

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091117\
 Data File : BF098430.D
 Acq On : 12 Sep 2017 4:15
 Operator : SJ/JU
 Sample : I5138-16
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-WM-TS002-01

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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	4.869	470	473	489	rVB	427375	752963	10.17%	1.367%
2	5.287	539	544	547	rBV	6589400	7141938	96.48%	12.966%
3	6.328	715	721	732	rBV	5778003	7402690	100.00%	13.440%
4	6.445	736	741	744	rBV	6710824	6696065	90.45%	12.157%
5	6.669	775	779	787	rBV	1739400	1556623	21.03%	2.826%
6	6.822	801	805	809	rBV	4461523	4489462	60.65%	8.151%
7	7.239	870	876	879	rBV	4281627	4432536	59.88%	8.047%
8	7.951	991	997	1000	rBV	2355243	2036740	27.51%	3.698%
9	9.028	1174	1180	1183	rBV	5227931	4514269	60.98%	8.196%
10	9.110	1189	1194	1198	rBV	111995	122017	1.65%	0.222%
11	9.422	1244	1247	1250	rVB	1351207	1068940	14.44%	1.941%
12	9.698	1288	1294	1298	rBV	2210815	1975324	26.68%	3.586%
13	10.410	1412	1415	1421	rBV2	80112	103886	1.40%	0.189%
14	10.492	1424	1429	1432	rBV	3123291	2933710	39.63%	5.326%
15	10.763	1472	1475	1477	rBV	204661	170975	2.31%	0.310%
16	10.839	1485	1488	1493	rVB	113355	107067	1.45%	0.194%
17	10.886	1493	1496	1499	rBV	169572	146990	1.99%	0.267%
18	10.957	1501	1508	1513	rBV3	127019	187696	2.54%	0.341%
19	11.069	1521	1527	1535	rBV2	134174	150115	2.03%	0.273%
20	11.180	1541	1546	1553	rBV	2018634	1724051	23.29%	3.130%
