

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF123115\
 Data File : BF084223.D
 Acq On : 1 Jan 2016 4:20
 Operator : UM/SJ
 Sample : G4981-06
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0533

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-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	4.441	204	206	210	rVB	116115	133224	1.45%	0.192%
2	5.093	260	263	269	rVB	823797	1087831	11.83%	1.571%
3	5.504	296	299	301	rBV	5310141	5198434	56.52%	7.507%
4	6.521	386	388	391	rBV	2500128	2961106	32.20%	4.276%
5	6.670	398	401	403	rBV	8214026	7881524	85.70%	11.382%
6	6.899	419	421	424	rVB	2399208	1963697	21.35%	2.836%
7	7.059	432	435	437	rBV	7616785	6814873	74.10%	9.842%
8	7.470	467	471	473	rBV	6033651	6836688	74.34%	9.873%
9	7.676	487	489	491	rBV2	156193	220112	2.39%	0.318%
10	8.190	531	534	536	rBV	2538995	2571583	27.96%	3.714%
11	9.265	625	628	631	rBV	8707246	9196797	100.00%	13.282%
12	9.653	660	662	665	rBV	576993	706751	7.68%	1.021%
13	9.939	685	687	690	rVB	2714640	2598225	28.25%	3.752%
14	10.362	722	724	727	rBV3	67788	138520	1.51%	0.200%
15	10.728	753	756	759	rBV	5553682	5913800	64.30%	8.541%
16	10.853	763	767	773	rVV3	107403	199317	2.17%	0.288%
17	11.310	804	807	810	rBV2	482755	662848	7.21%	0.957%
18	11.425	815	817	819	rBV	2963609	2464347	26.80%	3.559%
19	12.842	938	941	943	rBV	341789	295245	3.21%	0.426%
20	12.911	943	947	949	rVB	77383	99222	1.08%	0.143%
21	13.014	953	956	959	rBV	7627920	7435329	80.85%	10.738%
22	13.551	1000	1003	1004	rBV	140941	187066	2.03%	0.270%
23	13.916	1033	1035	1039	rBV	258595	342632	3.73%	0.495%
24	14.054	1045	1047	1050	rBV	1299267	1663438	18.09%	2.402%
