

Data Path : Z:\HPCHEM1\BNA F\DATA\BF123115\
 Data File : BF084221.D
 Acq On : 1 Jan 2016 3:25
 Operator : UM/SJ
 Sample : G4981-04
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0531

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-BF123115.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	4.224	175	187	189	rBV2	32077	136101	1.64%	0.212%
2	5.082	260	262	265	rVB	795877	893767	10.76%	1.394%
3	5.173	268	270	276	rVB2	50407	84177	1.01%	0.131%
4	5.504	296	299	301	rVB	2734591	3635855	43.76%	5.669%
5	6.522	386	388	391	rBV	2468598	2200036	26.48%	3.430%
6	6.670	398	401	403	rBV	6719348	6613213	79.59%	10.311%
7	6.899	419	421	424	rBV	2159405	1861888	22.41%	2.903%
8	7.059	432	435	437	rVB	7051060	6187974	74.47%	9.648%
9	7.470	467	471	473	rBV	5146349	6034630	72.62%	9.409%
10	7.916	507	510	513	rVB3	61200	90195	1.09%	0.141%
11	8.190	531	534	536	rBV	2523455	2420991	29.14%	3.775%
12	8.819	586	589	590	rVB	89355	90776	1.09%	0.142%
13	9.116	610	615	616	rBV2	50334	93589	1.13%	0.146%
14	9.265	625	628	631	rBV	8627964	8309559	100.00%	12.956%
15	9.653	660	662	664	rVB	168543	181377	2.18%	0.283%
16	9.882	679	682	685	rBV	79768	104667	1.26%	0.163%
17	9.939	685	687	689	rVV	2582408	2423336	29.16%	3.778%
18	9.973	689	690	692	rVB	130623	98535	1.19%	0.154%
19	10.236	708	713	717	rBV	107343	329242	3.96%	0.513%
20	10.373	722	725	729	rVB2	117733	218776	2.63%	0.341%
21	10.465	729	733	735	rBV2	98899	162436	1.95%	0.253%
22	10.591	741	744	746	rBV	2174977	2042463	24.58%	3.185%
