

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060615\
 Data File : BF079770.D
 Acq On : 6 Jun 2015 15:48
 Operator : TP/IZ
 Sample : PB83804BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB83804BL

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-BF060515.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	1.370	15	16	18	rVB	16339100	11241890	100.00%	33.861%
2	1.690	43	44	79	rVB3	171614	1382285	12.30%	4.164%
3	2.227	90	91	106	rVB	197854	388686	3.46%	1.171%
4	2.433	106	109	112	rBV	2249223	3110198	27.67%	9.368%
5	5.713	394	396	399	rBV	235132	219795	1.96%	0.662%
6	6.090	427	429	432	rBV	1268507	1572215	13.99%	4.736%
7	7.073	512	515	517	rBV	2316175	1979099	17.60%	5.961%
8	7.245	528	530	532	rBV	2403948	2007082	17.85%	6.045%
9	7.473	548	550	553	rBV	406723	477636	4.25%	1.439%
10	7.633	562	564	566	rBV	1309182	1479621	13.16%	4.457%
11	8.033	597	599	601	rBV	1245948	1067283	9.49%	3.215%
12	8.765	661	663	666	rBV	367890	470421	4.18%	1.417%
13	9.839	755	757	760	rBV	1532826	1730498	15.39%	5.212%
14	10.548	817	819	821	rVB	633026	572165	5.09%	1.723%
15	11.336	886	888	891	rBV	1113898	1014909	9.03%	3.057%
16	12.056	948	951	953	rBV	509483	599249	5.33%	1.805%
17	13.691	1091	1094	1096	rBV	2215577	2233488	19.87%	6.727%
18	14.902	1197	1200	1202	rBV	780704	805963	7.17%	2.428%
19	16.788	1362	1365	1372	rBV	473389	847403	7.54%	2.552%

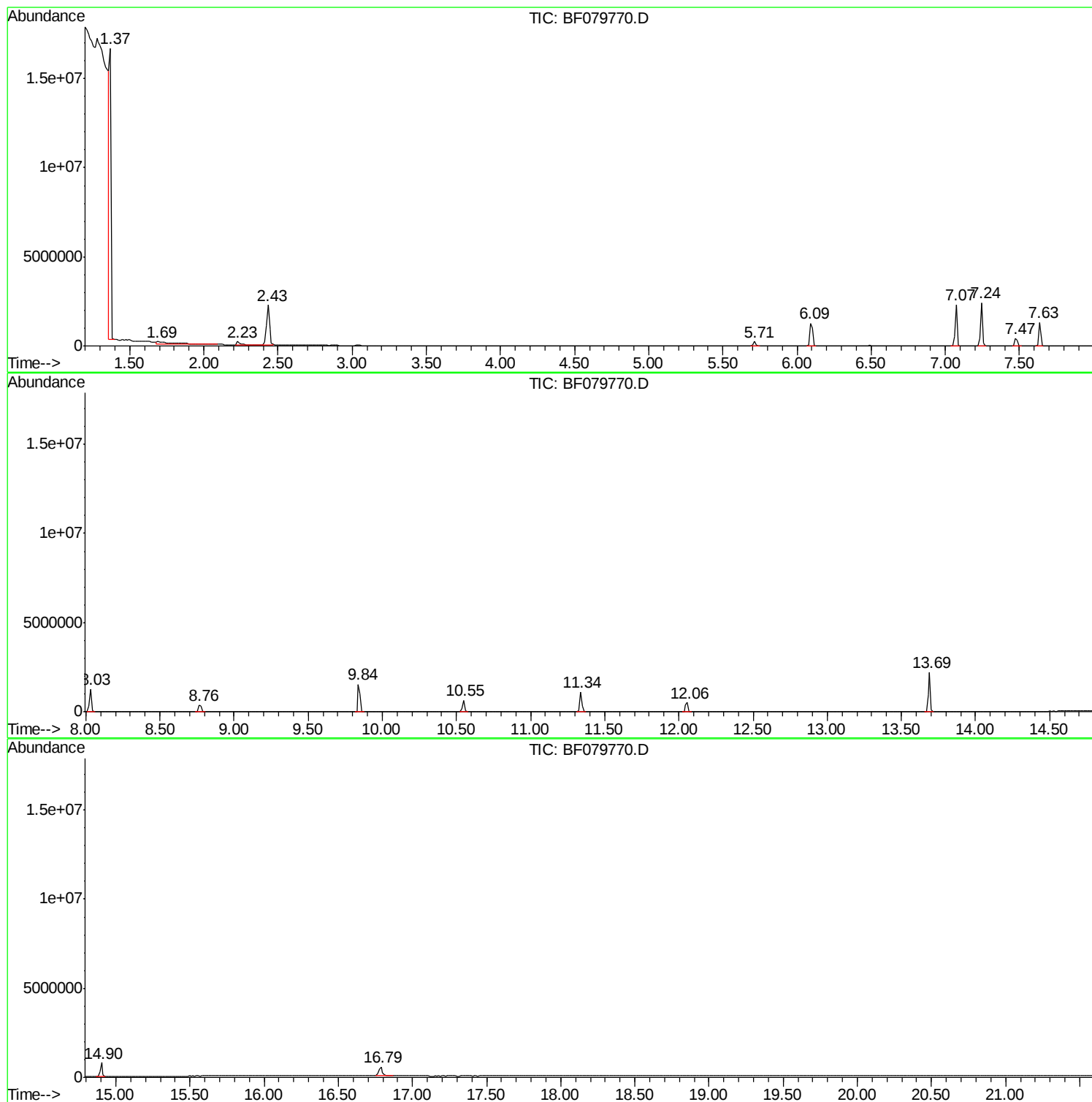