25	15.494	1170	1173	1176	rBV	1024225	1524480	16.58%	2.202%
26	16.477	1254	1259	1262	rBV	60605	147039	1.60%	0.212%

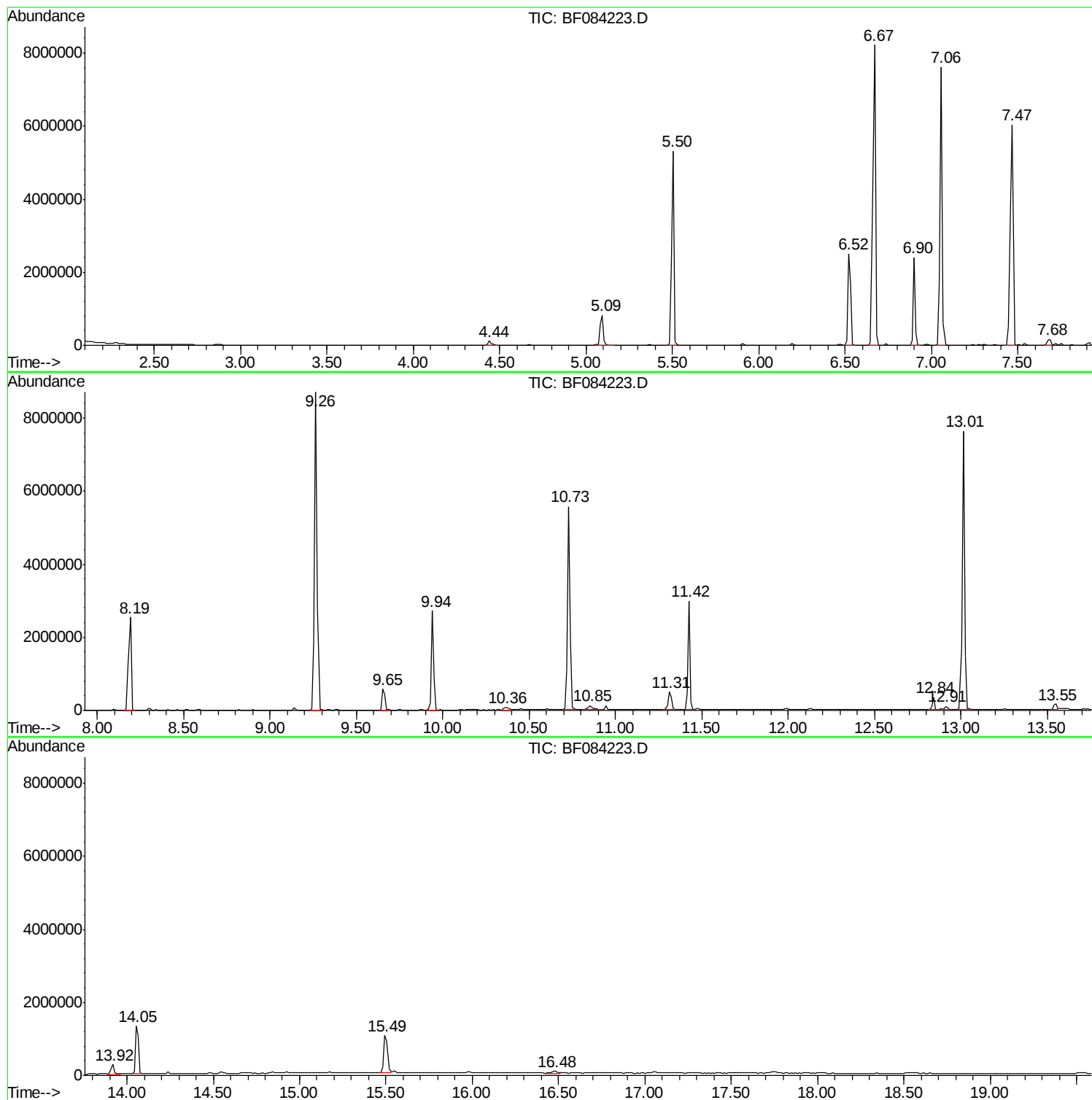
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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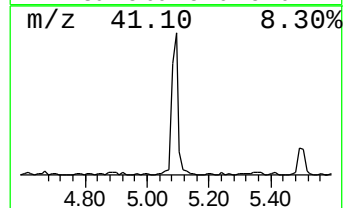
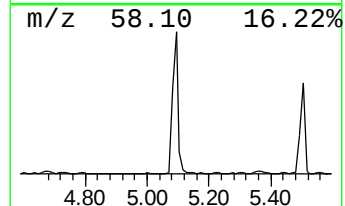
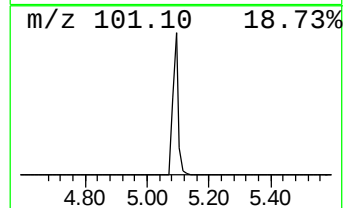
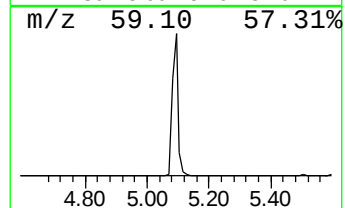
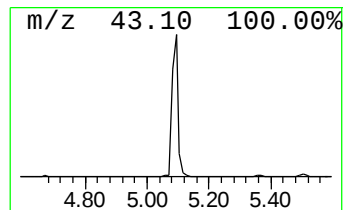
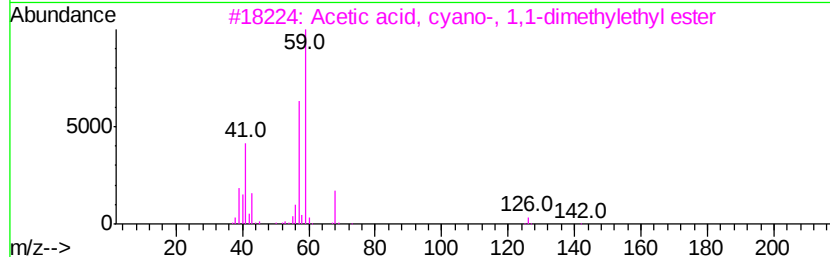
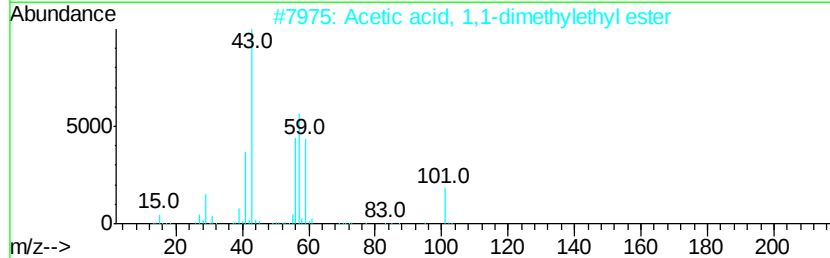
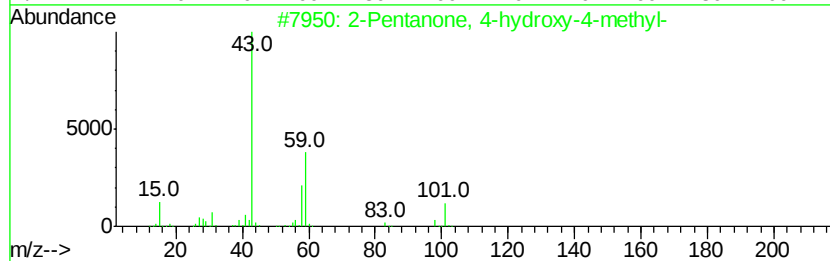
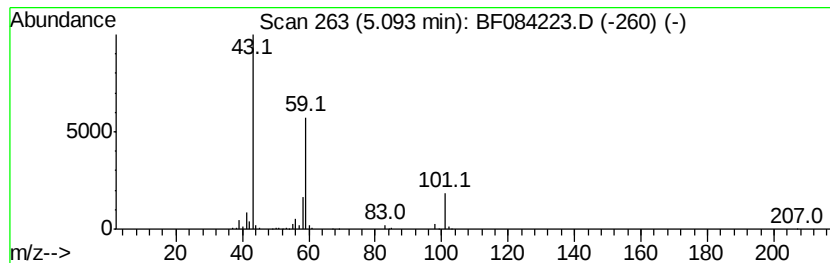
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	11.08 ng	1087830	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	59	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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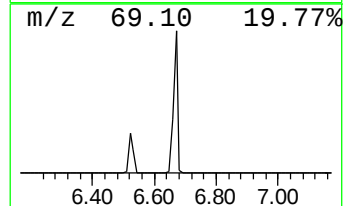
