

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
 Data File : BF096542.D
 Acq On : 6 Jul 2017 19:21
 Operator : SJ/MA
 Sample : I3999-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS4-1-4-COMP

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-BF070117.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	4.910	475	480	490	rBV	403064	587094	18.79%	2.218%
2	5.334	547	552	555	rBV	3072848	3106749	99.42%	11.735%
3	6.357	717	726	729	rBV	2839302	3124844	100.00%	11.804%
4	6.487	743	748	751	rBV	3104221	2957705	94.65%	11.172%
5	6.716	783	787	790	rBV	867385	757434	24.24%	2.861%
6	6.875	809	814	817	rBV	2306076	2249681	71.99%	8.498%
7	7.275	877	882	885	rBV	1941919	1891580	60.53%	7.145%
8	7.381	893	900	904	rBV2	37414	46234	1.48%	0.175%
9	7.992	1000	1004	1008	rBV	1021304	957456	30.64%	3.617%
10	9.075	1183	1188	1191	rBV	3028791	2775169	88.81%	10.483%
11	9.469	1251	1255	1258	rBV	598883	503131	16.10%	1.901%
12	9.698	1291	1294	1297	rVB	55954	48569	1.55%	0.183%
13	9.751	1298	1303	1307	rBV	932485	852907	27.29%	3.222%
14	10.192	1375	1378	1381	rVB	71189	59081	1.89%	0.223%
15	10.533	1432	1436	1440	rBV	1265440	1253765	40.12%	4.736%
16	10.669	1455	1459	1466	rBV	58327	72930	2.33%	0.275%
17	11.116	1531	1535	1538	rBV2	44491	41190	1.32%	0.156%
18	11.227	1551	1554	1557	rBV	755976	683975	21.89%	2.584%