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PB83804BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060515.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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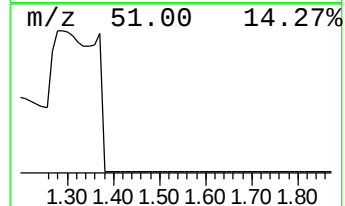
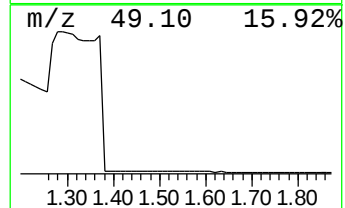
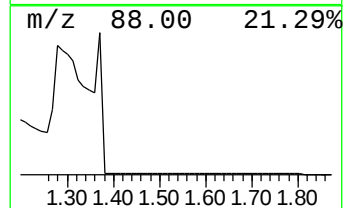
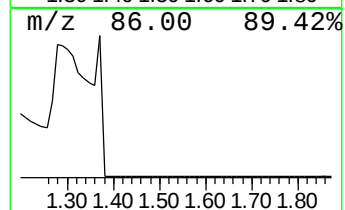
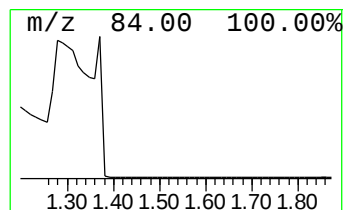
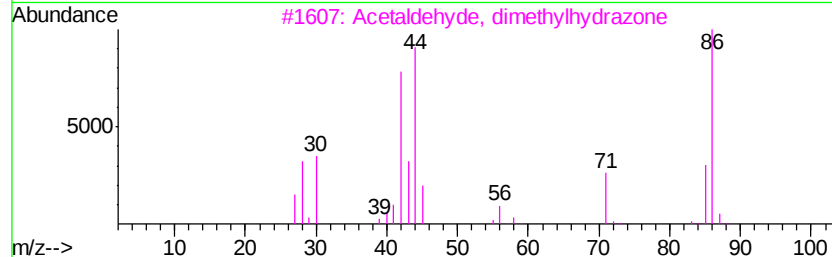
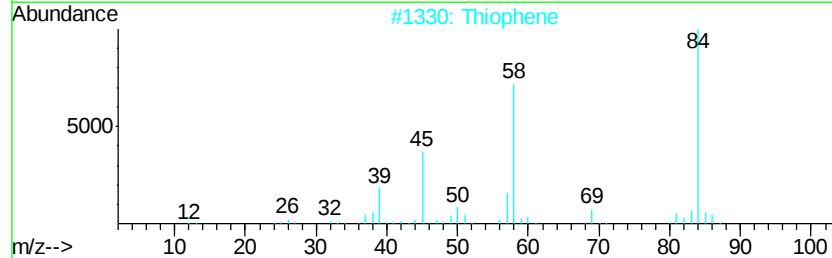
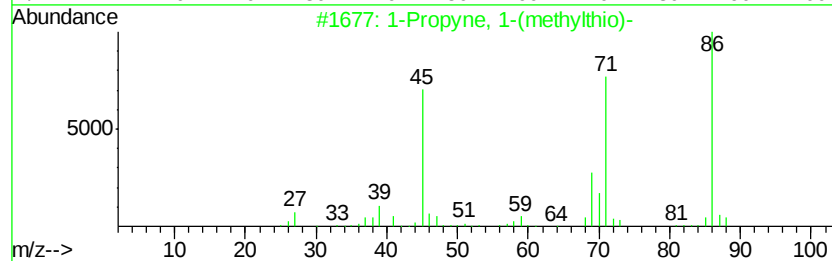
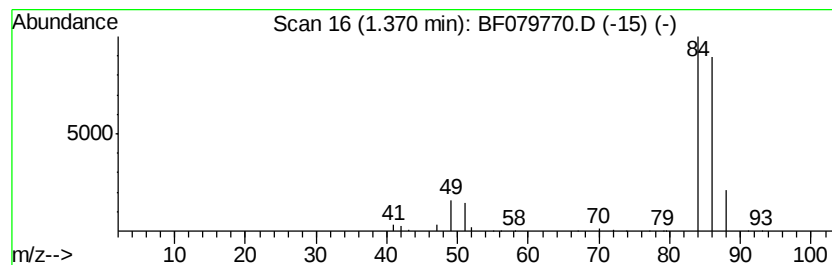
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	470.73 ng	11241900	1,4-Dichlorobenzene-d4	7.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propyne, 1-(methylthio)-	86	C4H6S	022174-51-2	4
2			Thiophene	84	C4H4S	000110-02-1	4