23	10.728	753	756	758	rBV	4914212	4715605	56.75%	7.352%
24	10.785	758	761	764	rVV	1770163	2155925	25.95%	3.361%
25	10.854	764	767	769	rVV	110398	146750	1.77%	0.229%
26	11.425	815	817	819	rBV	2425305	2066916	24.87%	3.223%
27	11.642	833	836	838	rBV	356813	439660	5.29%	0.686%
28	12.648	923	924	927	rBV	102327	142116	1.71%	0.222%
29	12.797	935	937	939	rBV	370050	398528	4.80%	0.621%
30	12.842	939	941	944	rVV2	169793	234266	2.82%	0.365%
31	13.014	953	956	959	rBV	6365514	5874597	70.70%	9.160%
32	13.551	1000	1003	1004	rBV	76492	111525	1.34%	0.174%
33	13.585	1004	1006	1008	rBV3	56733	103024	1.24%	0.161%
34	13.802	1022	1025	1027	rBV2	154650	227738	2.74%	0.355%

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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

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35	13.917	1032	1035	1040	rVB3	149075	346590	4.17%	0.540%
36	14.054	1045	1047	1050	rVB	1135300	1384249	16.66%	2.158%
37	14.682	1100	1102	1109	rVB3	76999	154024	1.85%	0.240%
38	15.505	1171	1174	1176	rBV	953850	1421030	17.10%	2.216%

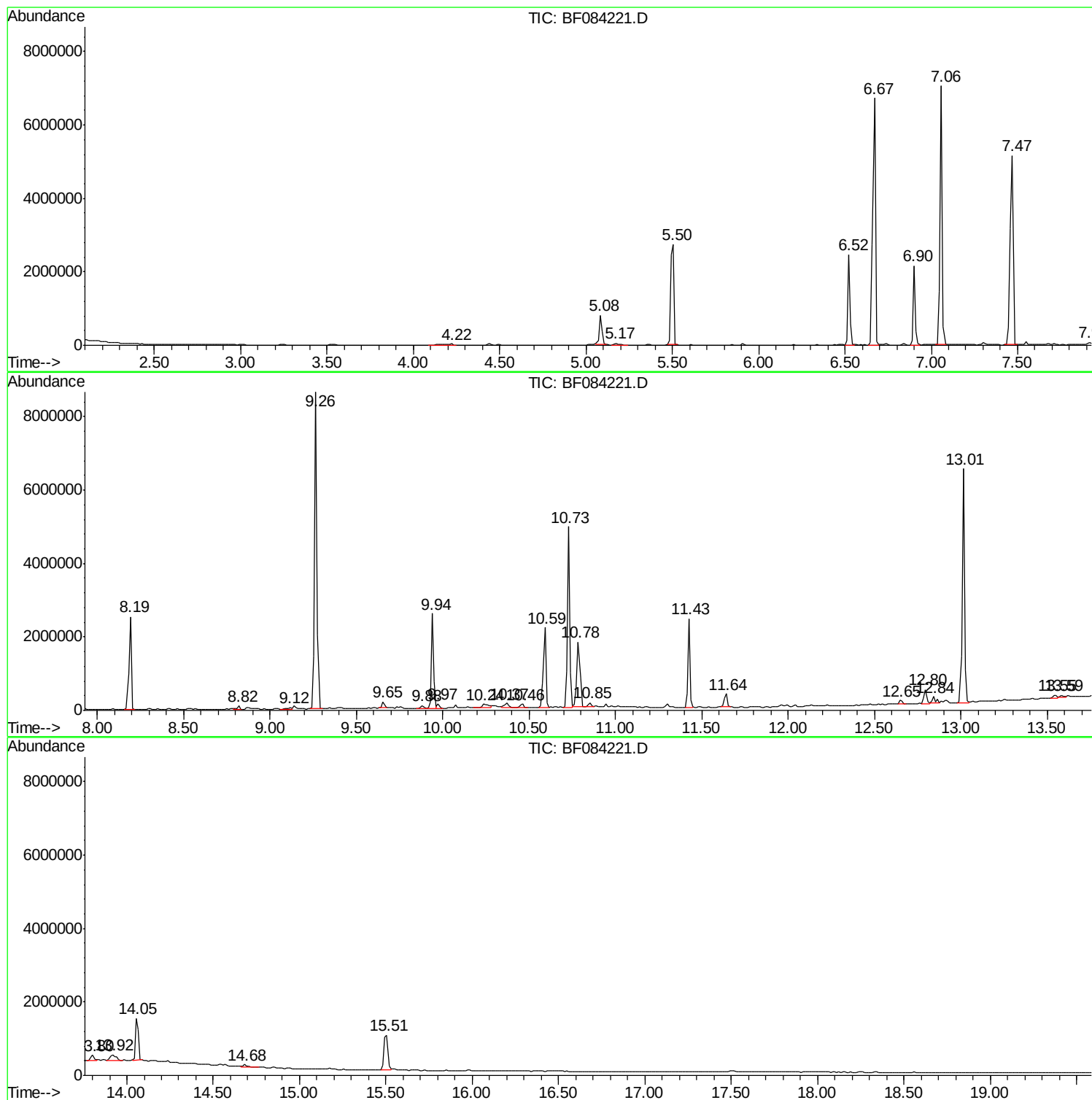
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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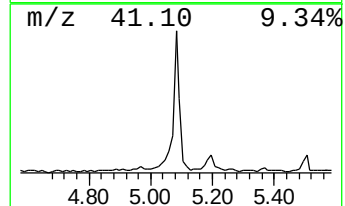
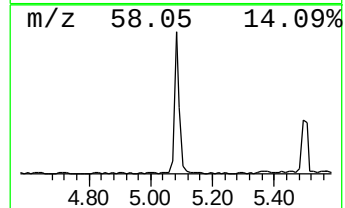
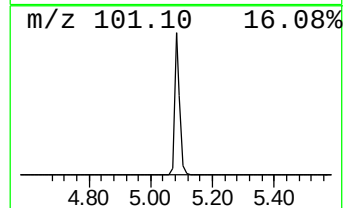
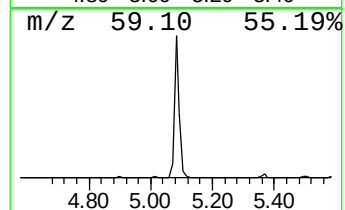
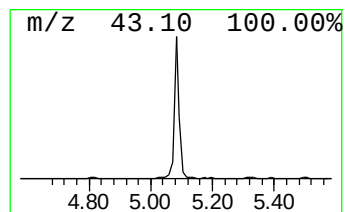
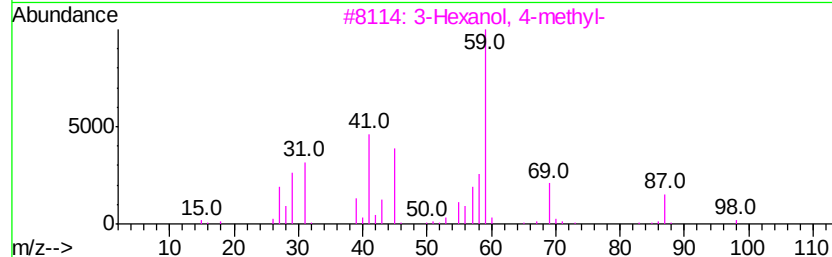