21	11.251	1553	1558	1561	rBV2	126503	137976	1.86%	0.250%
22	11.869	1659	1663	1670	rVB3	58504	76452	1.03%	0.139%
23	12.263	1725	1730	1732	rBV	204465	197406	2.67%	0.358%
24	12.280	1732	1733	1739	rVB3	132281	114780	1.55%	0.208%
25	12.427	1755	1758	1765	rVB	172906	151083	2.04%	0.274%
26	12.663	1793	1798	1803	rVB3	47082	86861	1.17%	0.158%
27	12.763	1811	1815	1818	rBV	2888199	2523511	34.09%	4.581%
28	13.663	1964	1968	1972	rBV	318595	340615	4.60%	0.618%
29	13.810	1988	1993	1997	rBV	1215676	1169749	15.80%	2.124%
30	14.286	2071	2074	2079	rBV2	102086	129057	1.74%	0.234%
31	14.886	2173	2176	2180	rBV	283849	311952	4.21%	0.566%
32	15.210	2227	2231	2240	rVB	915741	1204210	16.27%	2.186%
33	15.627	2298	2302	2308	rBV	214065	323552	4.37%	0.587%
34	17.086	2542	2550	2557	rVB7	170706	451274	6.10%	0.819%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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35	17.774	2663	2667	2672	rBV7	60412	148113	2.00%	0.269%
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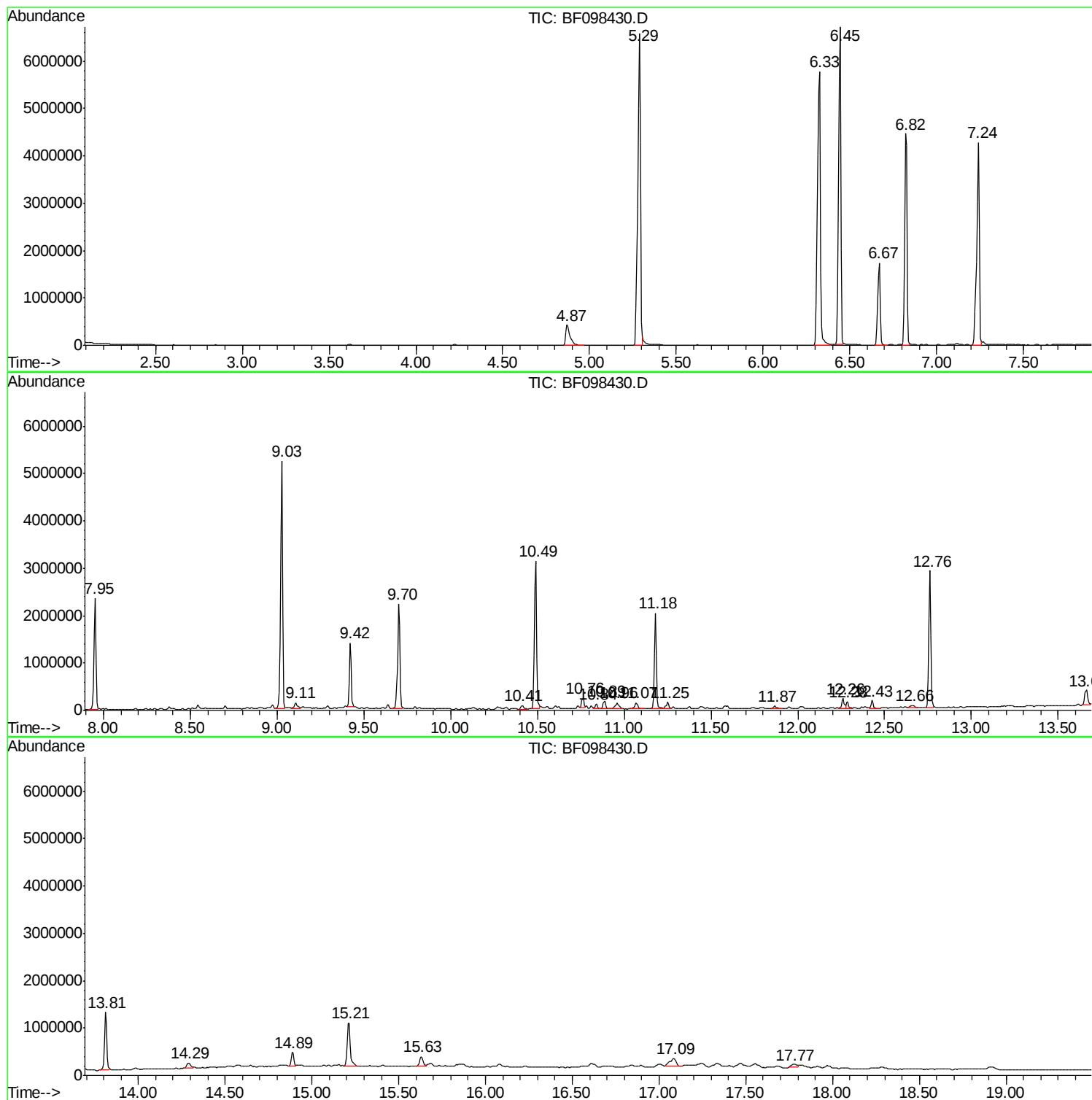
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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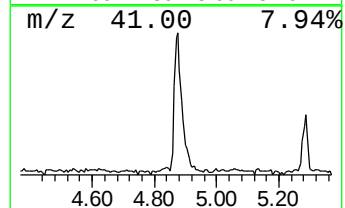
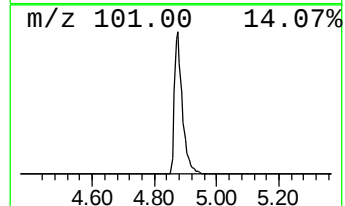
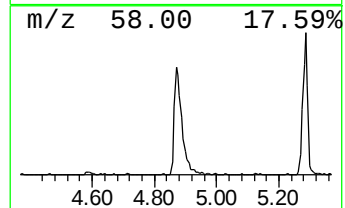
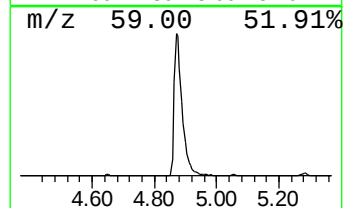
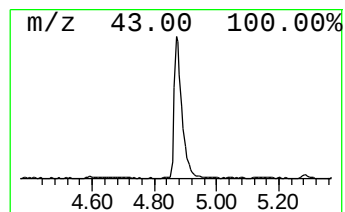
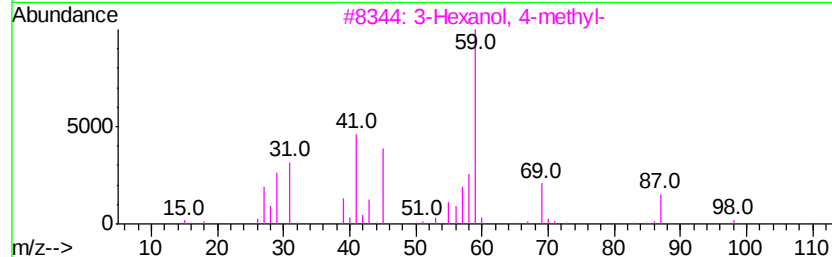
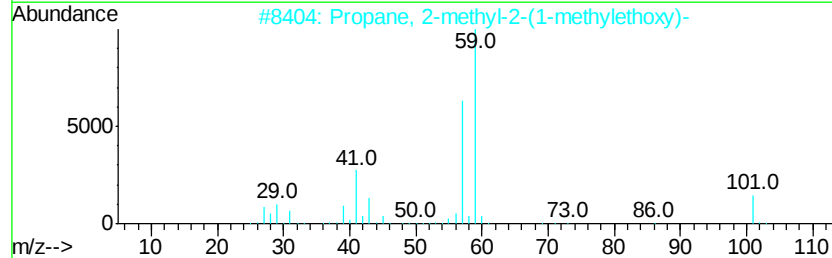