3			Acetaldehyde, dimethylhydrazone	86	C4H10N2	007422-90-4	4
4			1,4-Dioxin, 2,3-dihydro-	86	C4H6O2	000543-75-9	4
5			Methane-d, trichloro-	119	CDCl3	000865-49-6	4



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ClientSampled :
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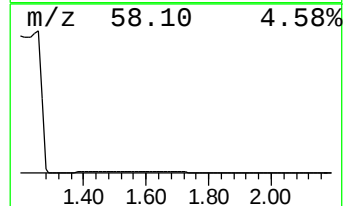
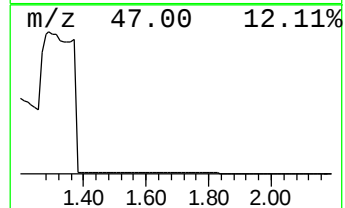
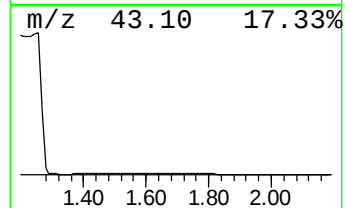
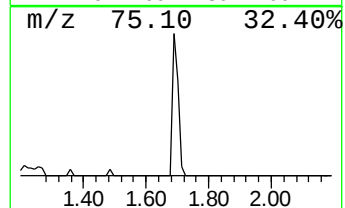
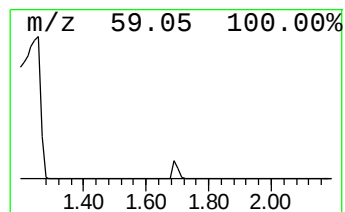
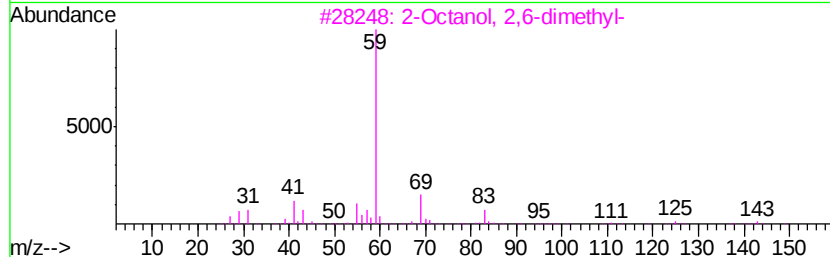
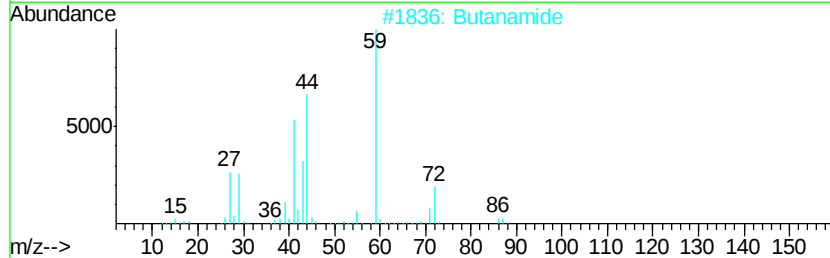
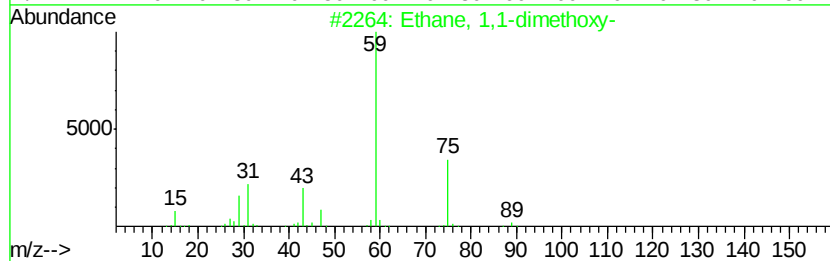
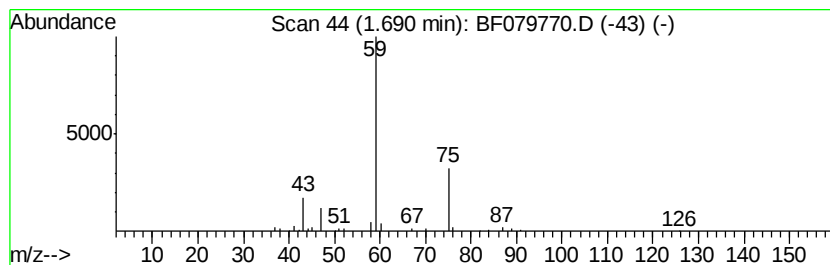
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	57.88 ng	1382290	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	83