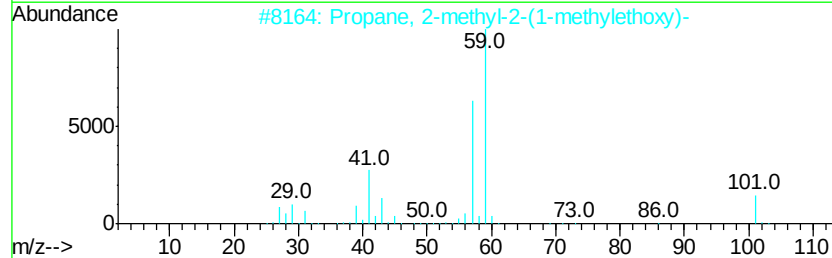
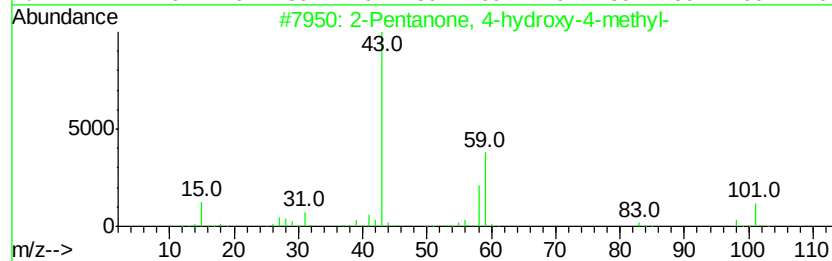
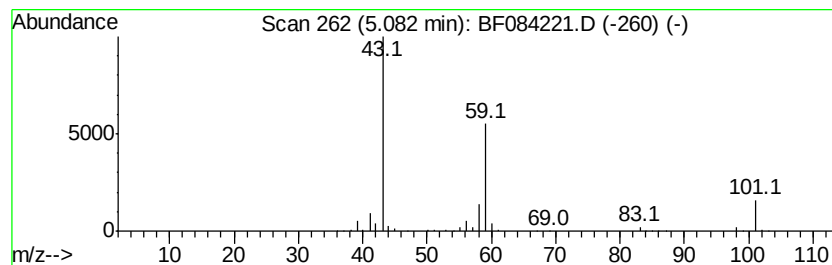
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.08	9.60 ng	893767	1,4-Dichlorobenzene-d4	6.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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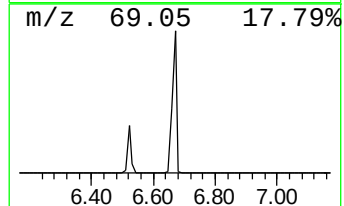
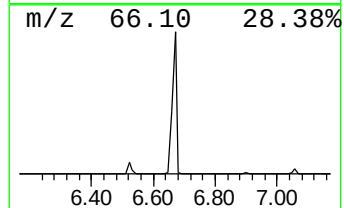
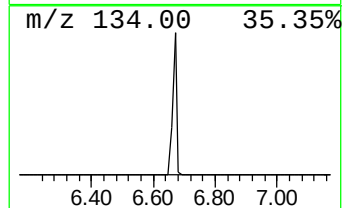
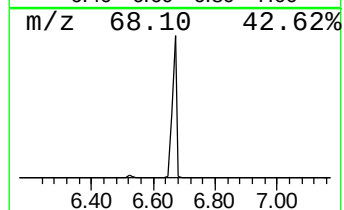
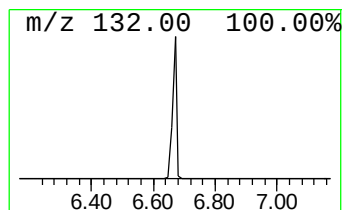
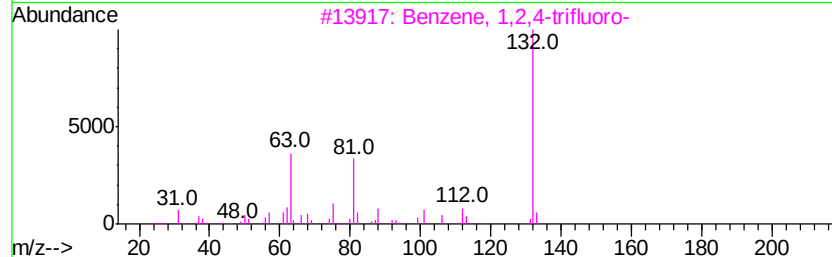
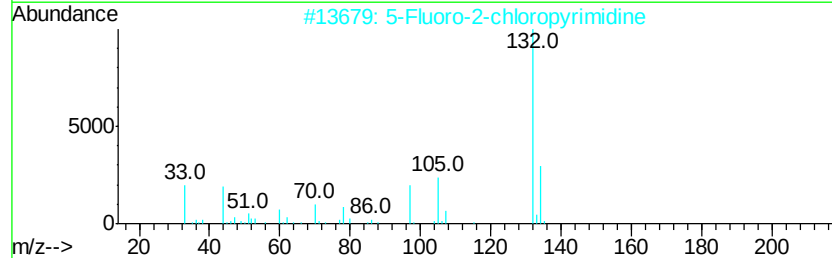
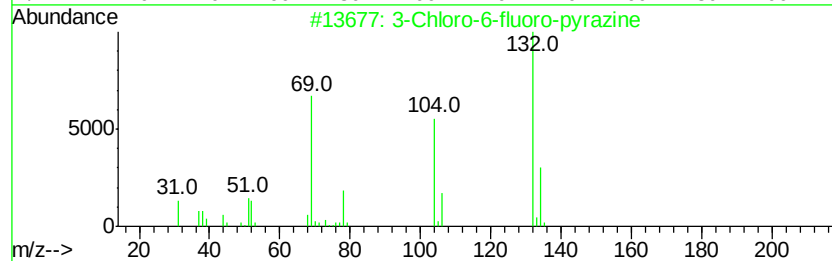
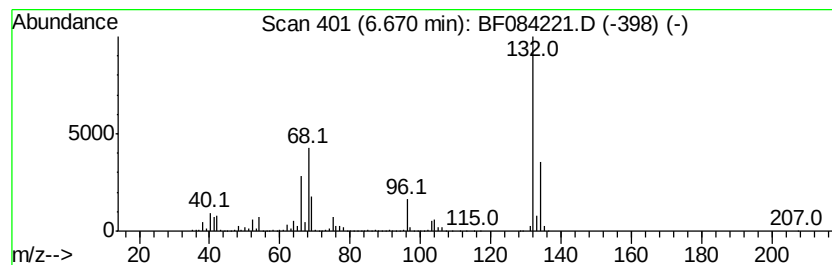
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	71.04 ng	6613210	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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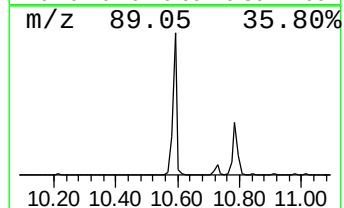
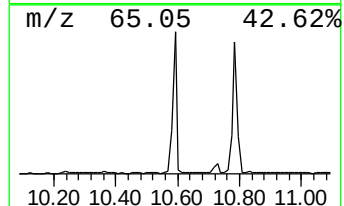
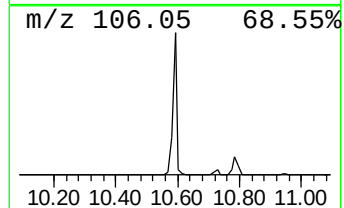
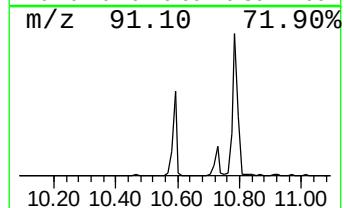
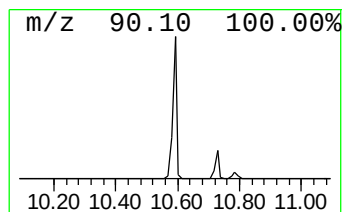
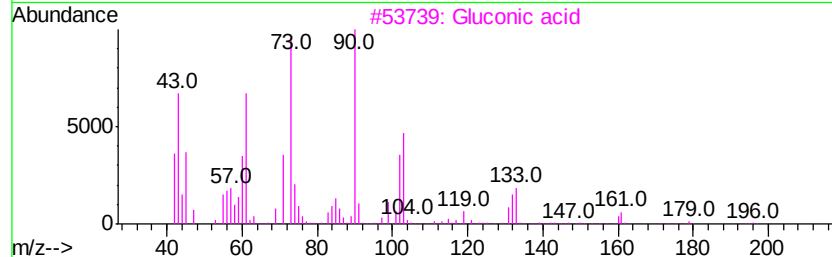
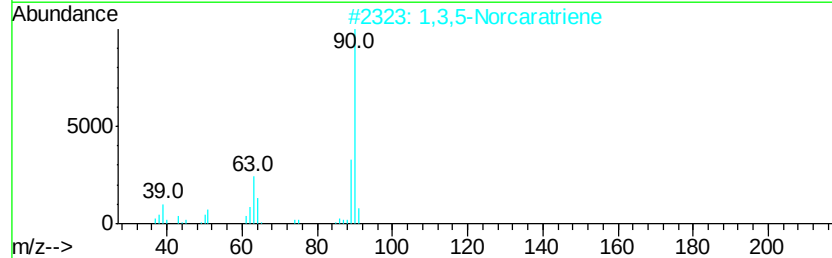
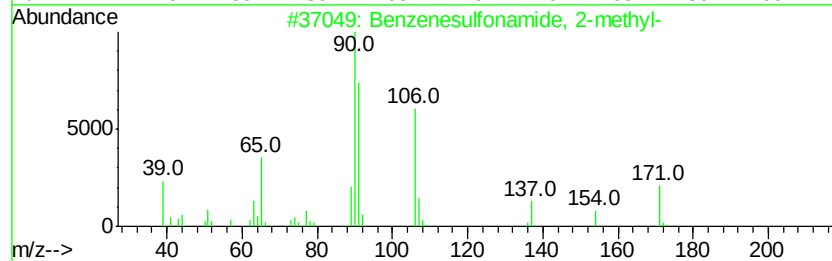
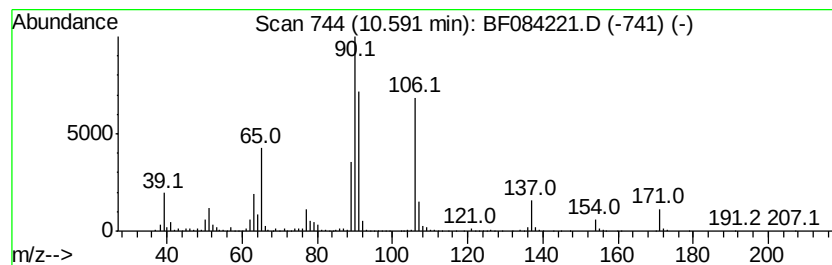
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.59	16.86 ng	2042460	Acenaphthene-d10		9.94
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	97
2	1,3,5-Norcaratriene	90	C7H6	004646-69-9	38