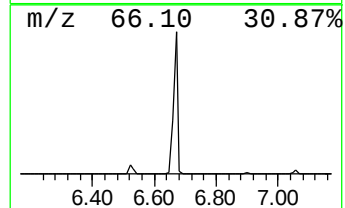
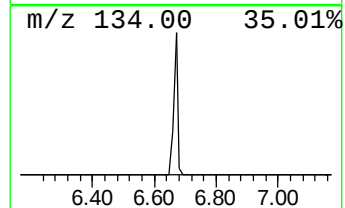
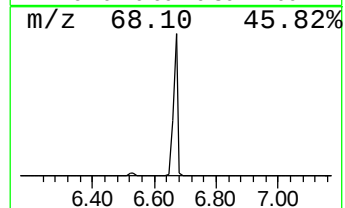
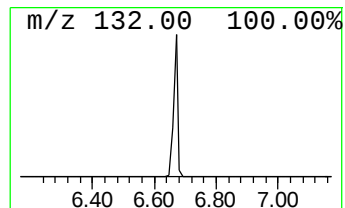
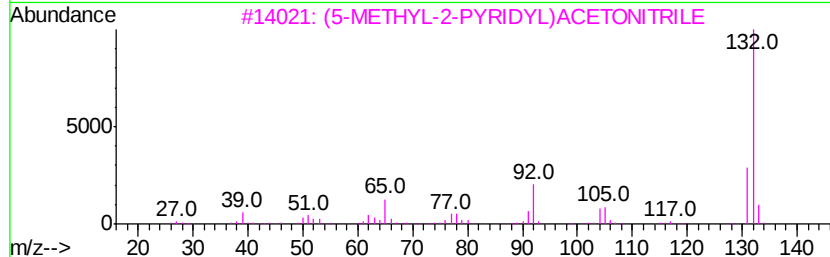
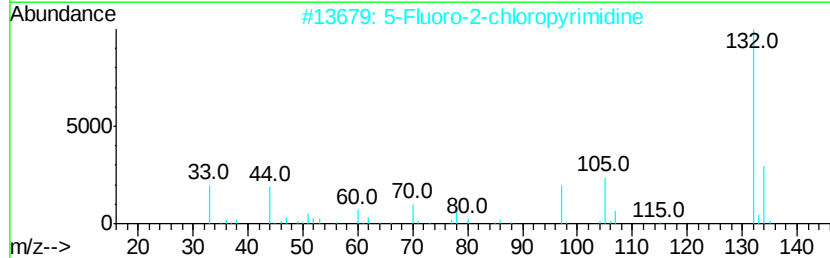
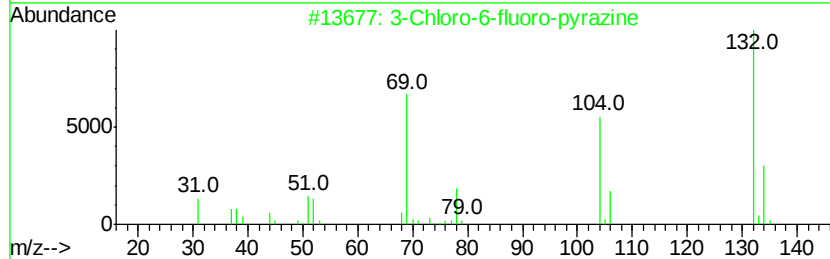
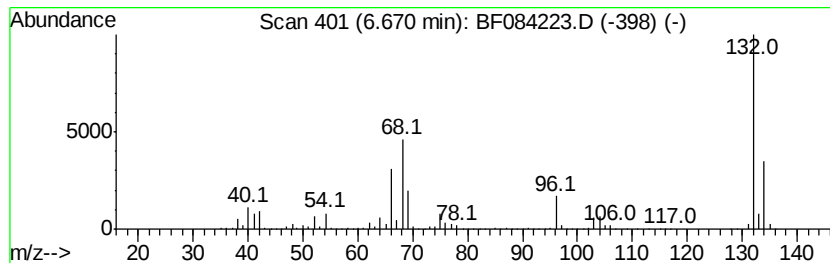
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	80.27 ng	7881520	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	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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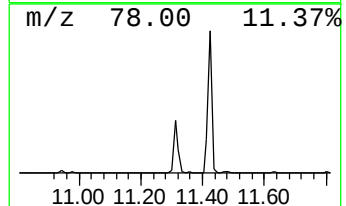
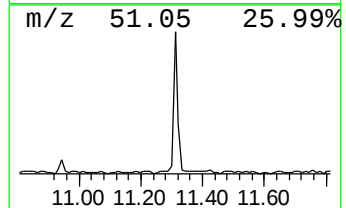
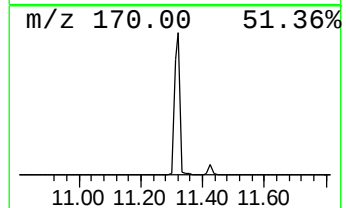
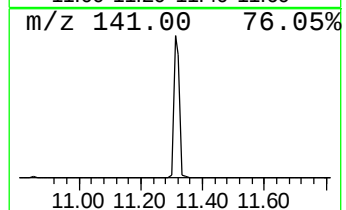
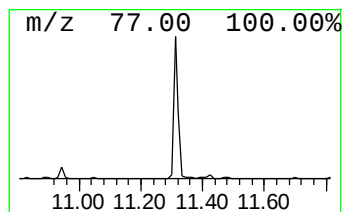