2		Butanamide	87	C4H9NO	000541-35-5	9
3		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	9
4		2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	9
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7



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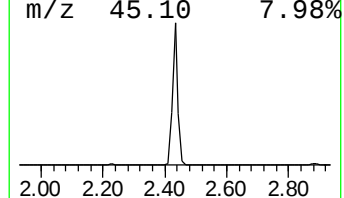
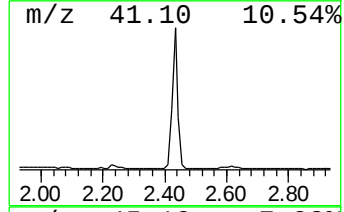
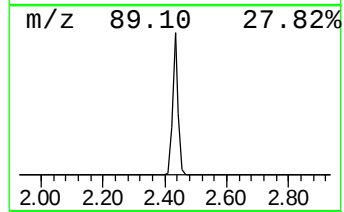
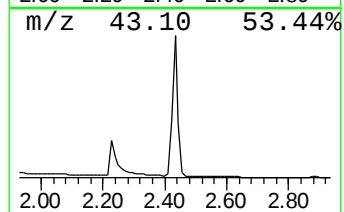
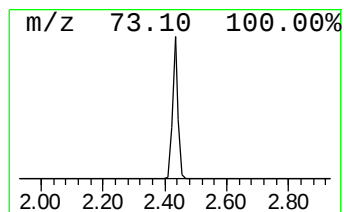
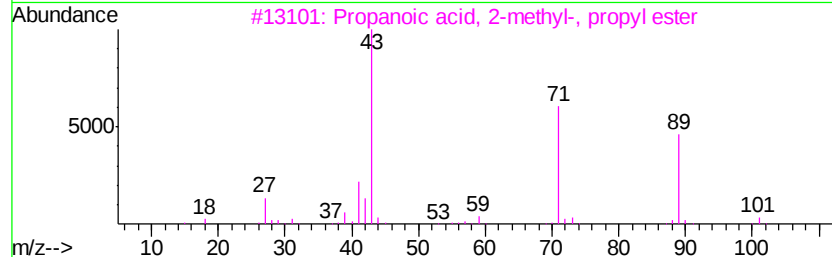
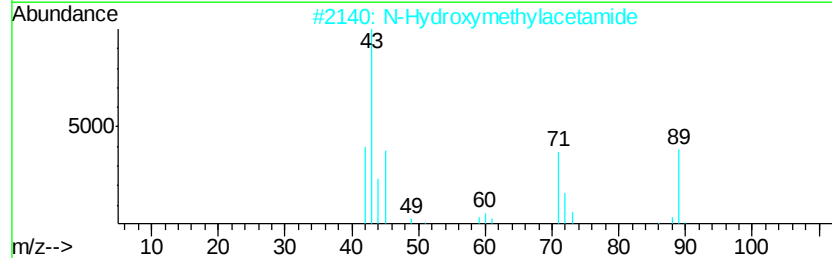
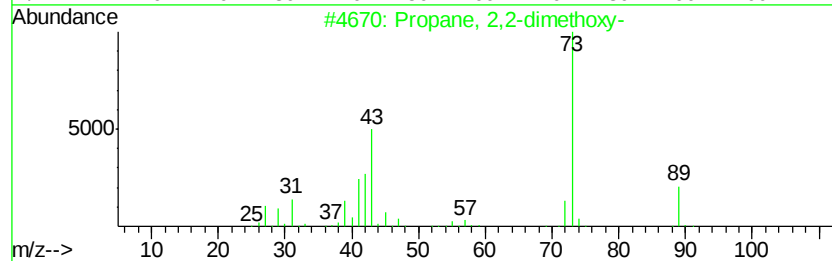
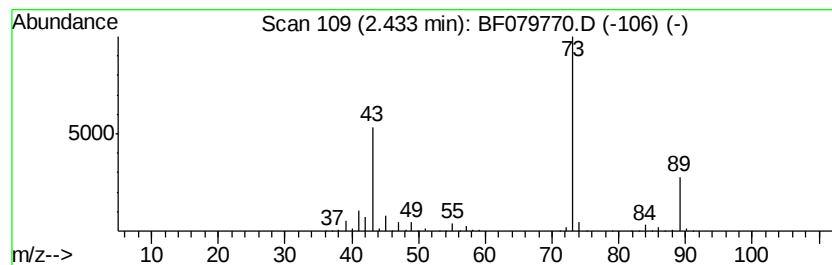
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	130.23 ng	3110200	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	59