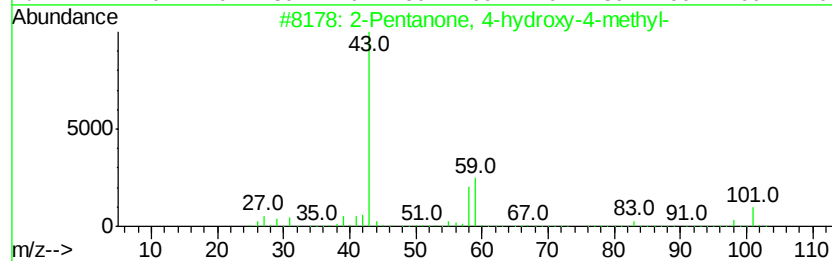
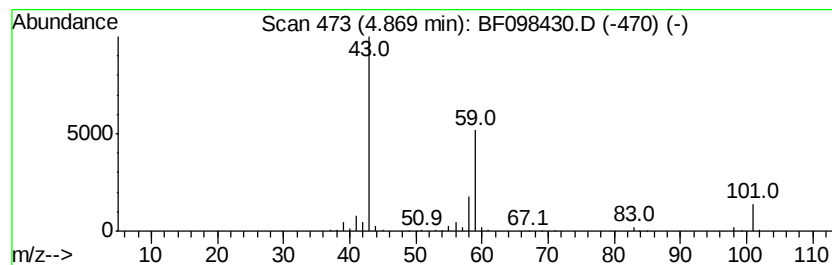
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	9.67 ng	752963	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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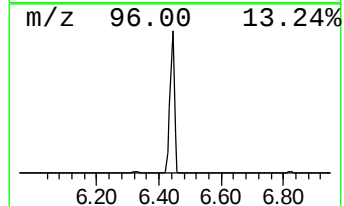
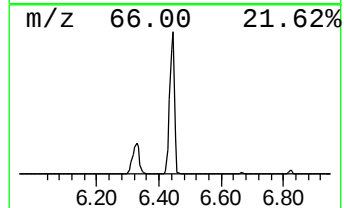
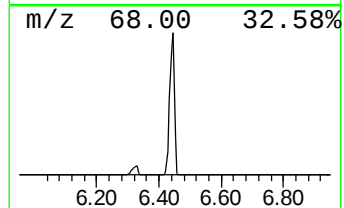
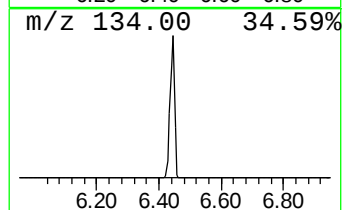
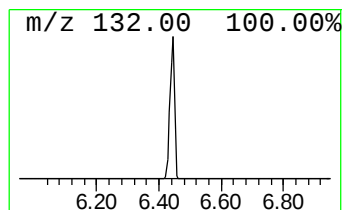
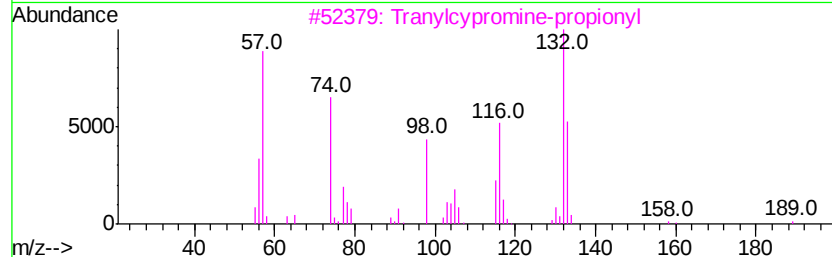
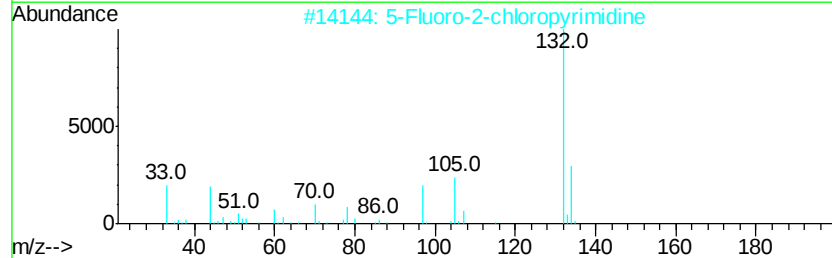
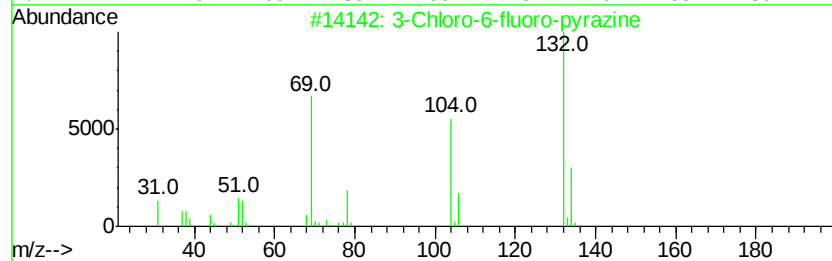
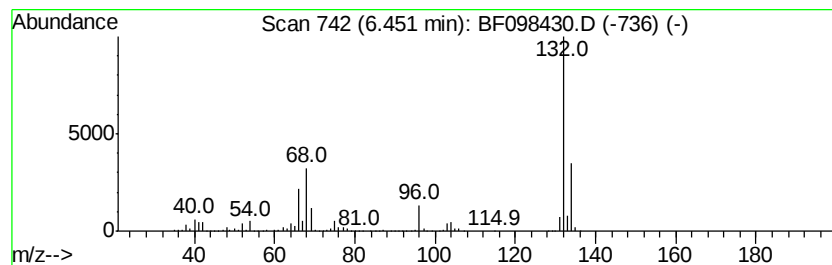
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	86.03 ng	6696070	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27		
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16		
3	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10		
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9		
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9		



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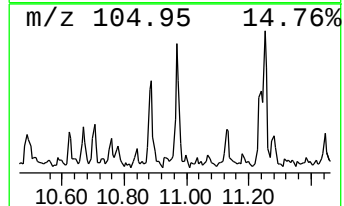
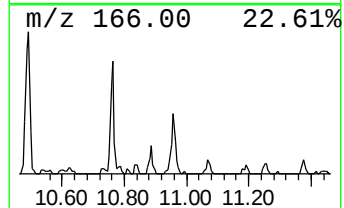
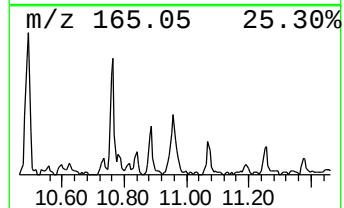
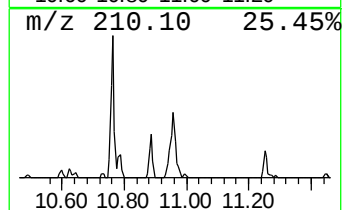
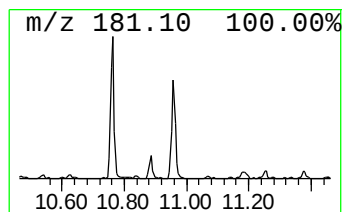
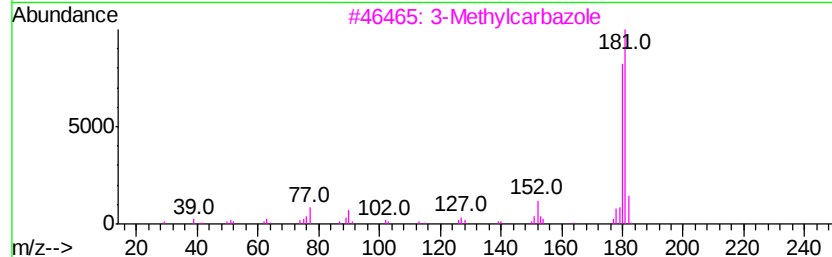
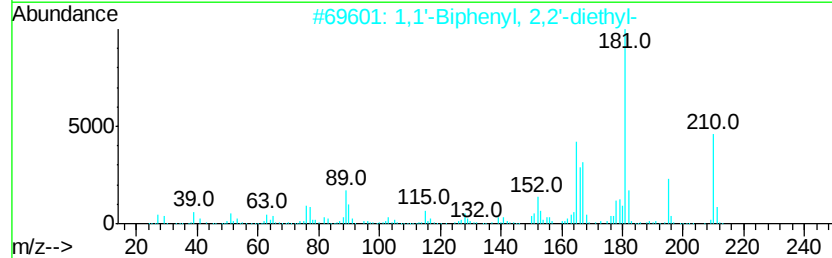
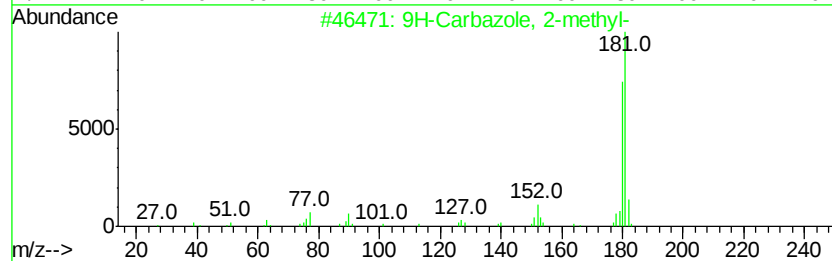
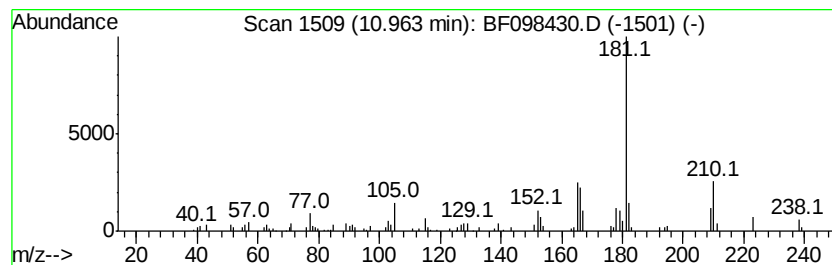