19	12.439	1756	1760	1764	rBV	115161	93358	2.99%	0.353%
20	12.663	1793	1798	1802	rBV2	87363	118187	3.78%	0.446%
21	12.816	1820	1824	1828	rBV	1958072	1982823	63.45%	7.490%
22	13.404	1922	1924	1929	rVB	50638	42567	1.36%	0.161%
23	13.610	1956	1959	1962	rBV4	32840	44054	1.41%	0.166%
24	13.721	1974	1978	1987	rBV2	265770	345477	11.06%	1.305%
25	13.862	1998	2002	2005	rBV	787982	744523	23.83%	2.812%
26	14.051	2031	2034	2036	rBV	94146	96463	3.09%	0.364%
27	14.351	2082	2085	2090	rBV	107425	133263	4.26%	0.503%
28	14.651	2133	2136	2138	rBV	70287	71147	2.28%	0.269%
29	14.780	2155	2158	2161	rBV	64158	71359	2.28%	0.270%
30	14.968	2187	2190	2199	rVB3	75783	139287	4.46%	0.526%
31	15.274	2238	2242	2247	rBV	455207	555701	17.78%	2.099%
32	16.627	2469	2472	2477	rBV4	30286	65801	2.11%	0.249%

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ClientSampleId :
SS4-1-4-COMP

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

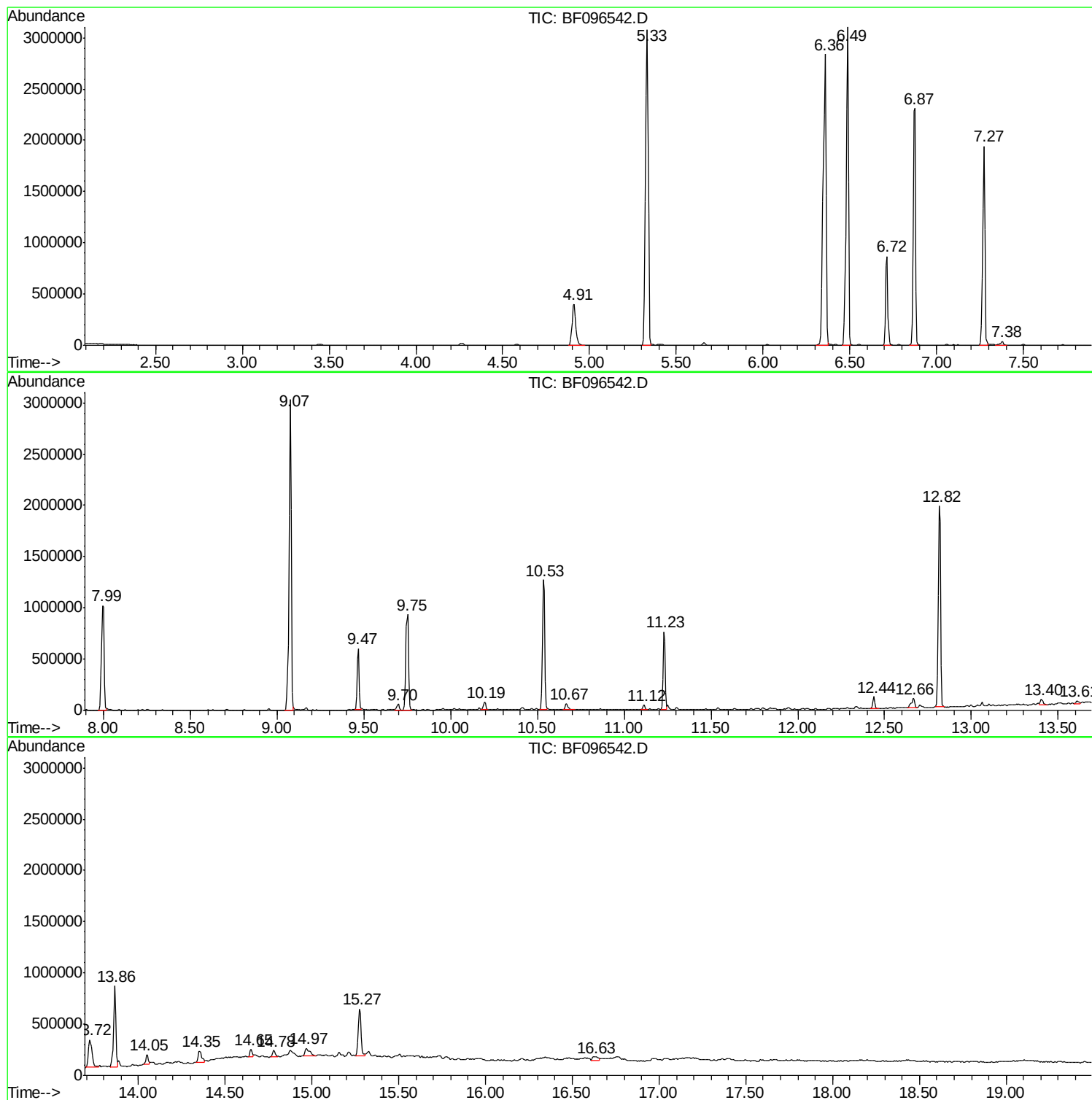
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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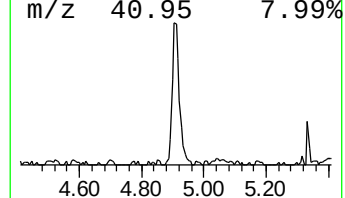
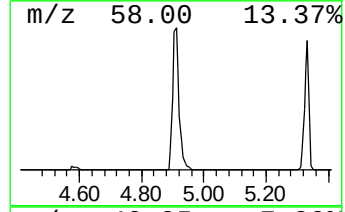
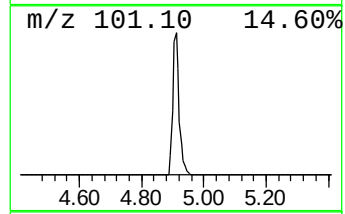
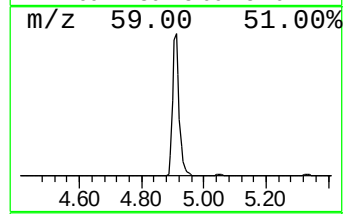
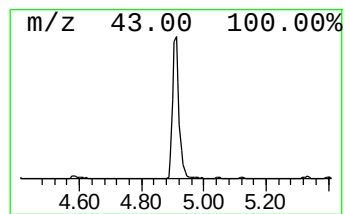