2		N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
3		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9



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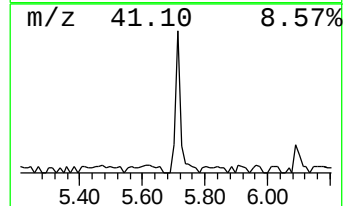
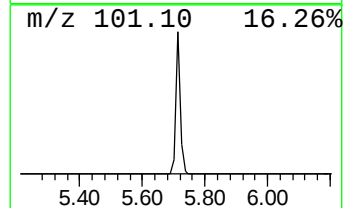
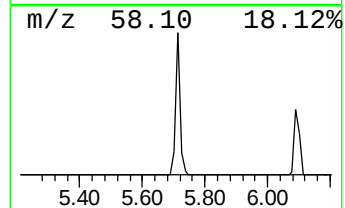
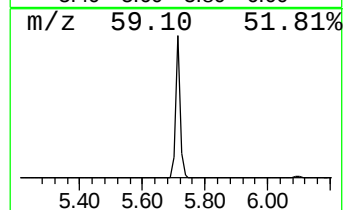
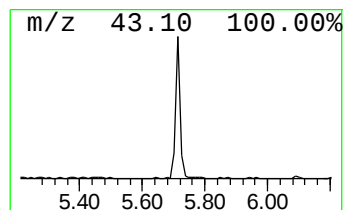
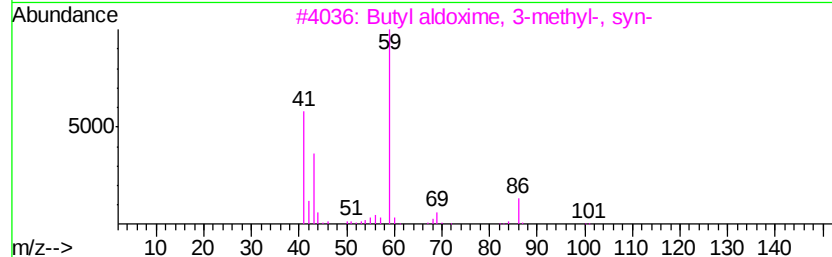
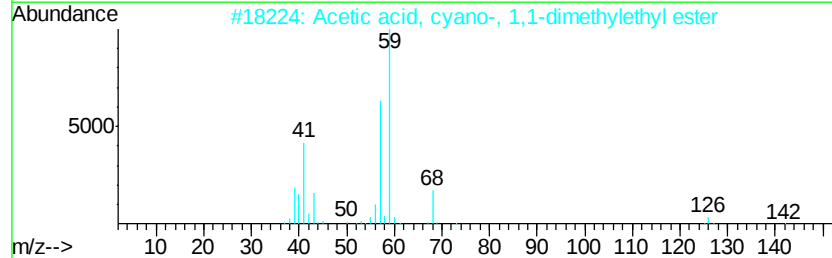
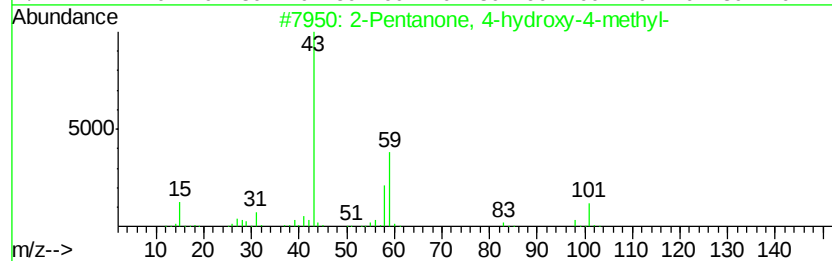
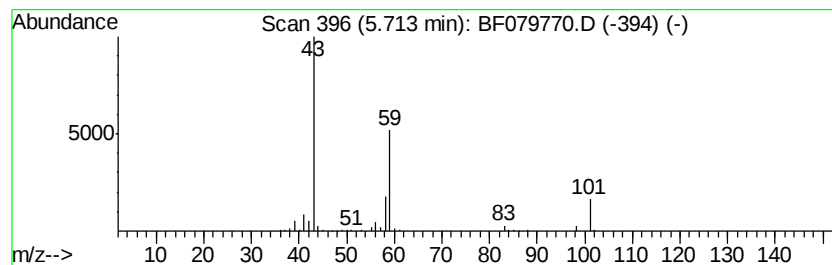
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	9.20 ng	219795	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		Acetone	58	C3H6O	000067-64-1	12