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9H-Carbazole, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	2.18 ng	187696	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9H-Carbazole, 2-methyl-	181	C13H11N	003652-91-3	78
2		1,1'-Biphenyl, 2,2'-diethyl-	210	C16H18	013049-35-9	70
3		3-Methylcarbazole	181	C13H11N	004630-20-0	60
4		7-Methyl-4-azafluorene	181	C13H11N	064291-99-2	58
5		Benzo[b]benzo[3,4]cyclobuta[1,2-...	210	C14H10O2	042896-18-4	58



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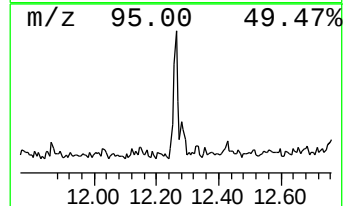
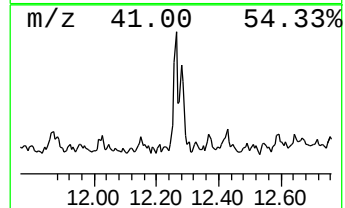
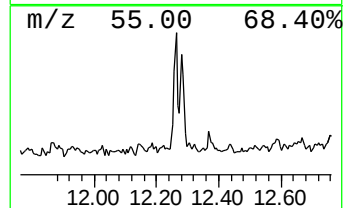
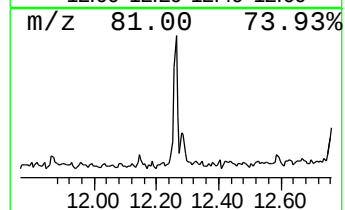
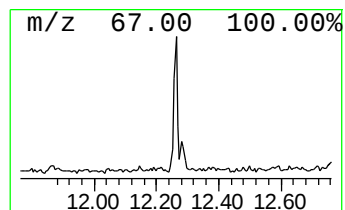
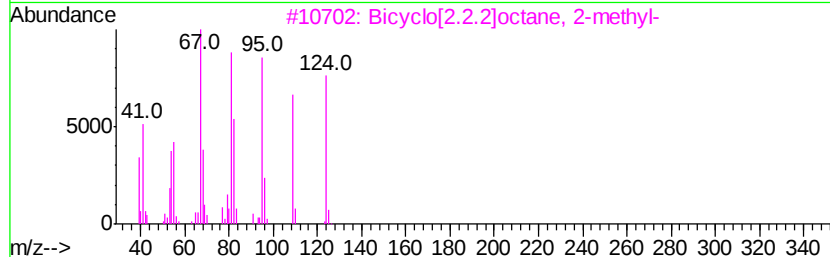
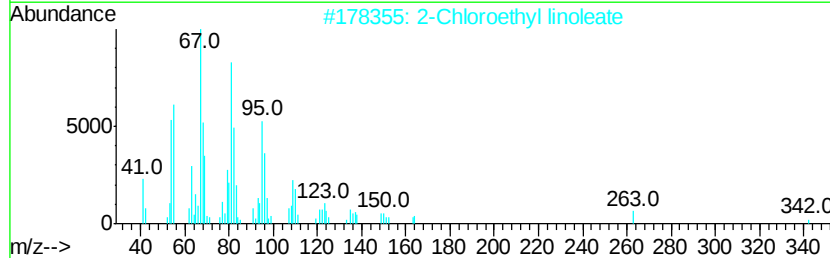
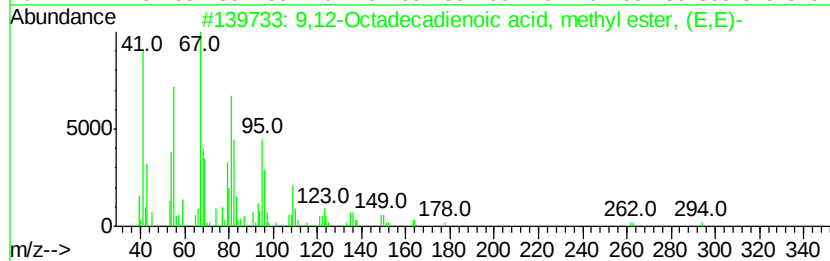
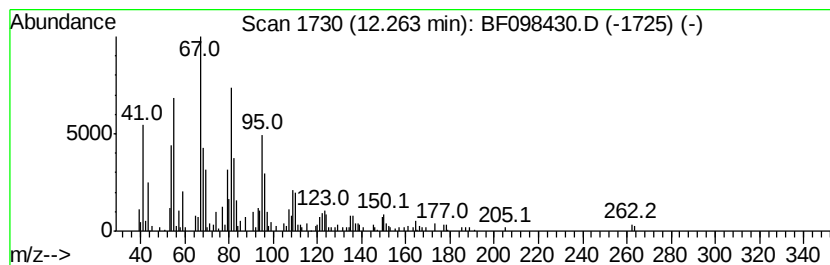
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.26	2.29 ng	197406	Phenanthrene-d10	11.18		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methyl-	294	C19H34O2	002566-97-4	92	
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90	
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	83	
4	11,14-Eicosadienoic acid, methyl-	322	C21H38O2	002463-02-7	70	
5	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	64	



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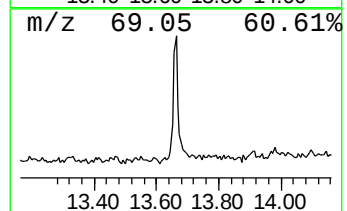
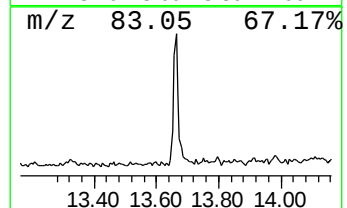
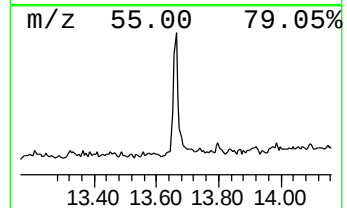