3	Gluconic acid	196	C6H12O7	000526-95-4	38
4	Thiourea, methyl-	90	C2H6N2S	000598-52-7	25
5	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	20



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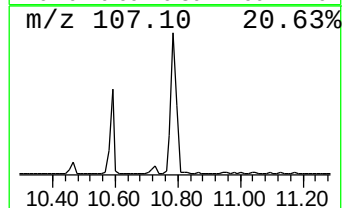
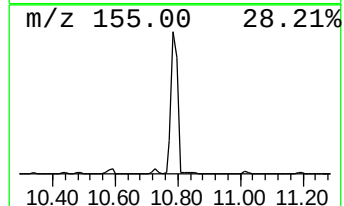
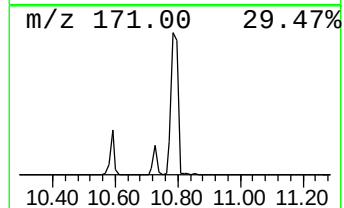
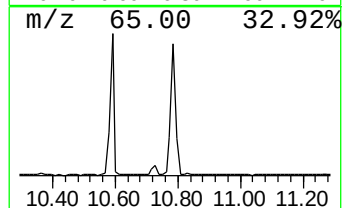
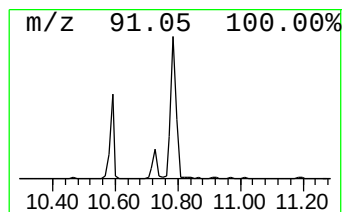
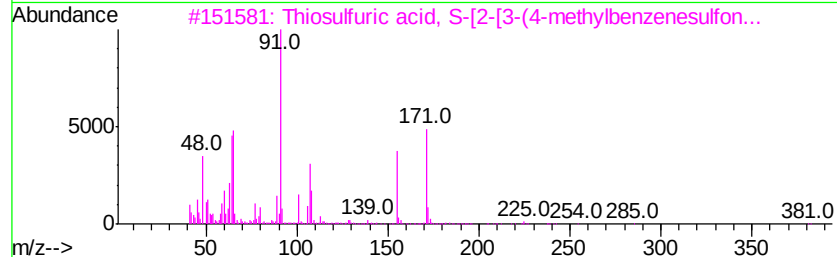
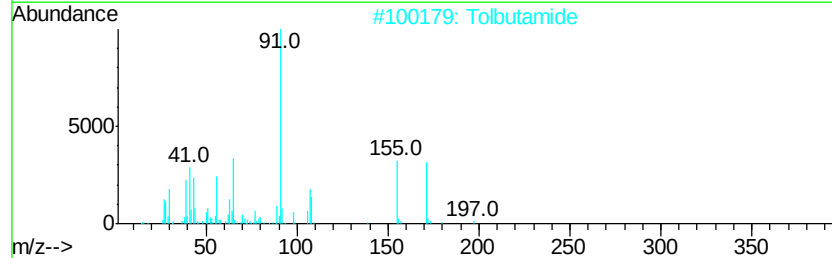
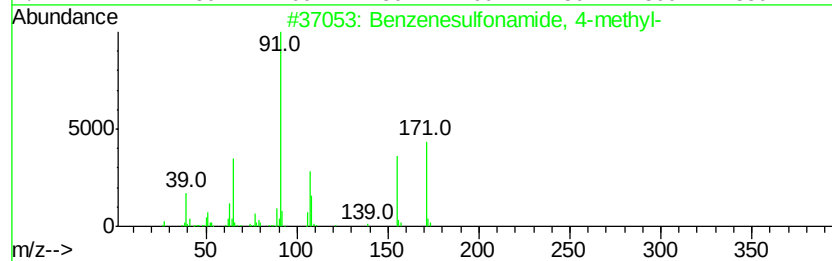
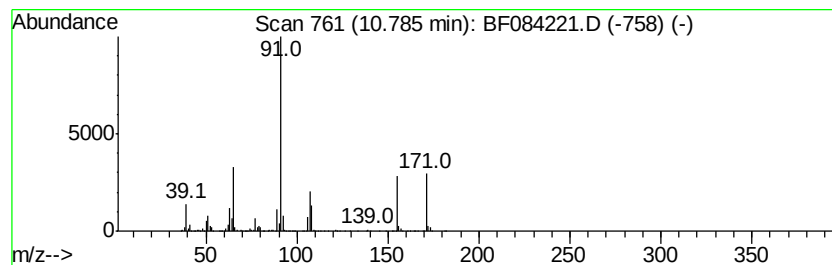
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	20.86 ng	2155930	Phenanthrene-d10	11.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2		Tolbutamide	270	C12H18N2O3S	000064-77-7	91
3		Thiosulfuric acid, S-[2-[3-(4-methyl-...]	381	C12H19N3O5S3	1000255-60-3	80
4		O-p-toluenesulfonyl-N-acetylserine	315	C13H17NO6S	1000126-44-8	72
5		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	68



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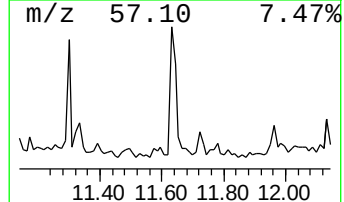
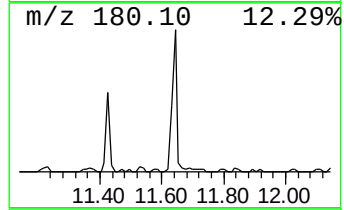
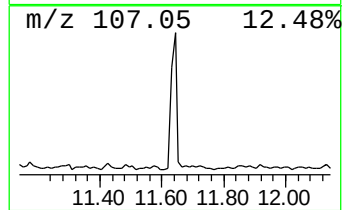
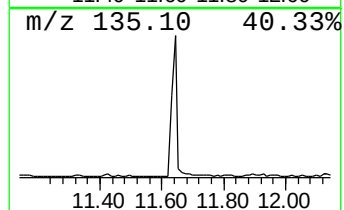
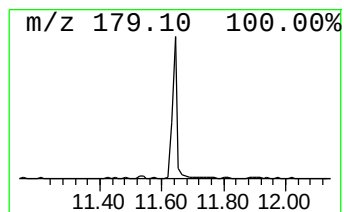
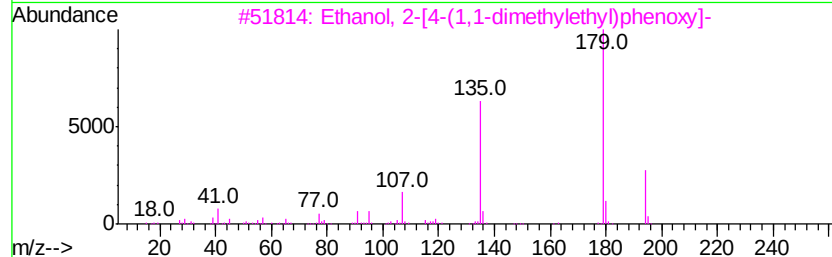
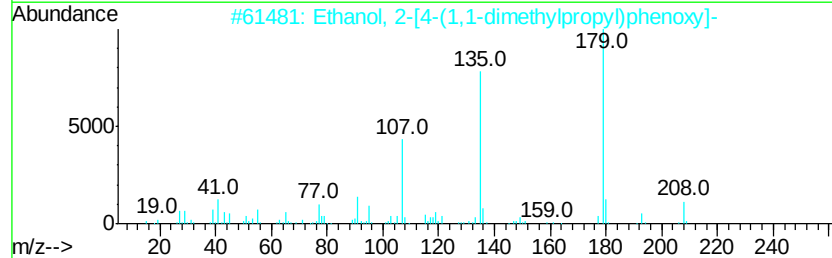
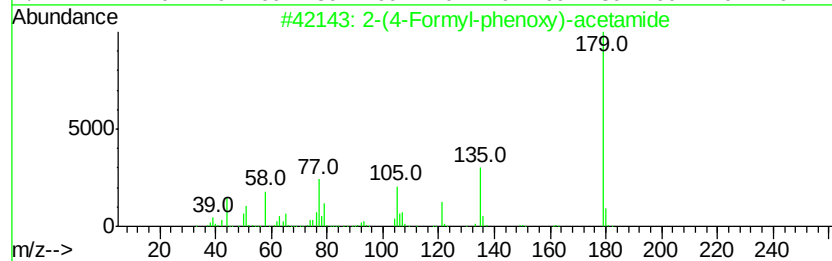
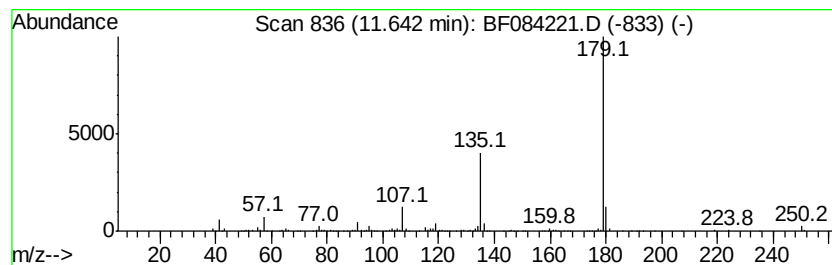