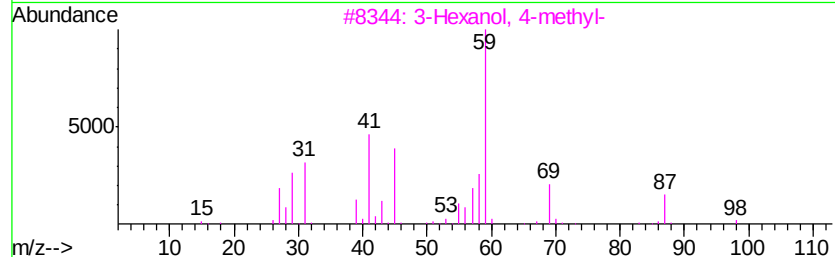
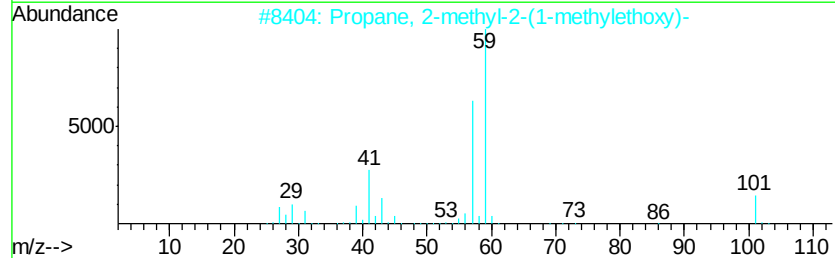
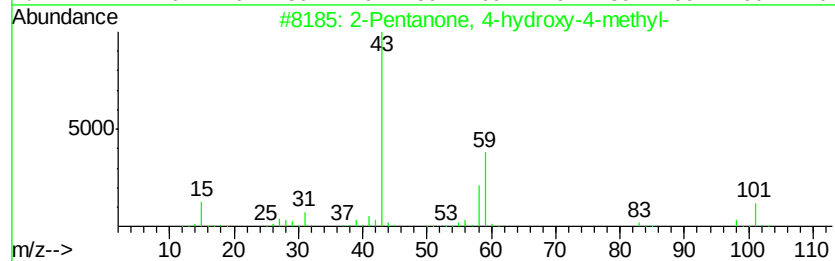
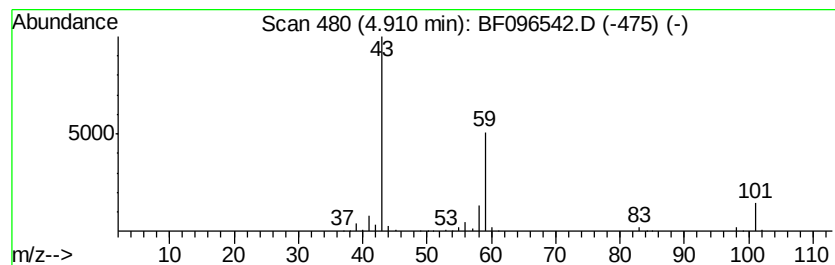
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	15.50 ng	587094	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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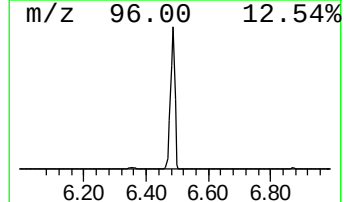
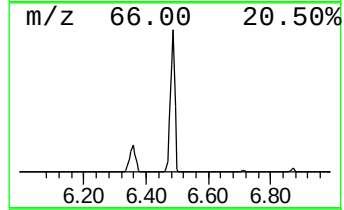
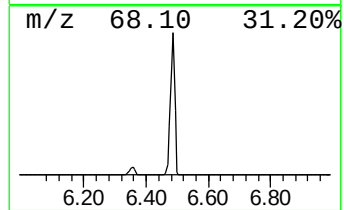
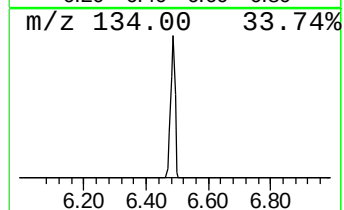
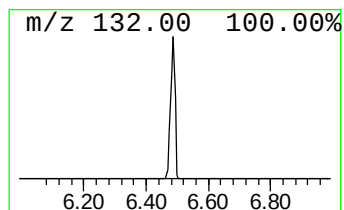
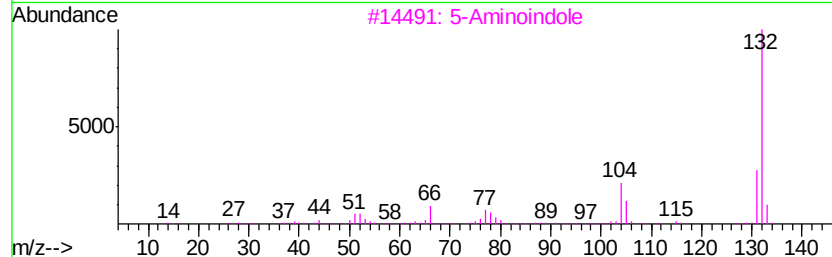
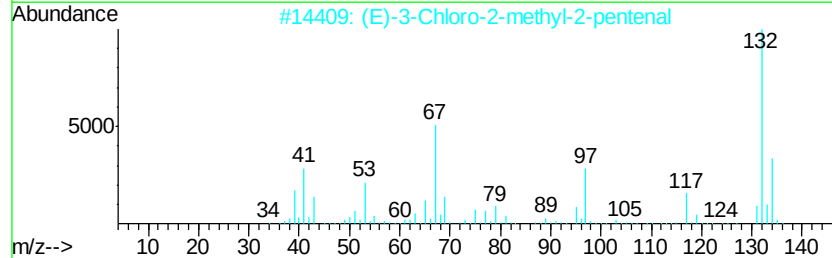
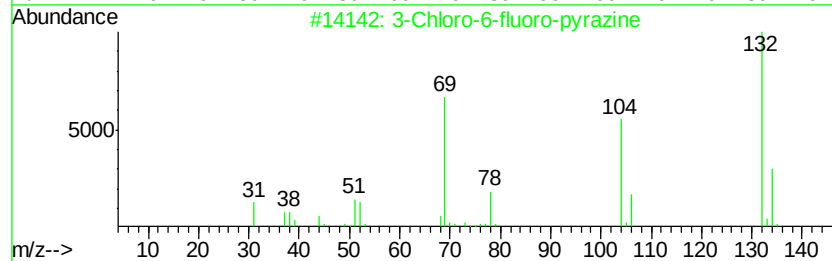
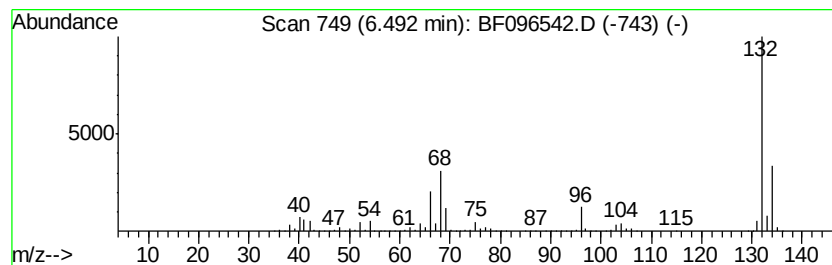
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	78.10 ng	2957710	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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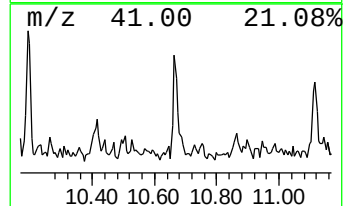
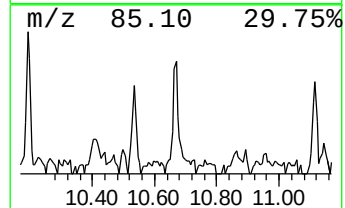
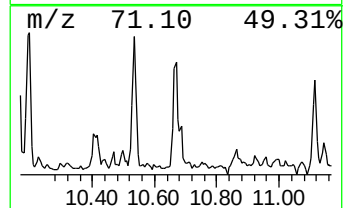
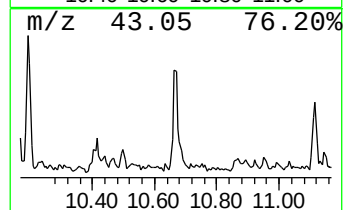
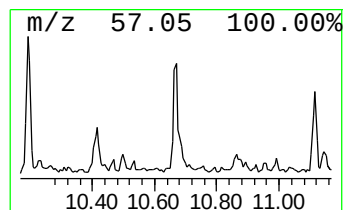
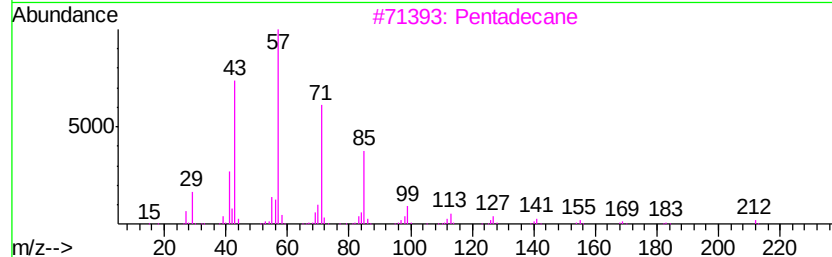
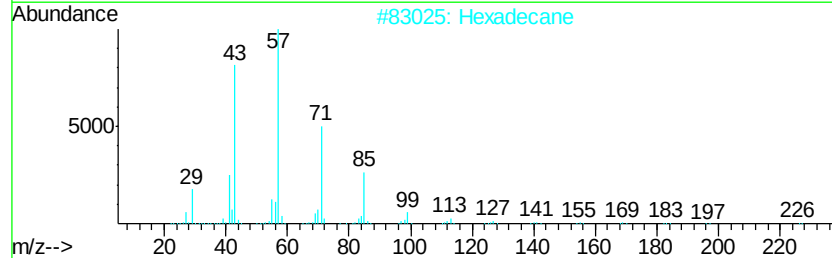
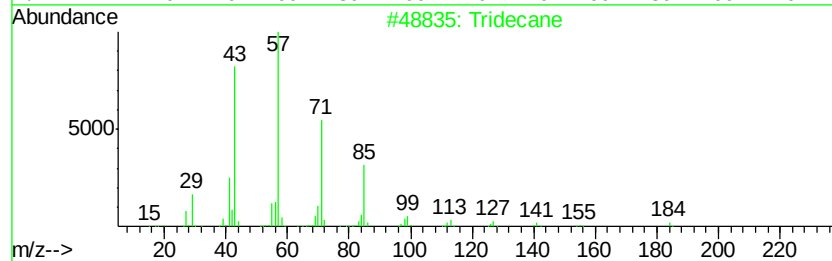
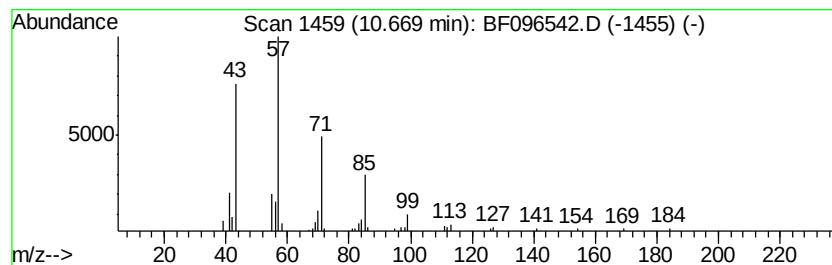