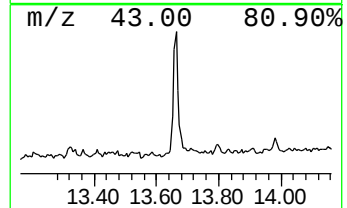
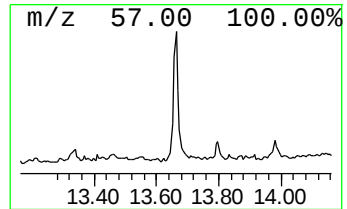
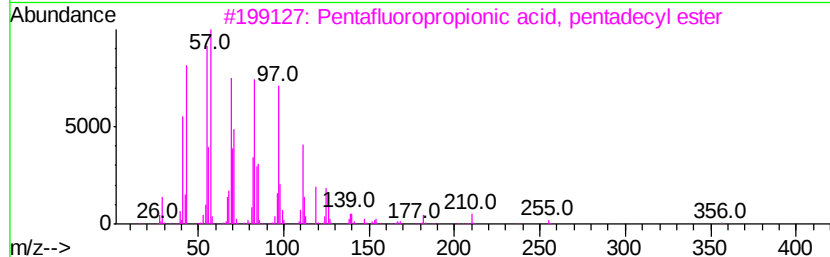
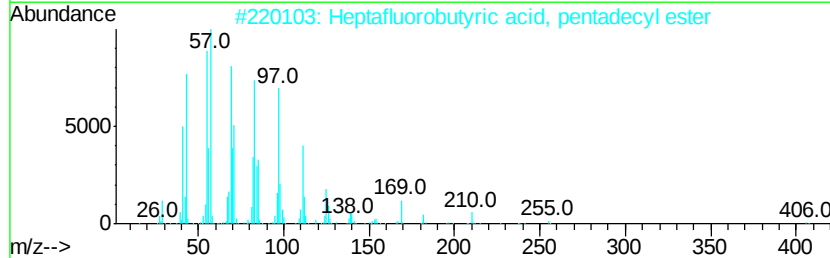
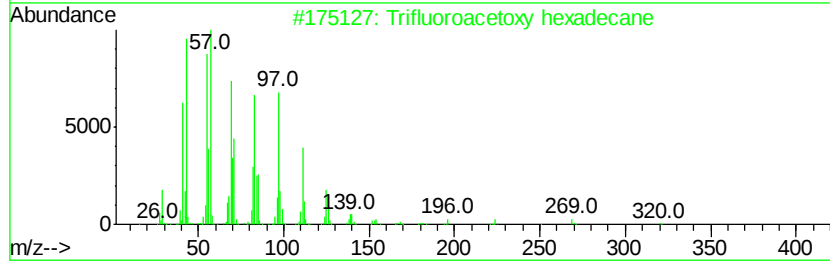
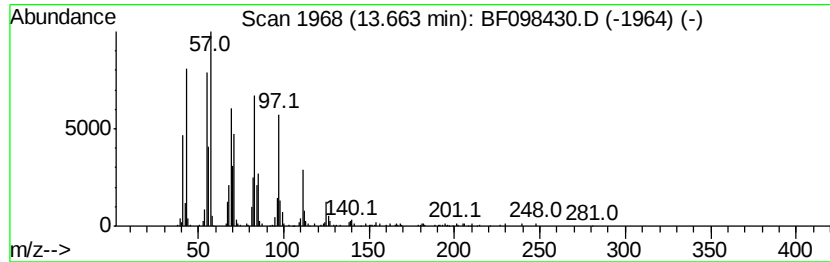
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.66	5.82 ng	340615	Chrysene-d12		13.81
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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Data File : BF098430.D
Acq On : 12 Sep 2017 4:15
Operator : SJ/JU
Sample : I5138-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-WM-TS002-01

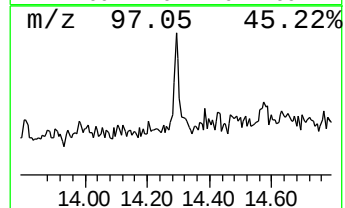
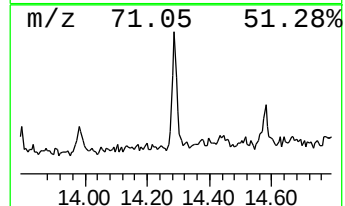
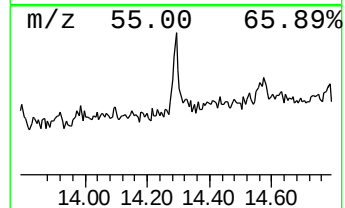
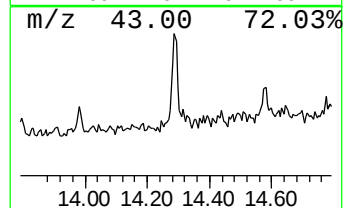
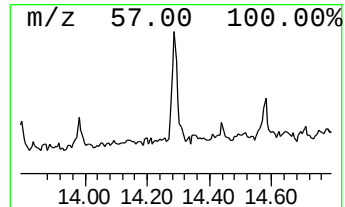
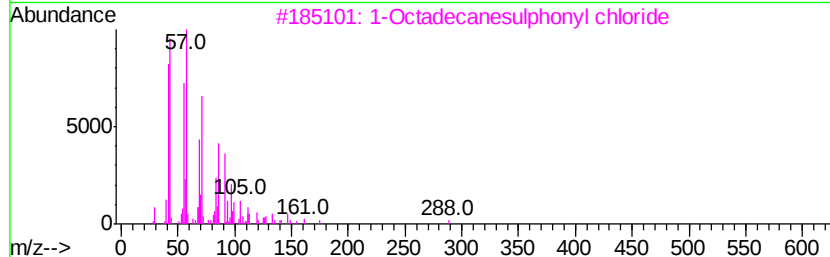
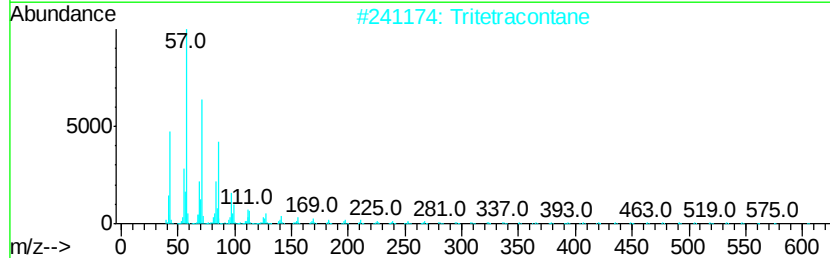
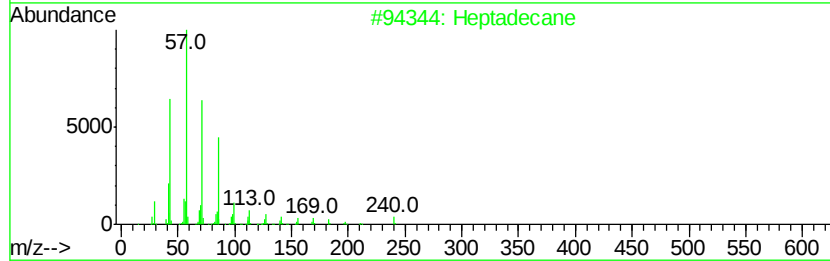
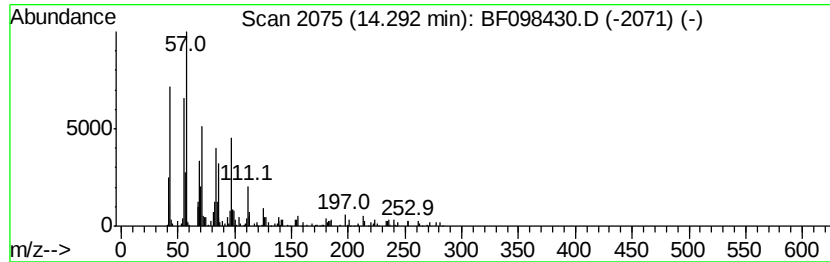
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.21 ng	129057	Chrysene-d12	13.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	94
2	Tritetracontane		605	C43H88	007098-21-7	87
3	1-Octadecanesulphonyl chloride		352	C18H37ClO2S	1000342-70-4	87
4	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	86
5	Sulfurous acid, 2-propyl tridecy...		306	C16H34O3S	1000309-12-4	86



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
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Operator : SJ/JU
