91243	4	11.23	829804	20.0
1-Heneicosyl formate	13.72	5.4	ng	356211	5	13.85	1322100	20.0
1-Decanol, 2-hexyl-	14.35	3.9	ng	260132	5	13.85	1322100	20.0
Eicosane	14.64	4.0	ng	180423	6	15.26	914670	20.0
Oxirane, tridecyl-	14.77	2.5	ng	112685	6	15.26	914670	20.0
Heneicosane	14.96	6.3	ng	289649	6	15.26	914670	20.0
Benzo[e]pyrene	15.14	3.2	ng	144963	6	15.26	914670	20.0
Octadecanal	15.49	2.2	ng	99423	6	15.26	914670	20.0
Heptadecane	15.72	6.7	ng	305101	6	15.26	914670	20.0