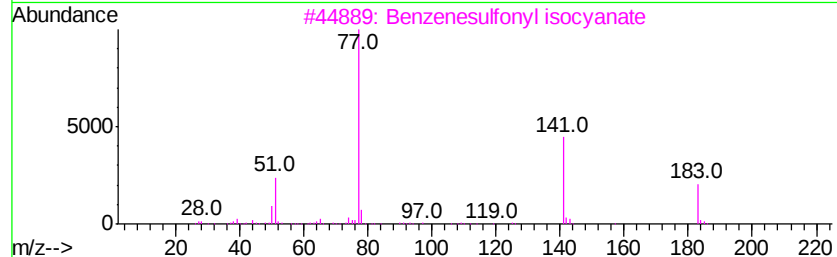
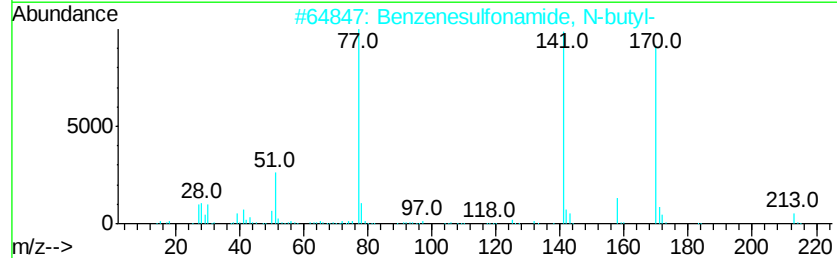
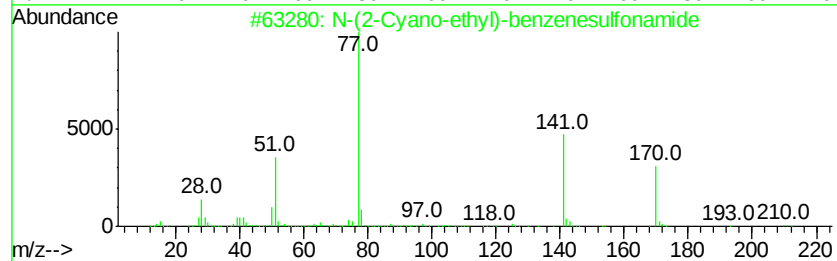
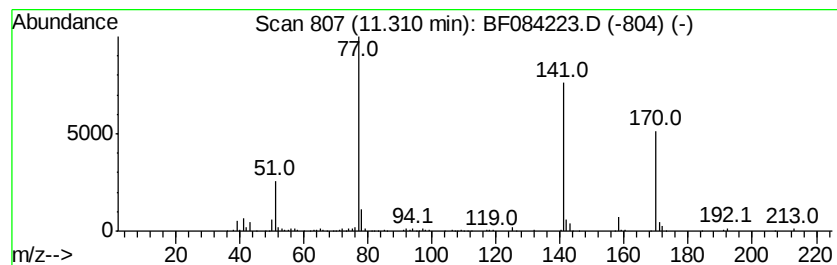
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 N-(2-Cyano-ethyl)-benzenesu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.31	5.38 ng	662848	Phenanthrene-d10		11.42	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	83
2		Benzenesulfonamide, N-butyl-	213	C10H15N02S	003622-84-2	83
3		Benzenesulfonyl isocyanate	183	C7H5N03S	002845-62-7	53
4		Benzenesulfonyl chloride	176	C6H5Cl02S	000098-09-9	53
5		N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6N03S	055734-41-3	53



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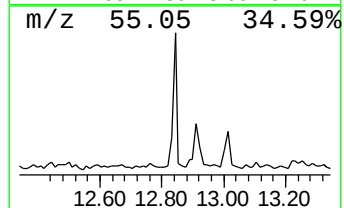
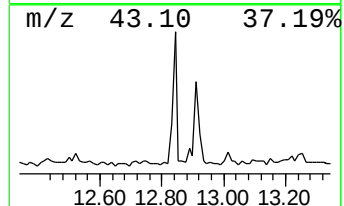
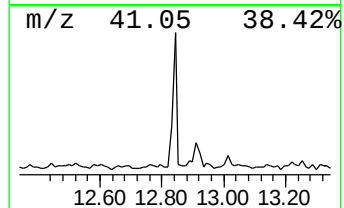