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Misc :
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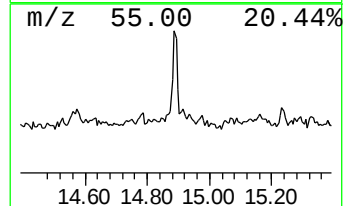
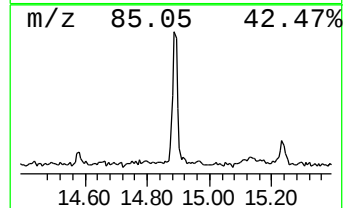
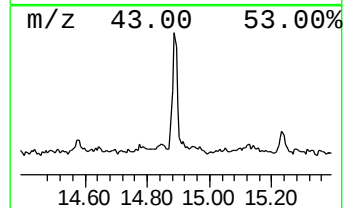
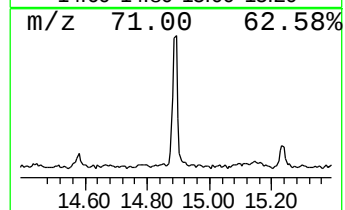
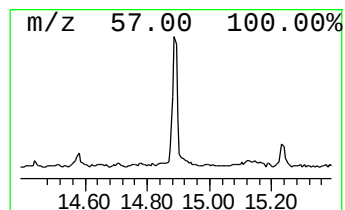
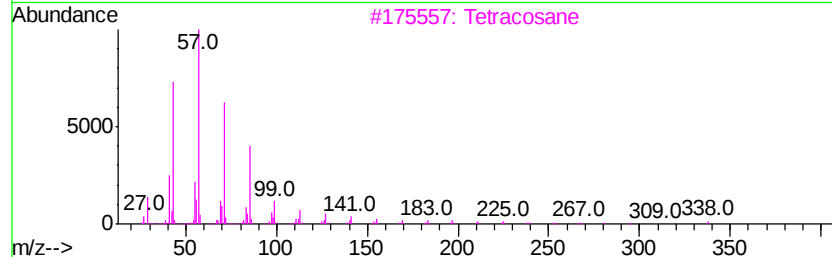
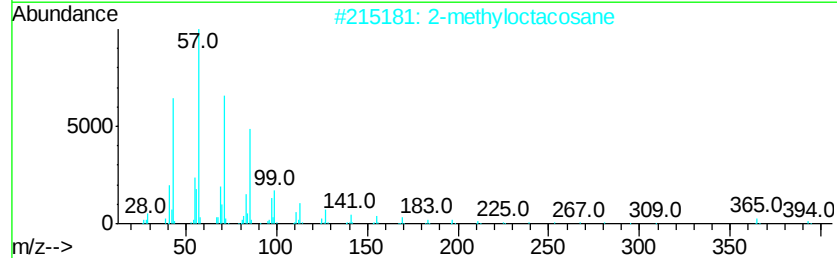
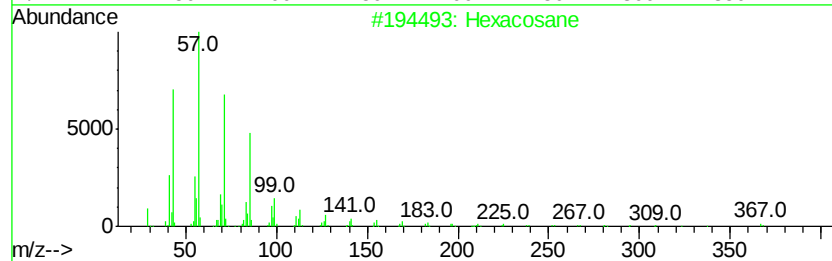
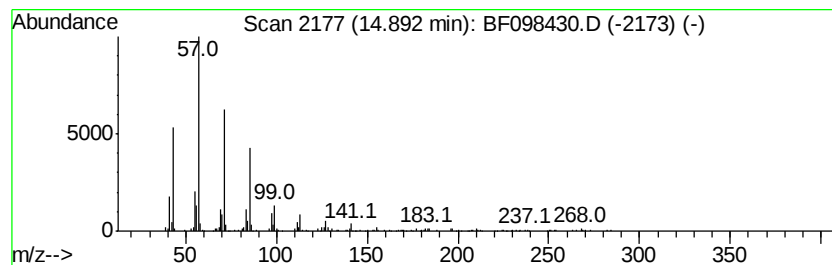
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	5.18 ng	311952	Perylene-d12	15.22
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	90
3	Tetracosane	338 C24H50	000646-31-1	87
4	Heptacosane	380 C27H56	000593-49-7	87
5	Heneicosane	296 C21H44	000629-94-7	83



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098430.D
Acq On : 12 Sep 2017 4:15
Operator : SJ/JU
Sample : I5138-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

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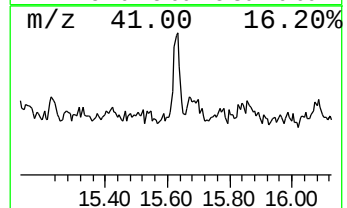
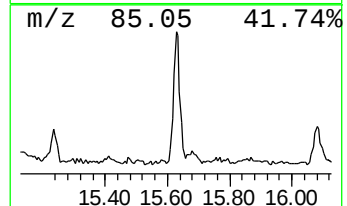
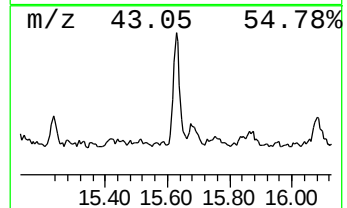
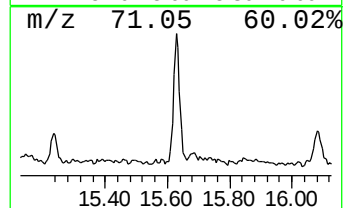
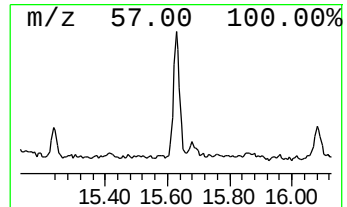
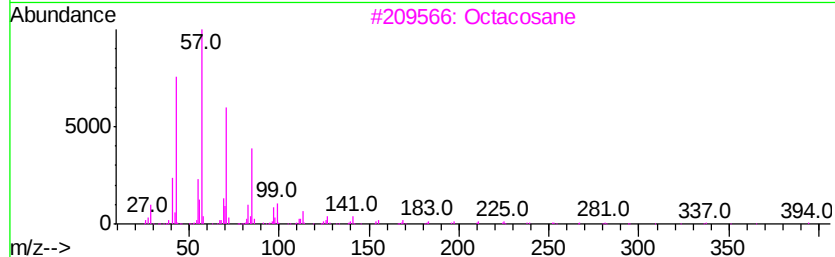
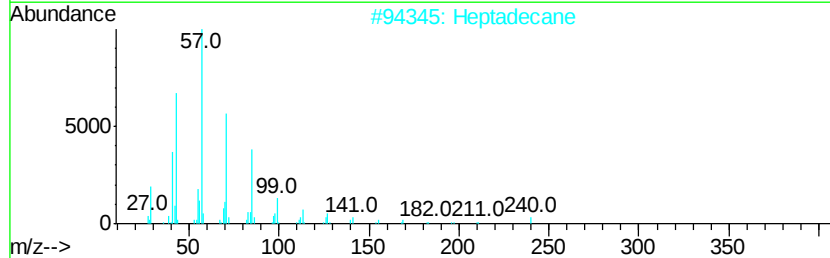
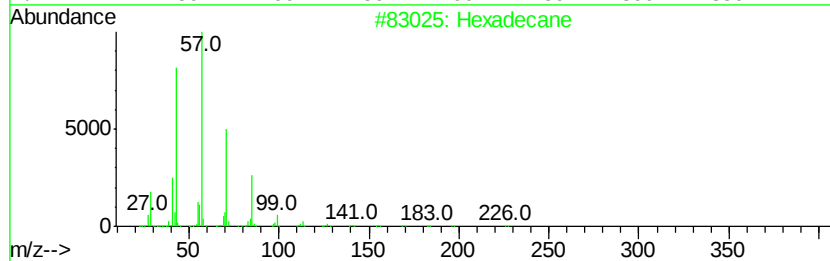
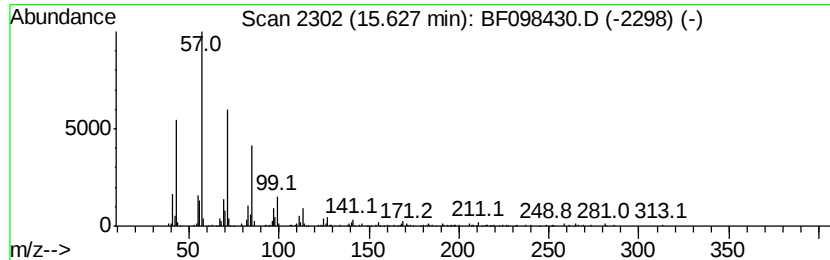