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.67	2.13 ng	72930	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tritetracontane	605	C43H88	007098-21-7	86
5	Dodecane	170	C12H26	000112-40-3	83



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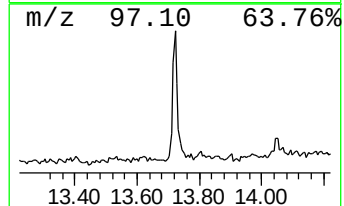
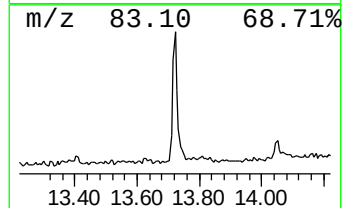
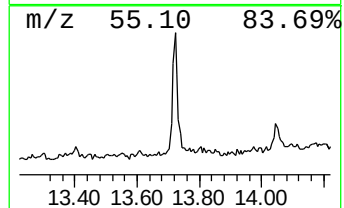
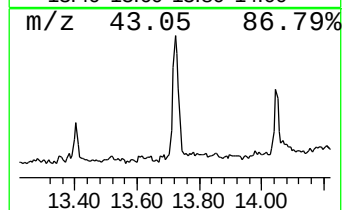
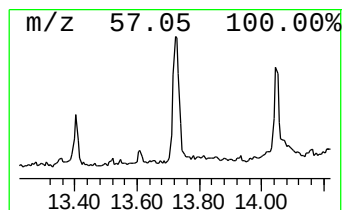
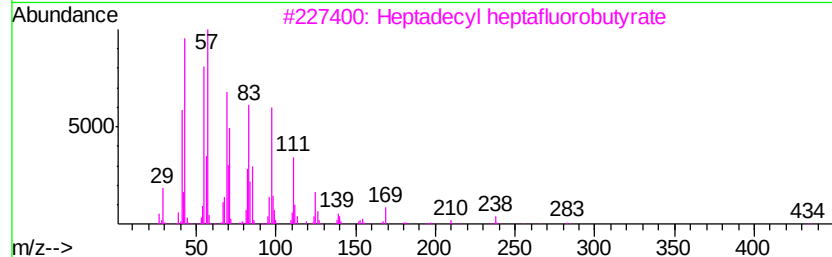
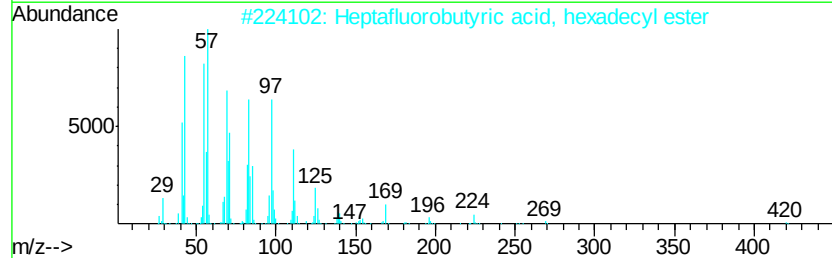
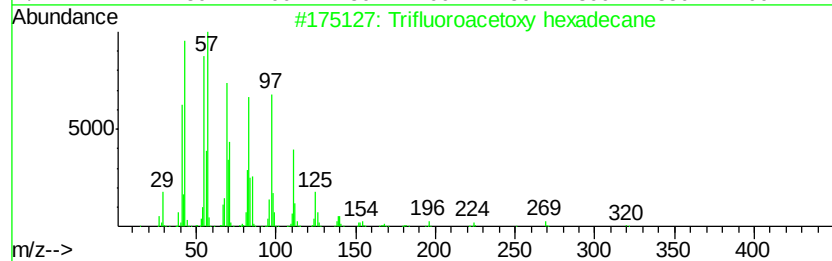
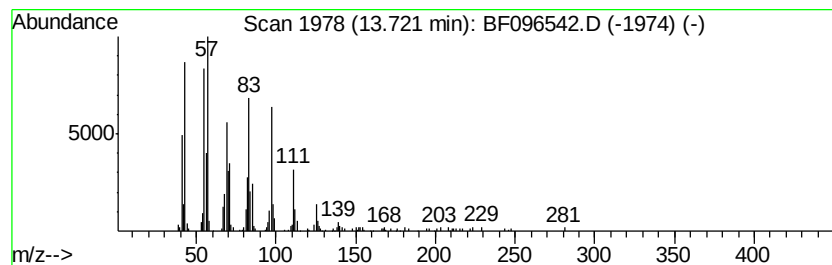
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.72	9.28 ng	345477	Chrysene-d12	13.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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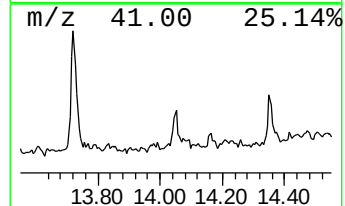
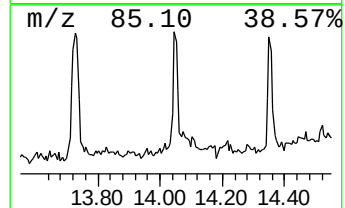
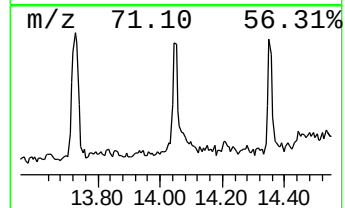
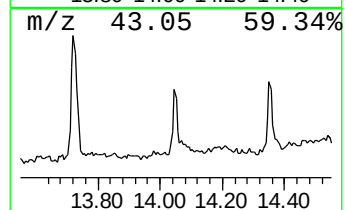
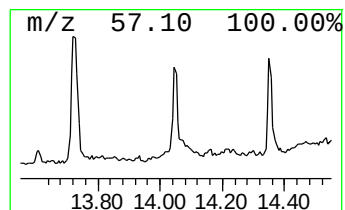
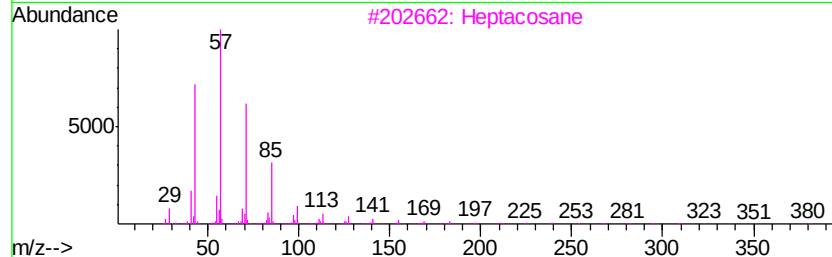
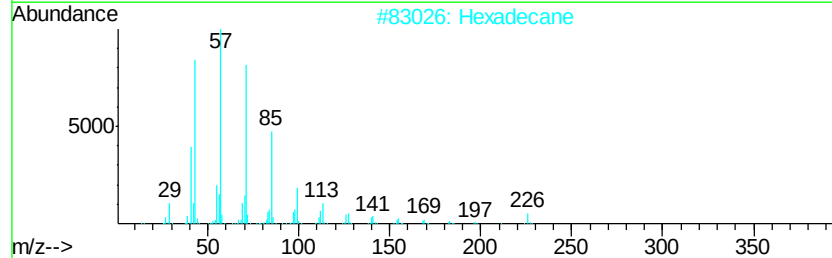
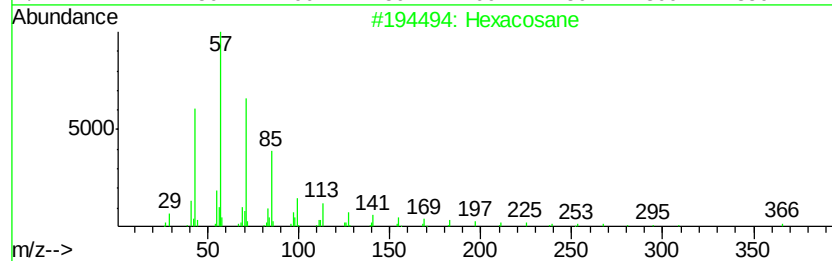
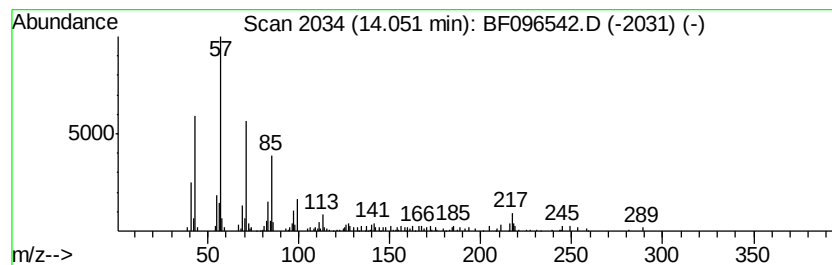
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.05	2.59 ng	96463	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	80
2	Hexadecane	226	C16H34	000544-76-3	72