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 2-(4-Formyl-phenoxy)-acetamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	4.25 ng	439660	Phenanthrene-d10	11.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(4-Formyl-phenoxy)-acetamide	179	C9H9NO3	135857-20-4	72
2		Ethanol, 2-[4-(1,1-dimethylpropyl)phenoxy]-	208	C13H20O2	006382-07-6	64
3		Ethanol, 2-[4-(1,1-dimethylethyl)phenoxy]-	194	C12H18O2	000713-46-2	50
4		1,3-Dioxolane, 2-(4-methoxyphenyl)-	194	C11H14O3	036881-00-2	40
5		Acetic acid, [2-[(2-propenylamino)oxy]phenyl]-	235	C12H13NO4	000119-45-9	28



Data Path : Z:\HPCHEM1\BNA F\DATA\BF123115\
Data File : BF084221.D
Acq On : 1 Jan 2016 3:25
Operator : UM/SJ
Sample : G4981-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

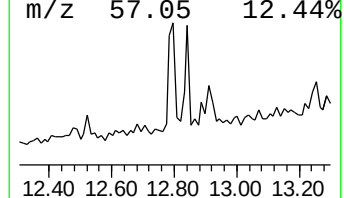
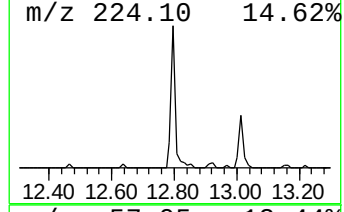
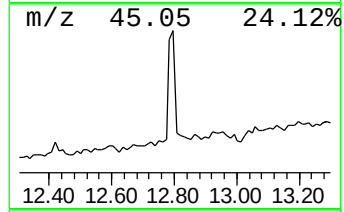
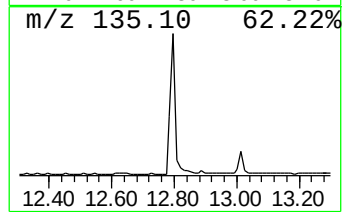
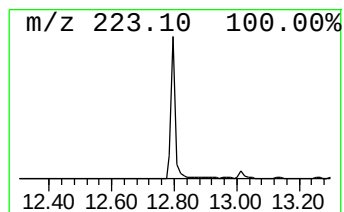
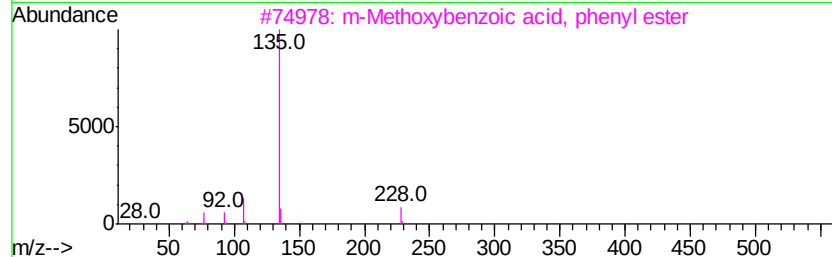
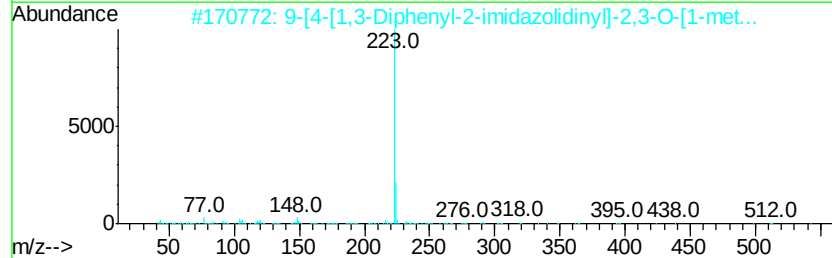
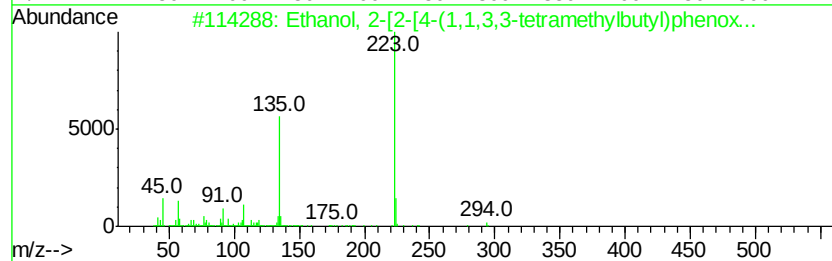
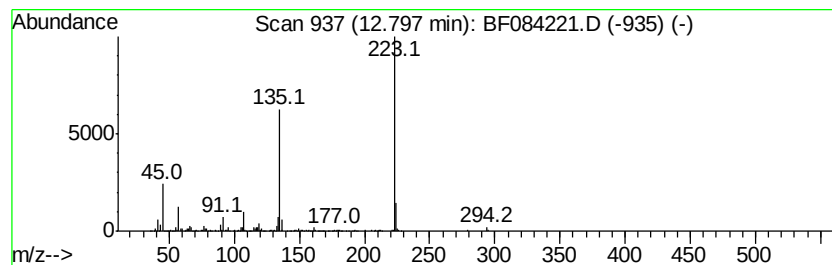
Instrument :
BNA_F
ClientSampleId :
S8-0531

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.80	5.76 ng	398528	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	94
2		9-[4-[1,3-Diphenyl-2-imidazolidi...	542	C28H30N8O4	1000214-46-0	35
3		m-Methoxybenzoic acid, phenyl ester	228	C14H12O3	065853-67-0	22
4		((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	14