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	5.37 ng	323552	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Heptadecane	240	C17H36	000629-78-7	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098430.D
Acq On : 12 Sep 2017 4:15
Operator : SJ/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

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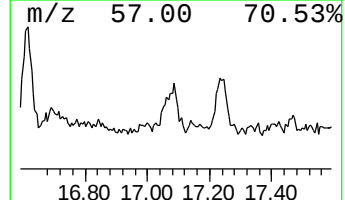
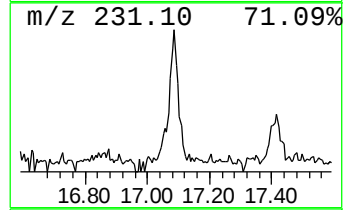
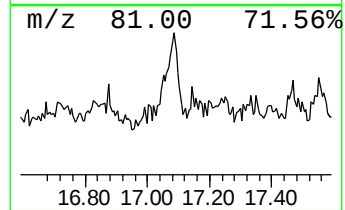
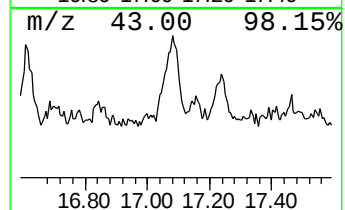
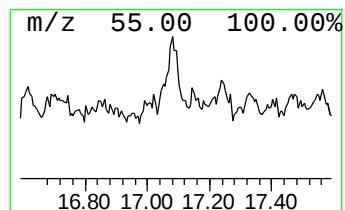
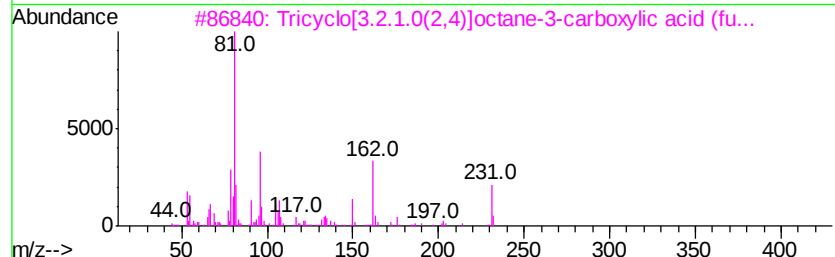
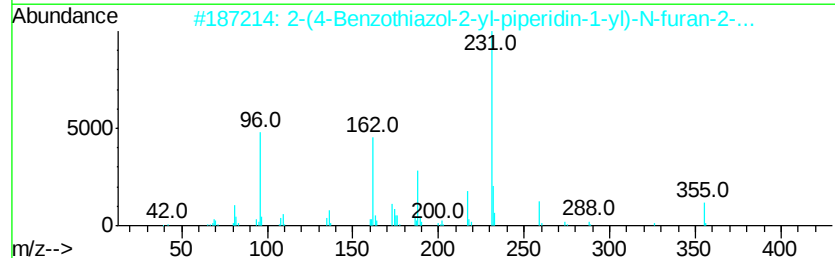
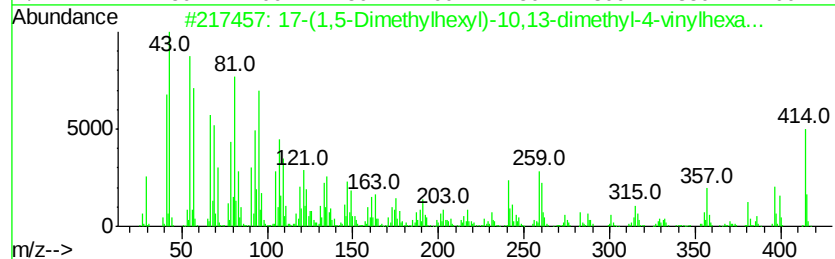
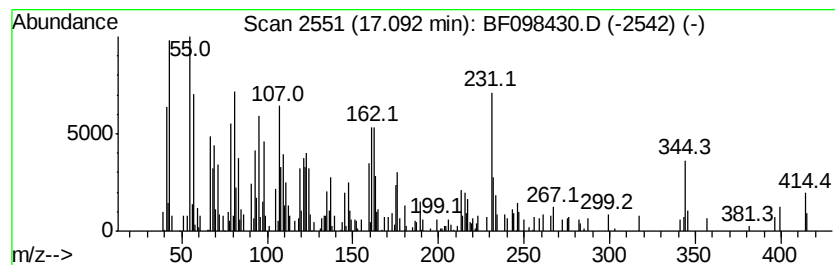
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.09 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	7.49 ng	451274	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25
2		2-(4-Benzothiazol-2-yl-piperidin...	355	C19H21N3O2S	1000322-21-0	25
3		Tricyclo[3.2.1.0(2,4)]octane-3-car...	231	C14H17N02	1000297-39-2	22
4		Adenine, N4-trifluoroacetyl-	231	C7H4F3N5O	1000374-88-1	22
5		6-epi-shyobunol	222	C15H26O	1000374-18-3	15



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098430.D
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Operator : SJ/JU
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Misc :
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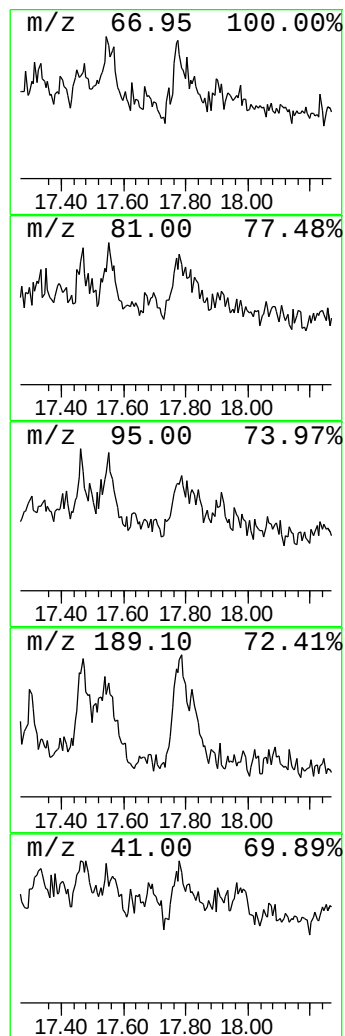
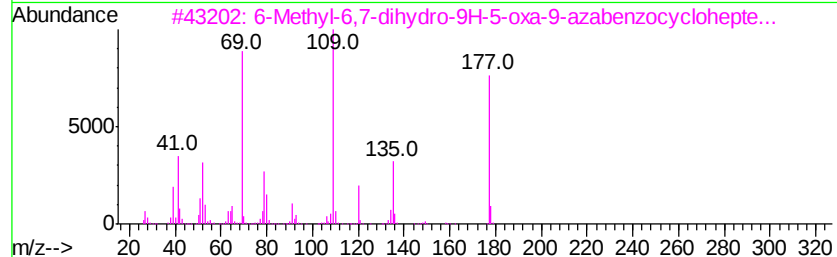
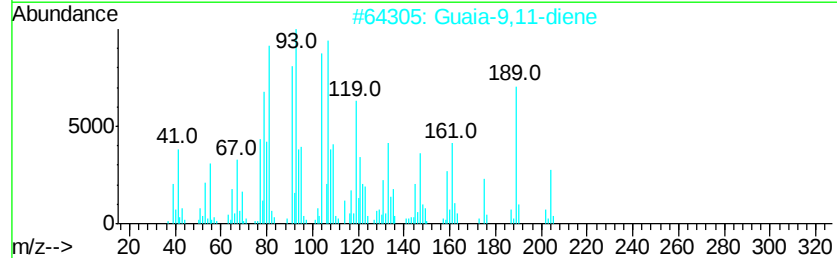