3	Heptacosane	380	C27H56	000593-49-7	72
4	Tritetracontane	605	C43H88	007098-21-7	72
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	68



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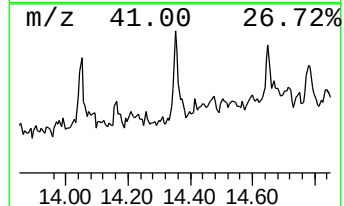
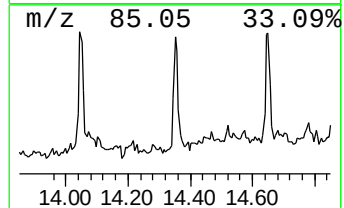
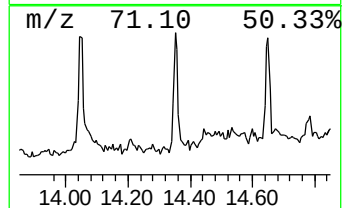
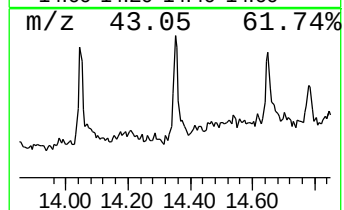
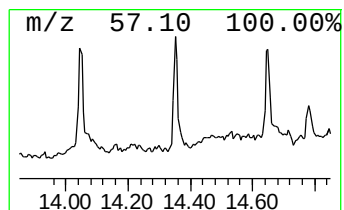
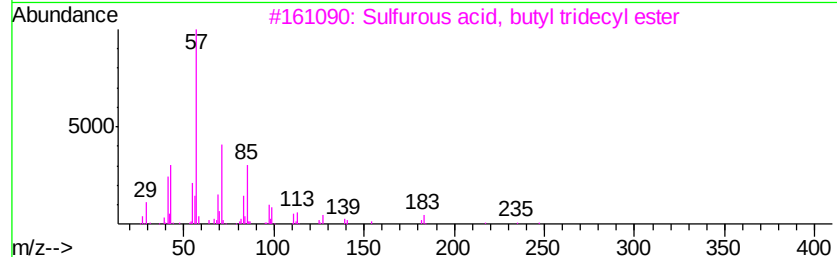
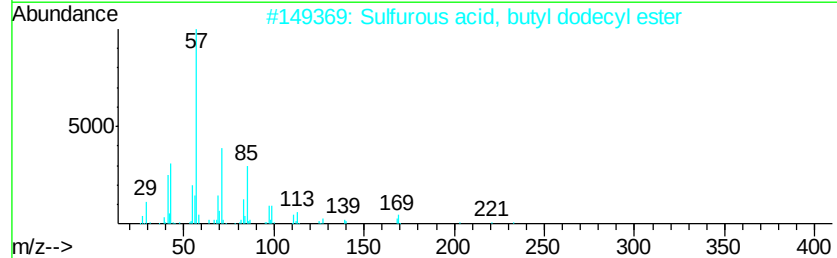
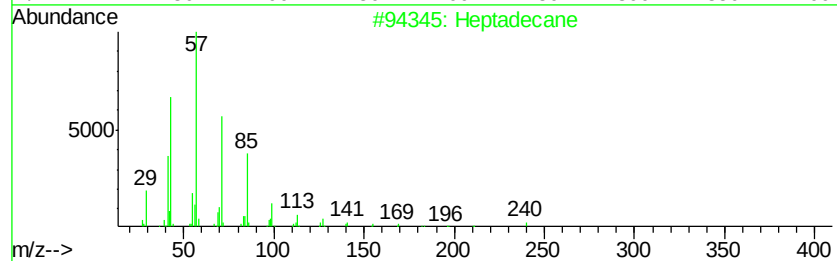
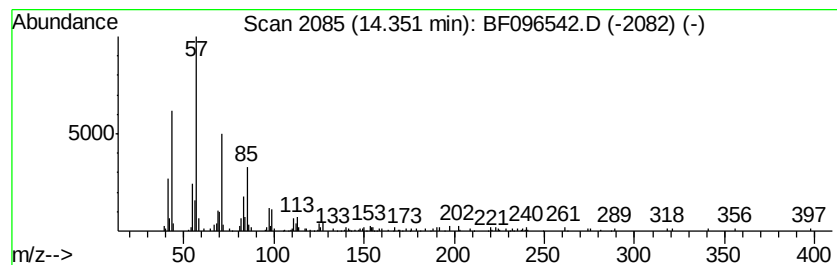
Instrument :
BNA_F
ClientSampleId :
SS4-1-4-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.58 ng	133263	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	Sulfurous acid, butyl dodecyl ester	306 C16H34O3S	1000309-17-9	83
3	Sulfurous acid, butyl tridecyl e...	320 C17H36O3S	1000309-18-0	83
4	Tetradecane, 1-chloro-	232 C14H29Cl	002425-54-9	83
5	Hexatriacontane	507 C36H74	000630-06-8	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096542.D
Acq On : 6 Jul 2017 19:21
Operator : SJ/MA
Sample : I3999-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS4-1-4-COMP

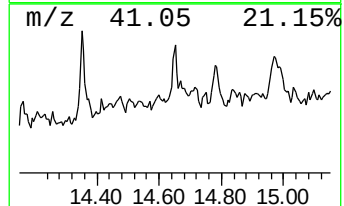
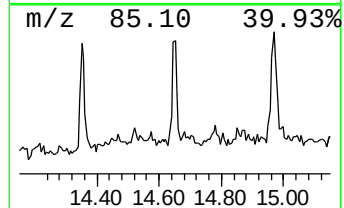
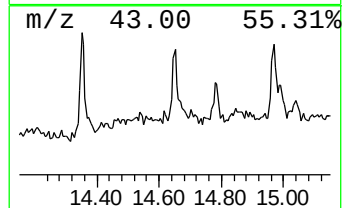
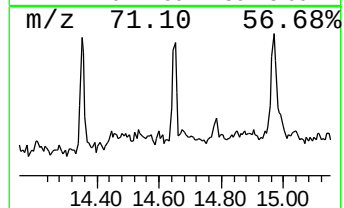