5		1,4-Benzenediamine, N-(1-methylh...	220	C14H24N2	039563-50-3	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF123115\
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Instrument :
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ClientSampleId :
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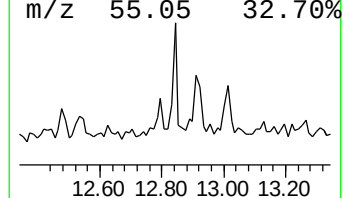
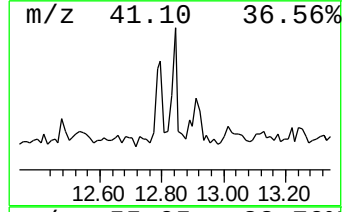
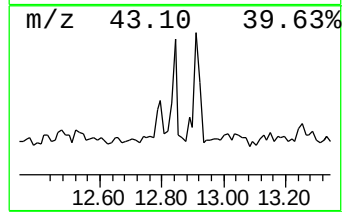
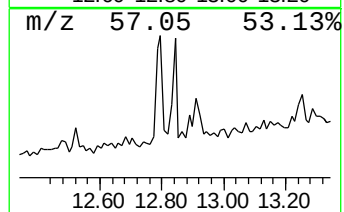
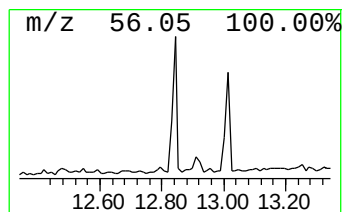
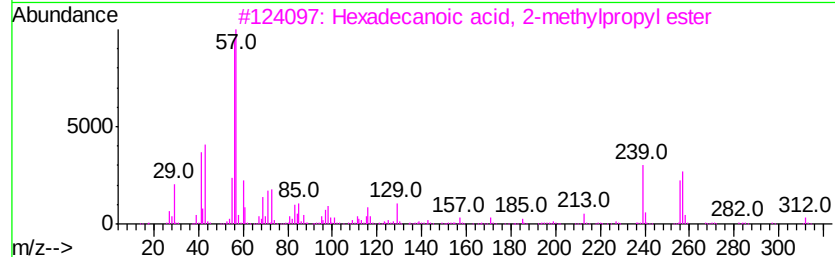
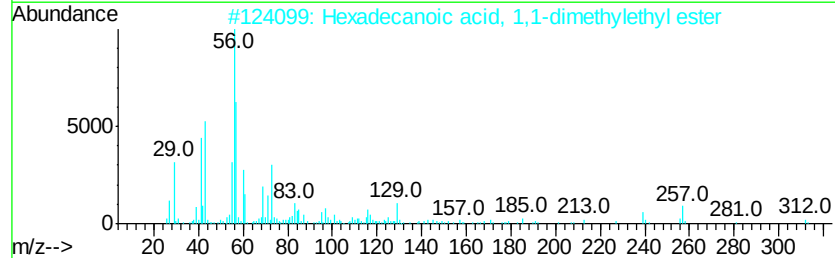
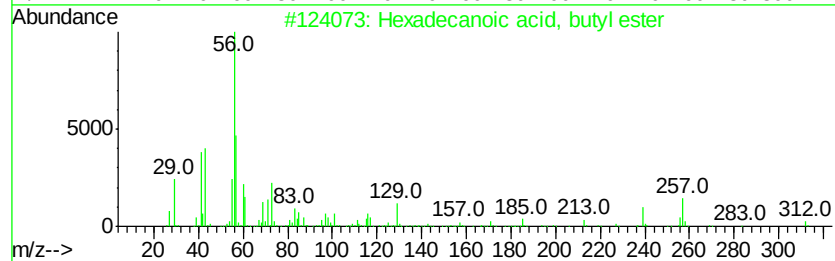
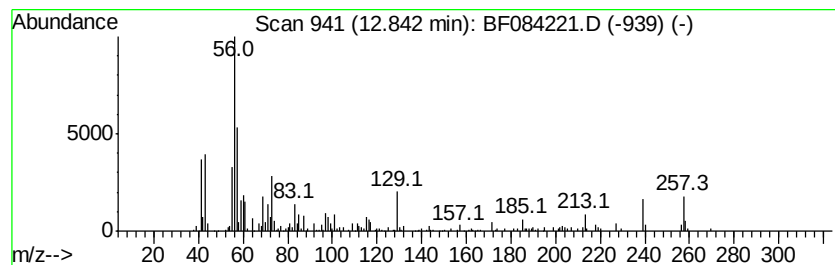
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	3.38 ng	234266	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	59
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
4		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
5		Cyclohexanol, 2-amino-, trans-	115	C6H13NO	006982-39-4	38



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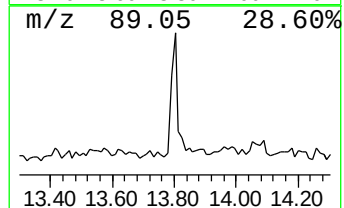
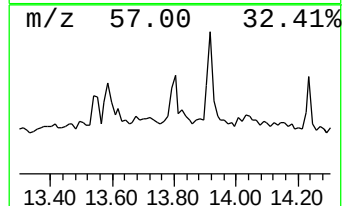
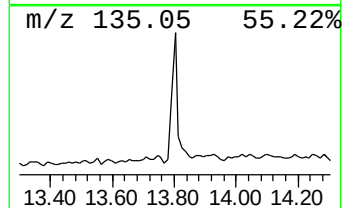
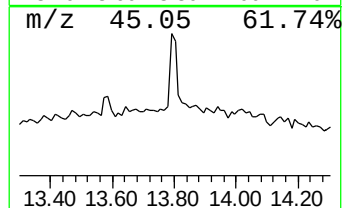
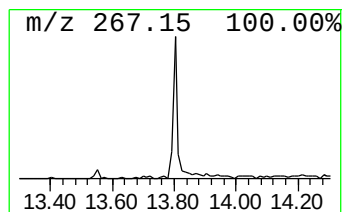
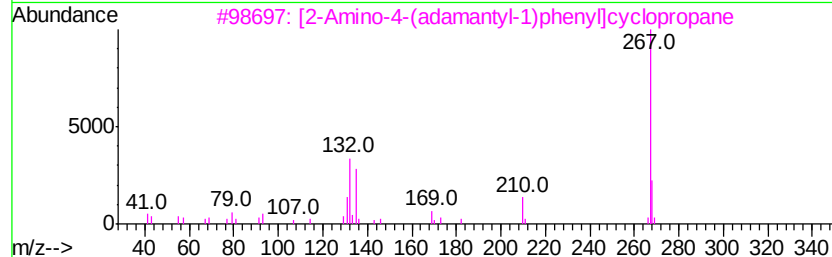
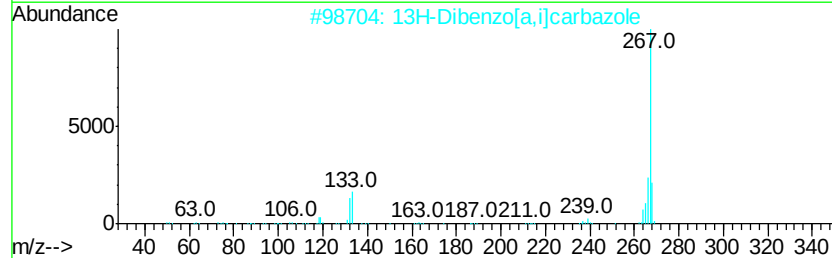
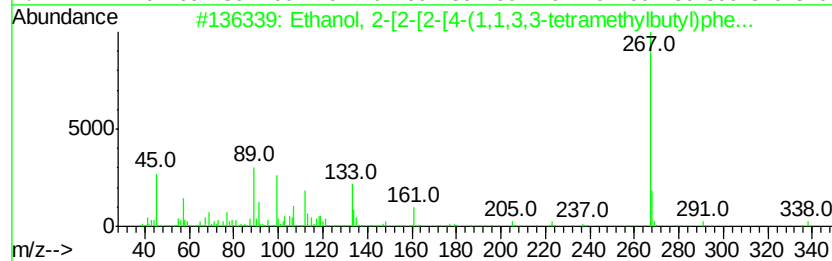
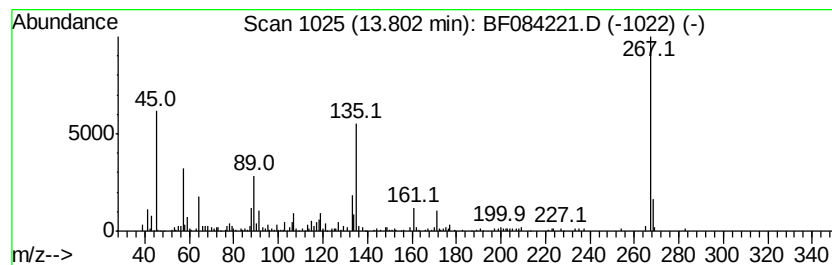