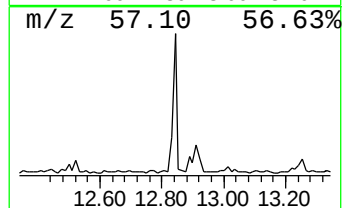
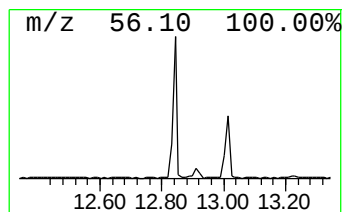
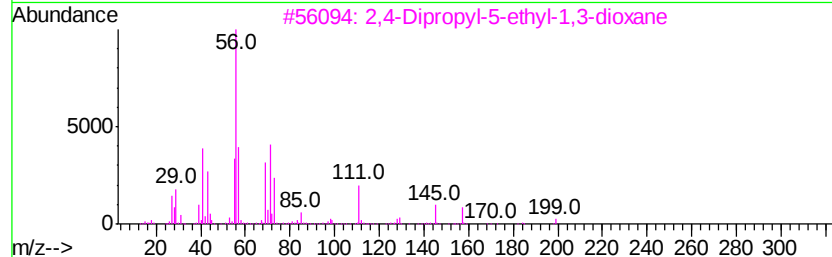
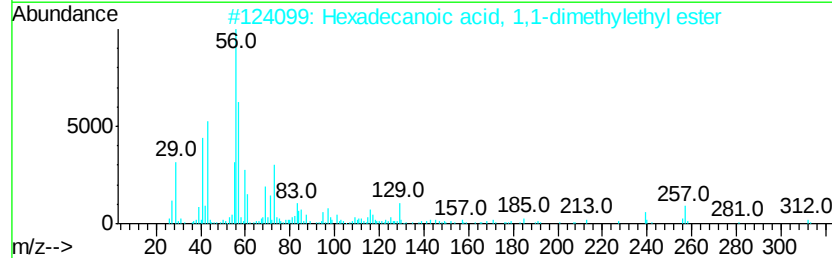
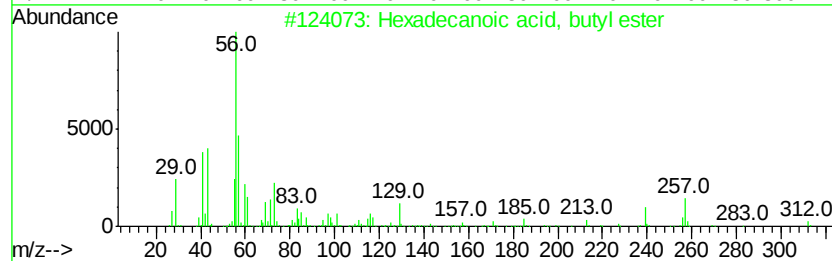
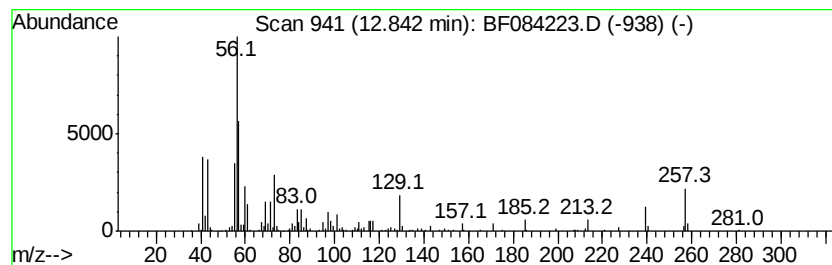
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	3.55 ng	295245	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
4		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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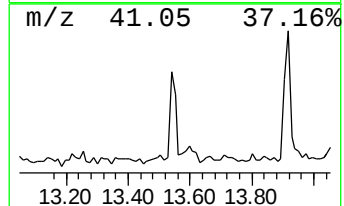
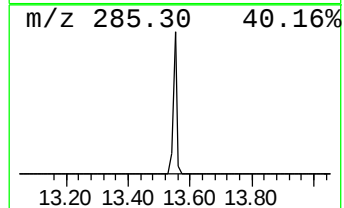
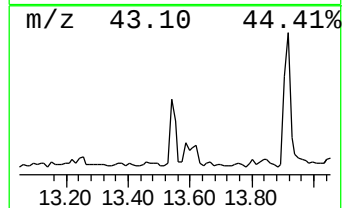
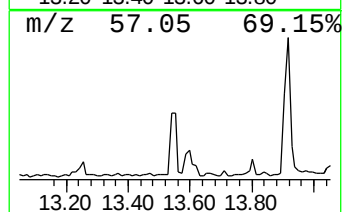
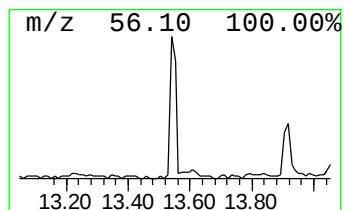
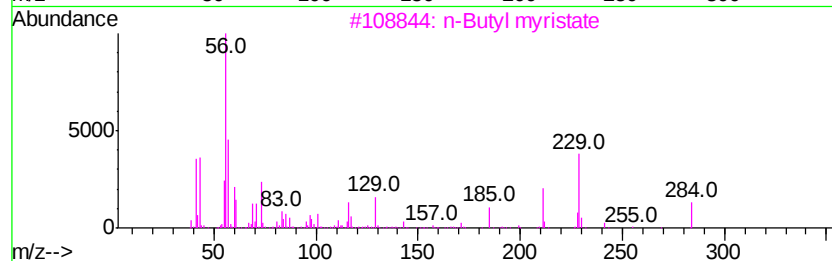
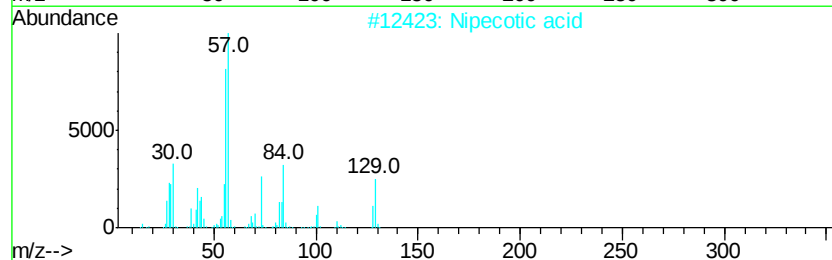
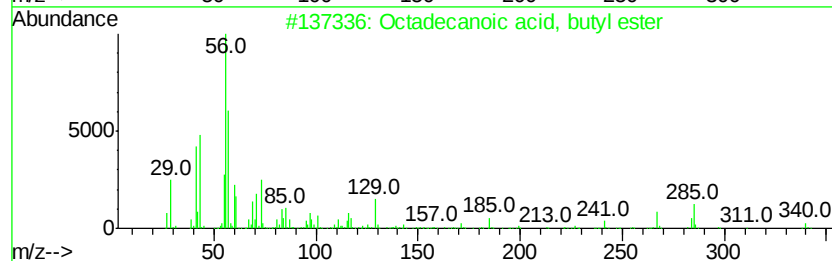
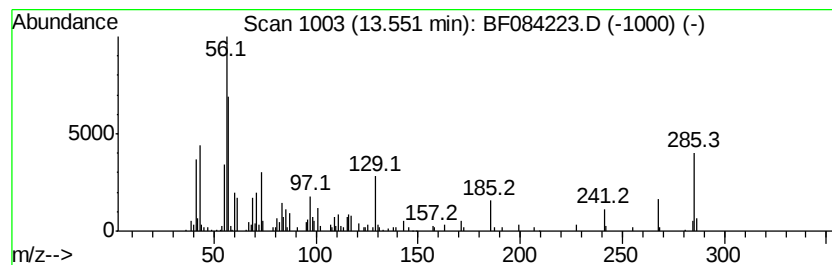