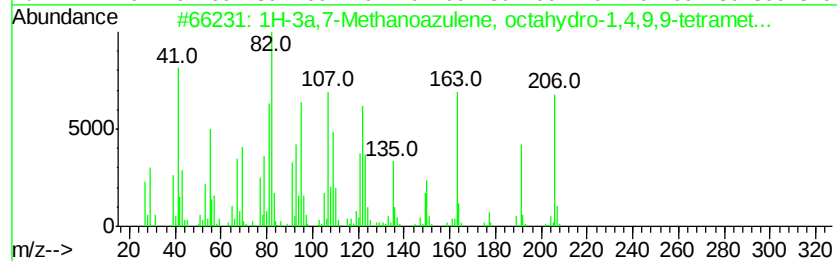
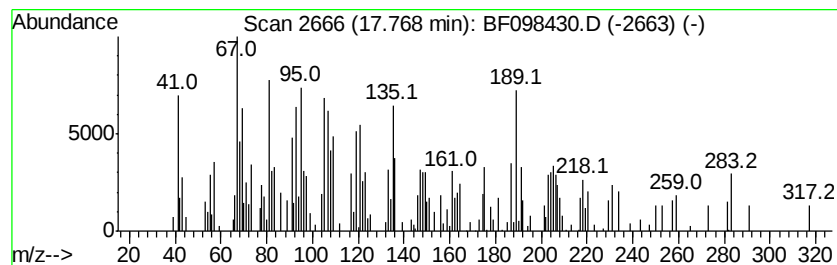
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1H-3a,7-Methanoazulene, oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	2.46 ng	148113	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1H-3a,7-Methanoazulene, octahydr...	206 C15H26	003724-42-3	50
2	Guaia-9,11-diene	204 C15H24	1000374-19-8	25
3	6-Methyl-6,7-dihydro-9H-5-oxa-9-...	177 C10H11N02	1000210-20-2	18
4	2(E),4-Pentadienamide, N-[1-(dim...	206 C12H18N2O	075378-94-8	18
5	1H-Cycloprop[e]azulen-4-ol, deca...	222 C15H26O	000552-02-3	18



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091117\
Data File : BF098430.D
Acq On : 12 Sep 2017 4:15
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Sample : I5138-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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
2-Pentanone, 4-hy...	4.87	9.7	ng	752963	1	6.67	1556620	20.0
unknown6.45	6.45	86.0	ng	6696070	1	6.67	1556620	20.0
9H-Carbazole, 2-m...	10.96	2.2	ng	187696	4	11.18	1724050	20.0
9,12-Octadecadien...	12.26	2.3	ng	197406	4	11.18	1724050	20.0
Trifluoroacetoxy ...	13.66	5.8	ng	340615	5	13.81	1169750	20.0
Heptadecane	14.29	2.2	ng	129057	5	13.81	1169750	20.0
Hexacosane	14.89	5.2	ng	311952	6	15.22	1204210	20.0
Hexadecane	15.63	5.4	ng	323552	6	15.22	1204210	20.0
unknown17.09	17.09	7.5	ng	451274	6	15.22	1204210	20.0
1H-3a,7-Methanoaz...	17.77	2.5	ng	148113	6	15.22	1204210	20.0