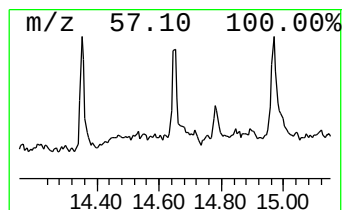
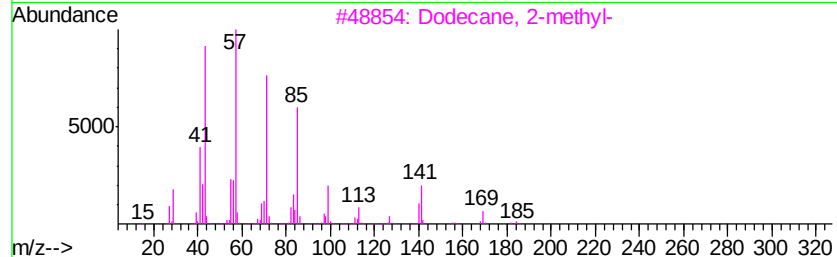
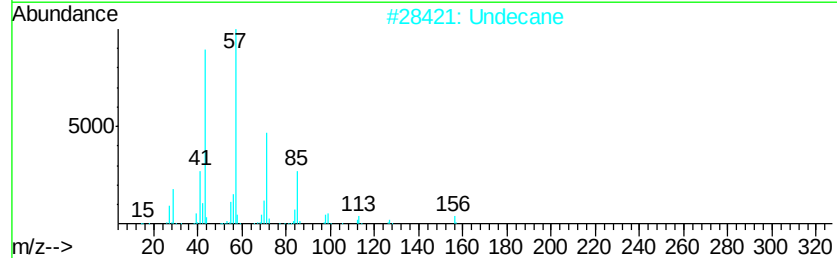
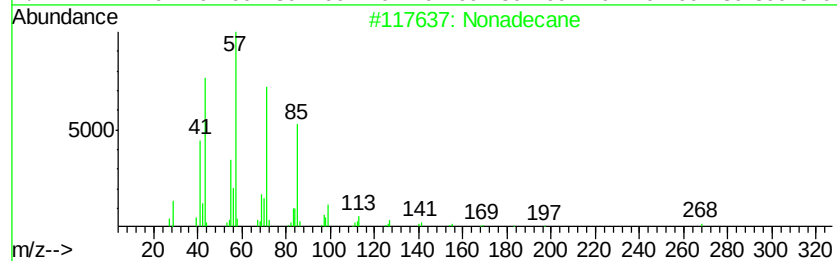
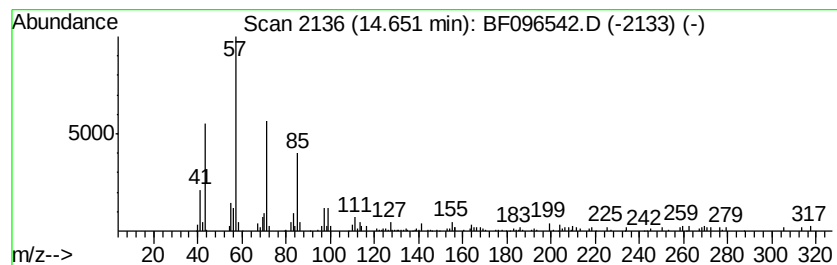
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.56 ng	71147	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	89
2	Undecane		156	C11H24	001120-21-4	80
3	Dodecane, 2-methyl-		184	C13H28	001560-97-0	76
4	Heptacosane		380	C27H56	000593-49-7	72
5	Tetradecane		198	C14H30	000629-59-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096542.D
Acq On : 6 Jul 2017 19:21
Operator : SJ/MA
Sample : I3999-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS4-1-4-COMP

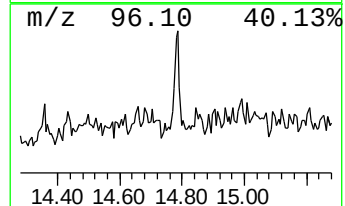
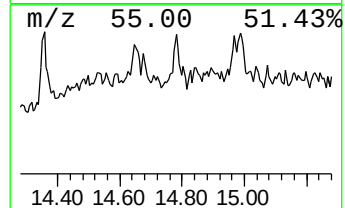
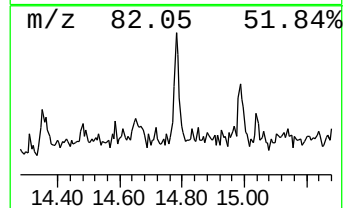
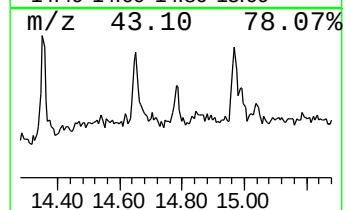
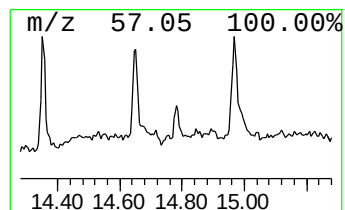
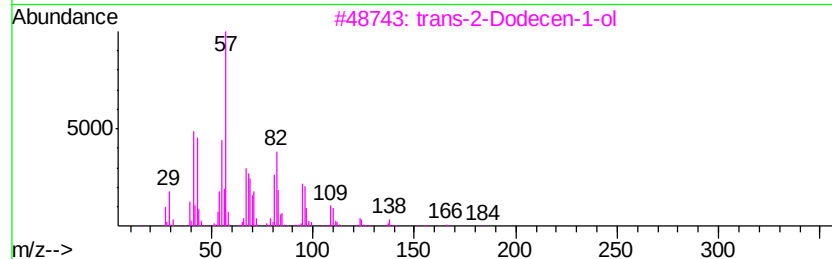
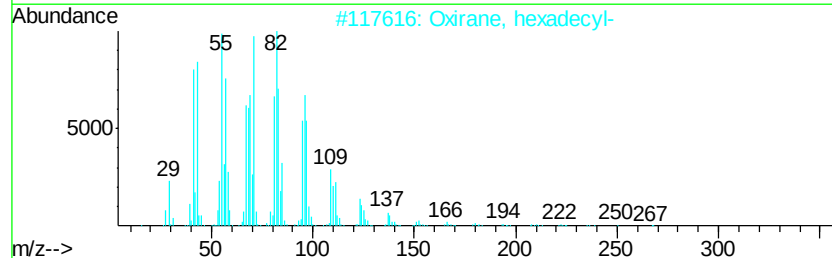
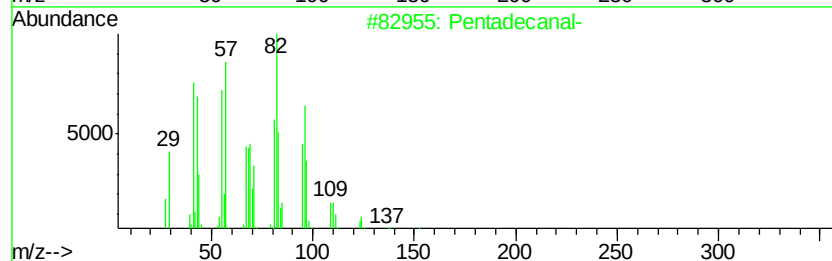
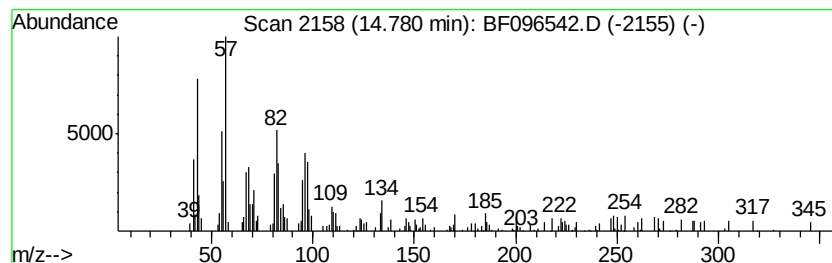
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecanal- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.57 ng	71359	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanal-	226	C15H30O	002765-11-9	81
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