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Ethanol, 2-[2-[2-[4-(1,1,3,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.80	3.29 ng	227738	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol,	2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	62
2	13H-Dibenzo[a,	ilcarbazole	267	C20H13N	000239-64-5	35
3	[2-Amino-4-(adamantyl-1)phenyl]c...		267	C19H25N	1000140-61-3	25
4	2-Methyl-5-(3,4-methylenedioxy)ci...		267	C16H13NO3	094298-70-1	12
5	8-Amino-6-oxo-6H-5-oxa-7-thia-cy...		365	C20H15NO4S	1000294-54-7	12



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Sample : G4981-04
Misc :
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Instrument :
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ClientSampleId :
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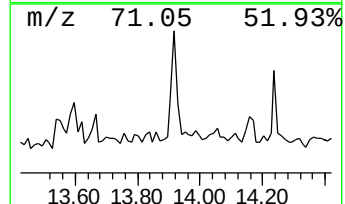
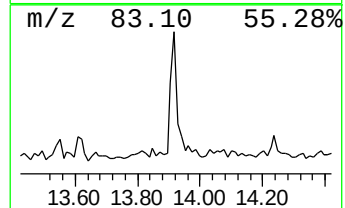
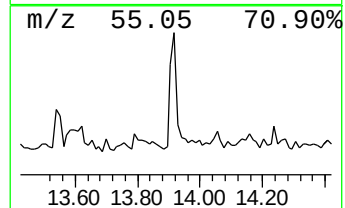
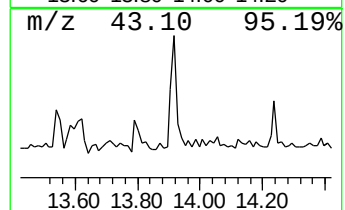
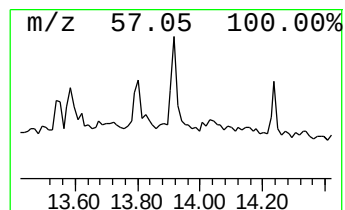
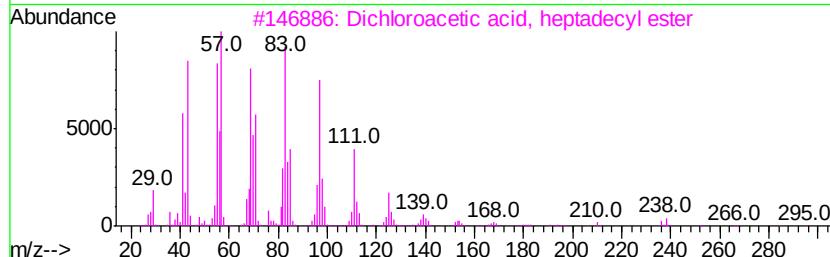
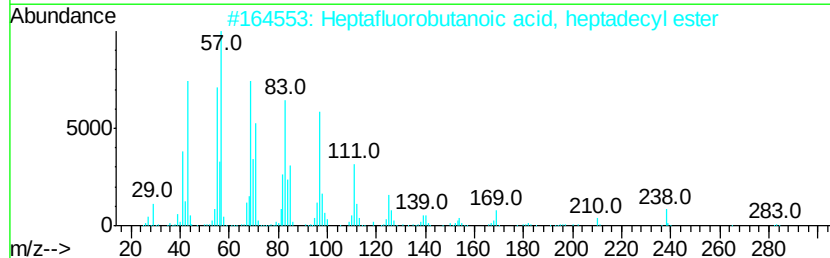
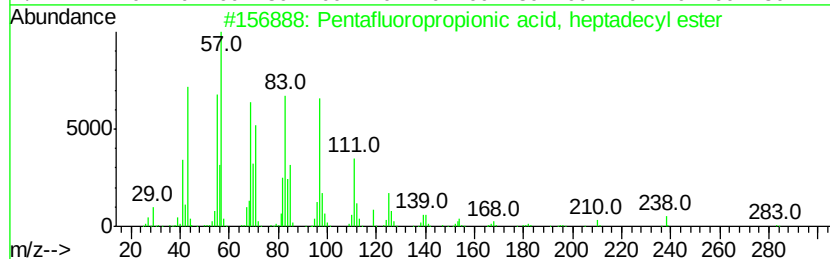
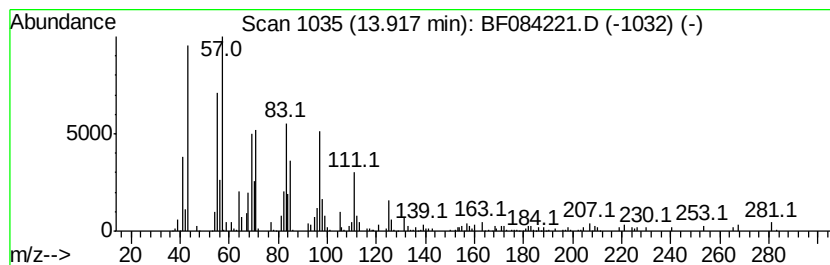
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	5.01 ng	346590	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
2			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	80
5			17-Pentatriacontene	491	C35H70	006971-40-0	74



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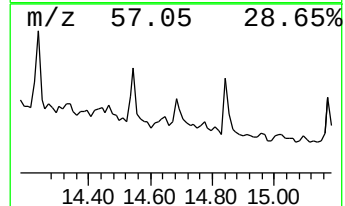