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.25 ng	187066	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	68
2		Nipecotic acid	129	C6H11NO2	000498-95-3	43
3		n-Butyl myristate	284	C18H36O2	000110-36-1	37
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	25
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	25



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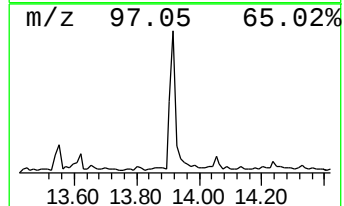
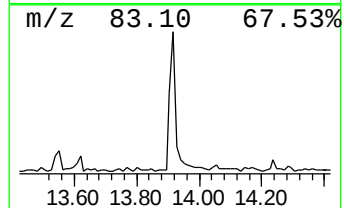
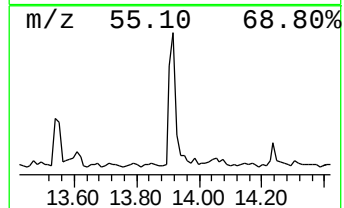
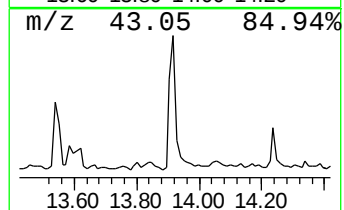
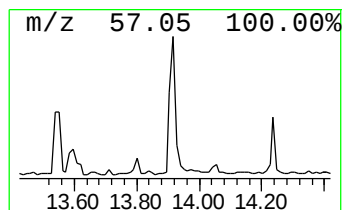
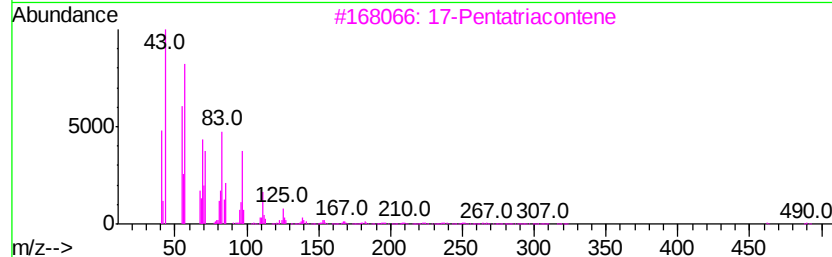
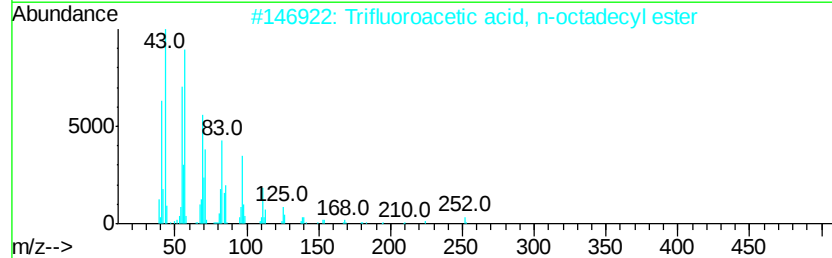
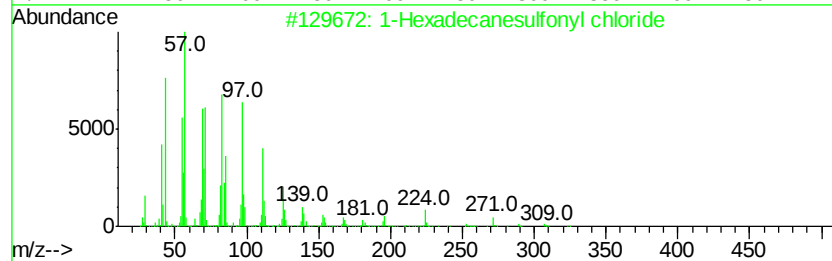
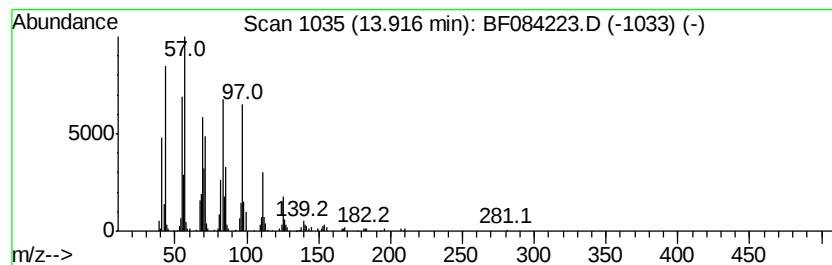
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexadecanesulfonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.12 ng	342632	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	90
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
5		1-Docosene	308	C22H44	001599-67-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF123115\
Data File : BF084223.D
Acq On : 1 Jan 2016 4:20
Operator : UM/SJ
Sample : G4981-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0533

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	11.1	ng	1087830	1	6.90	1963700	20.0
unknown6.67	6.67	80.3	ng	7881520	1	6.90	1963700	20.0
N-(2-Cyano-ethyl)...	11.31	5.4	ng	662848	4	11.42	2464350	20.0
Hexadecanoic acid...	12.84	3.5	ng	295245	5	14.07	1663440	20.0
Octadecanoic acid...	13.55	2.3	ng	187066	5	14.07	1663440	20.0
1-Hexadecanesulfo...	13.92	4.1	ng	342632	5	14.07	1663440	20.0