3		trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	70
4		Octadecanal	268	C18H36O	000638-66-4	70
5		Heptadecanal	254	C17H34O	1000376-70-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096542.D
Acq On : 6 Jul 2017 19:21
Operator : SJ/MA
Sample : I3999-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

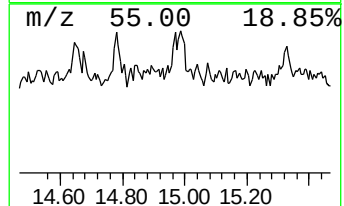
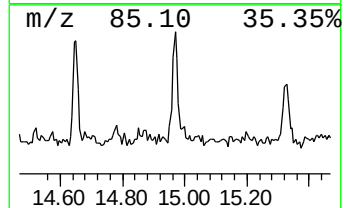
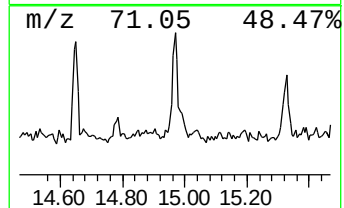
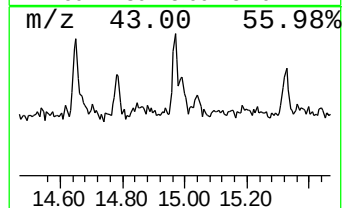
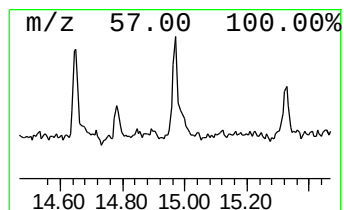
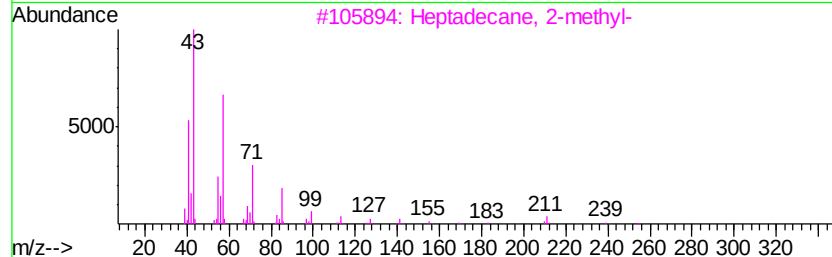
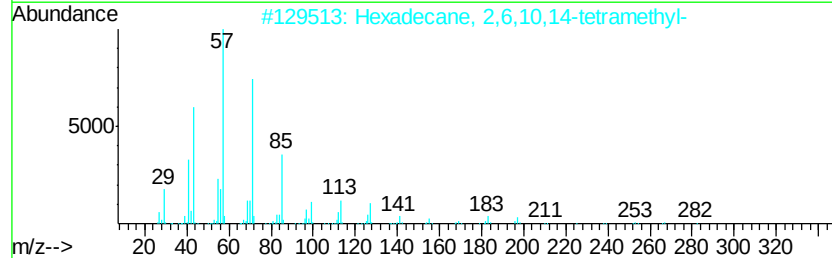
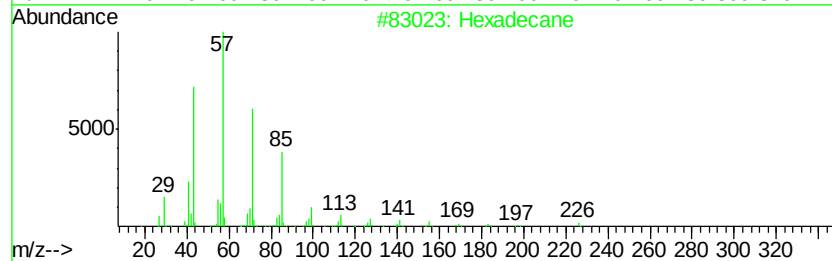
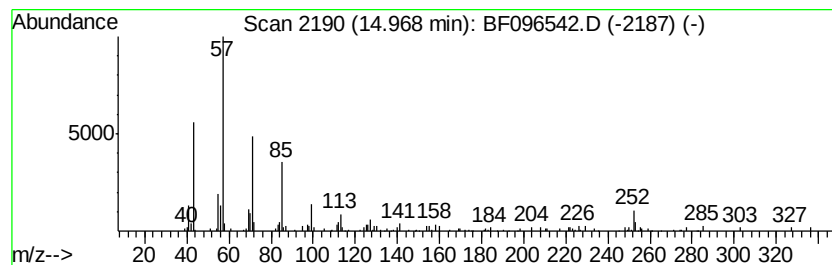
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.97	5.01 ng	139287	Perylene-d12	15.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	76
4	Tetracosane	338	C24H50	000646-31-1	68
5	Pentadecane	212	C15H32	000629-62-9	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096542.D
Acq On : 6 Jul 2017 19:21
Operator : SJ/MA
Sample : I3999-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS4-1-4-COMP

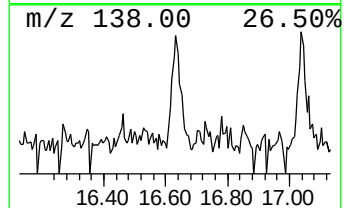
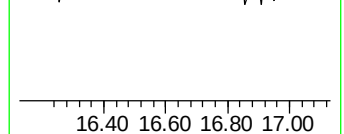
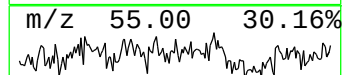
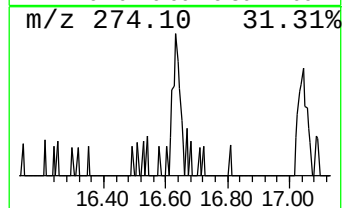