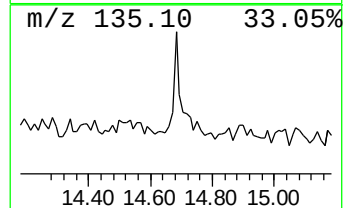
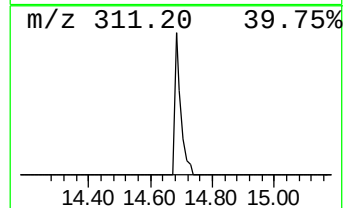
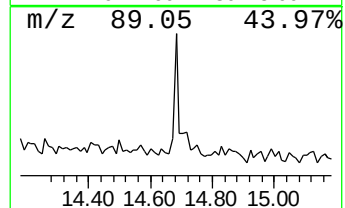
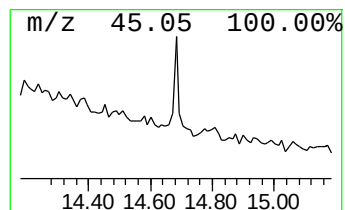
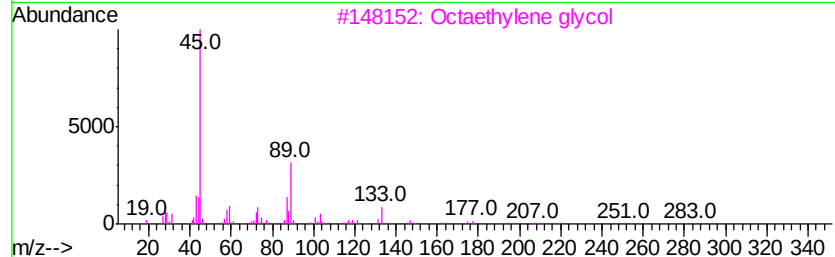
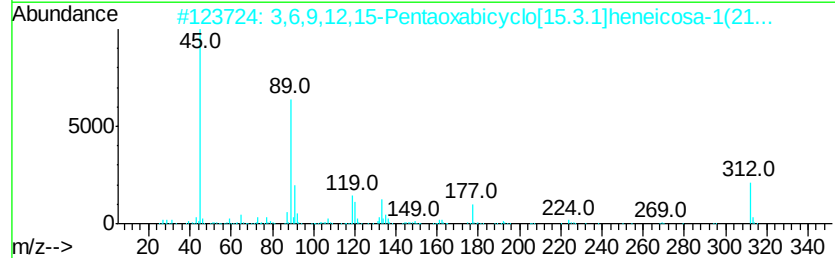
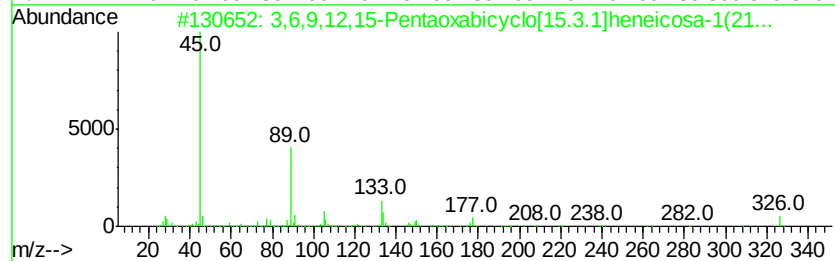
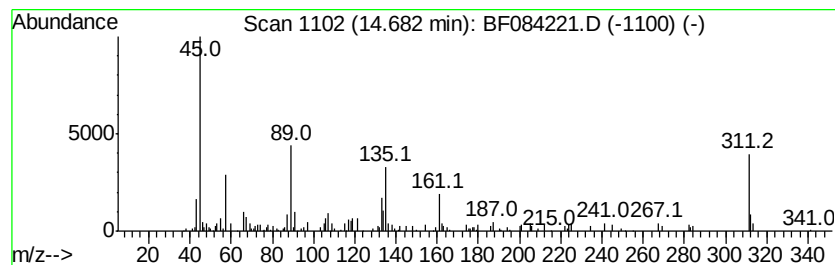
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown14.68 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	2.23 ng	154024	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	43		
2	3,6,9,12,15-Pentaoxabicyclo[15.3...	312	C16H24O6	065112-36-9	37		
3	Octaethylene glycol	370	C16H34O9	1000289-34-2	32		
4	1,4,7,10,13,16-Hexaoxonadecane...	320	C16H32O6	1000163-65-3	32		
5	1-Methoxy-3-(2-trimethylsilyloxy...	274	C15H34O2Si	1000216-82-7	32		



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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	9.6	ng	893767	1	6.90	1861890	20.0
unknown6.67	6.67	71.0	ng	6613210	1	6.90	1861890	20.0
Benzenesulfonamid...	10.59	16.9	ng	2042460	3	9.94	2423340	20.0
Benzenesulfonamid...	10.79	20.9	ng	2155930	4	11.43	2066920	20.0
2-(4-Formyl-pheno...	11.64	4.3	ng	439660	4	11.43	2066920	20.0
Ethanol, 2-[2-[4-...	12.80	5.8	ng	398528	5	14.05	1384250	20.0
Hexadecanoic acid...	12.84	3.4	ng	234266	5	14.05	1384250	20.0
Ethanol, 2-[2-[2-...	13.80	3.3	ng	227738	5	14.05	1384250	20.0
Pentafluoropropio...	13.92	5.0	ng	346590	5	14.05	1384250	20.0
unknown14.68	14.68	2.2	ng	154024	5	14.05	1384250	20.0