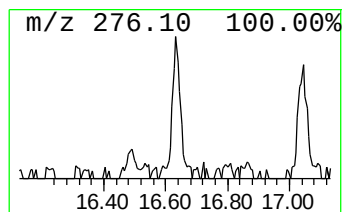
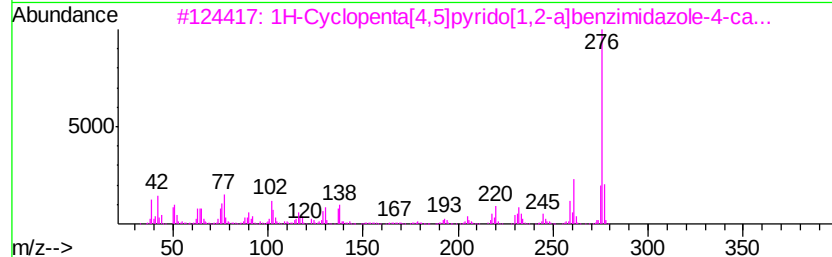
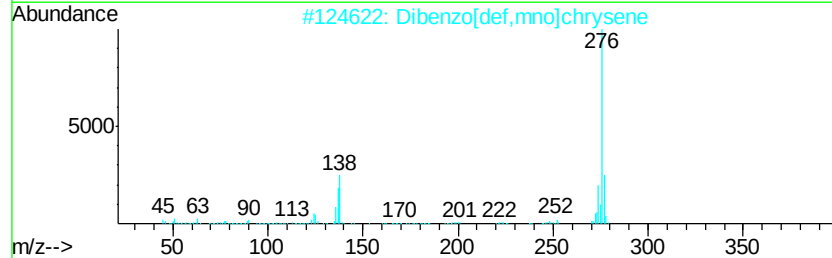
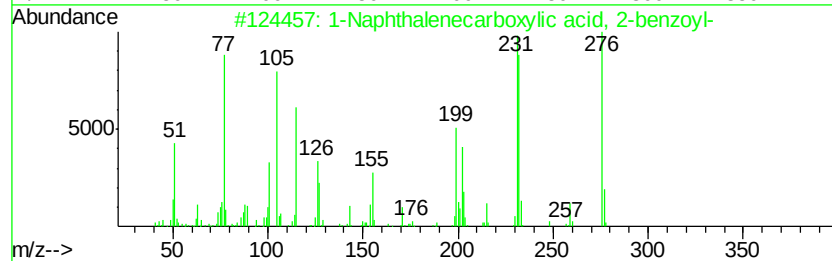
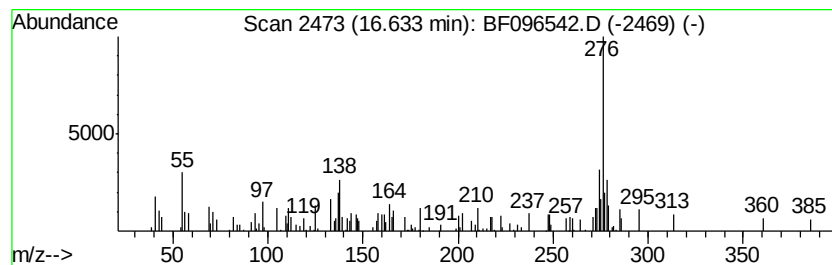
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Naphthalenecarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.37 ng	65801	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Naphthalenecarboxylic acid, 2-...	276	C18H12O3	038119-11-8	86
2		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	50
3		1H-Cyclopenta[4,5]pyrido[1,2-a]b...	276	C17H16N4	329707-31-5	46
4		Benzo[ghi]perylene	276	C22H12	000191-24-2	45
5		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096542.D
Acq On : 6 Jul 2017 19:21
Operator : SJ/MA
Sample : I3999-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.91	15.5	ng	587094	1	6.72	757434	20.0
unknown6.49	6.49	78.1	ng	2957710	1	6.72	757434	20.0
Tridecane	10.67	2.1	ng	72930	4	11.23	683975	20.0
Trifluoroacetoxy ...	13.72	9.3	ng	345477	5	13.86	744523	20.0
Hexacosane	14.05	2.6	ng	96463	5	13.86	744523	20.0
Heptadecane	14.35	3.6	ng	133263	5	13.86	744523	20.0
Nonadecane	14.65	2.6	ng	71147	6	15.27	555701	20.0
Pentadecanal-	14.78	2.6	ng	71359	6	15.27	555701	20.0
Hexadecane	14.97	5.0	ng	139287	6	15.27	555701	20.0
1-Naphthalenecarb...	16.63	2.4	ng	65801	6	15.27	555701	20.0