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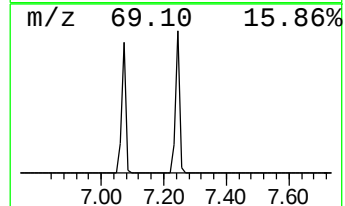
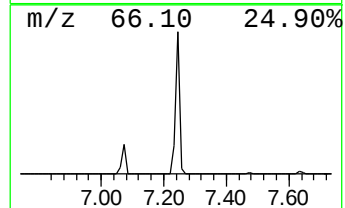
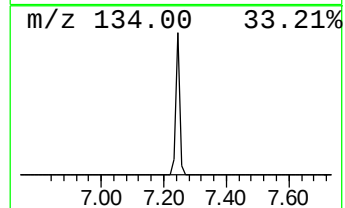
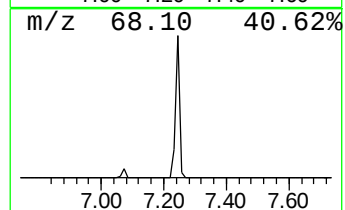
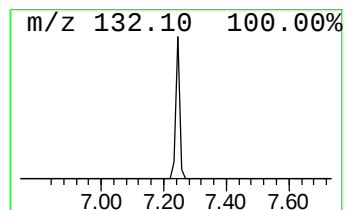
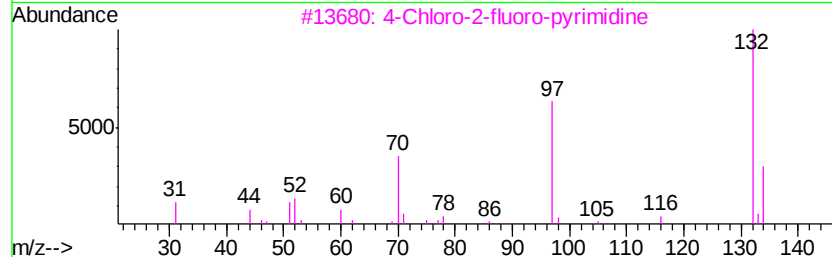
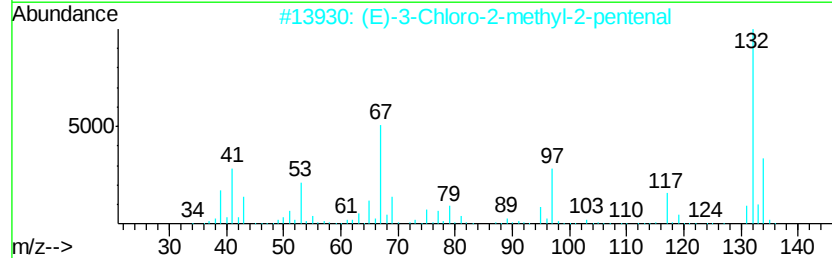
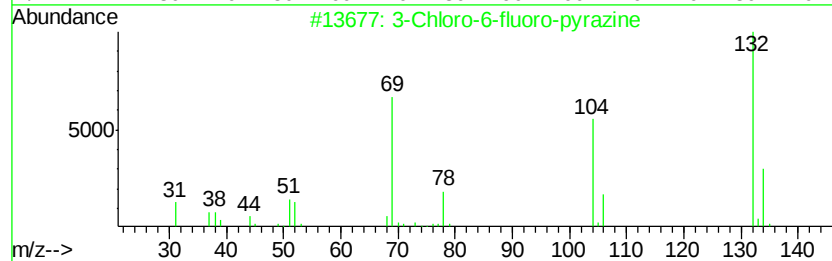
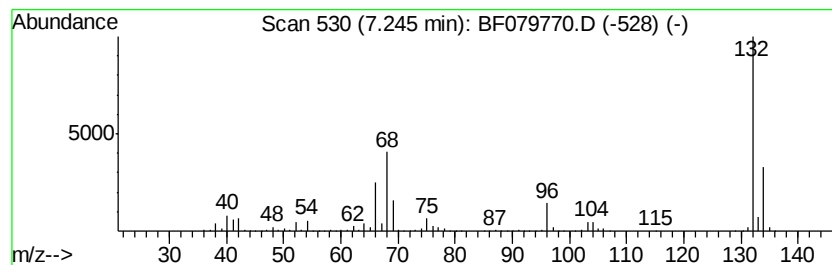
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	84.04 ng	2007080	1,4-Dichlorobenzene-d4	7.47

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	12
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethane, 1,1-dimet...	1.69	57.9	ng	1382290	1	7.47	477636	20.0
Propane, 2,2-dime...	2.43	130.2	ng	3110200	1	7.47	477636	20.0
2-Pentanone, 4-hy...	5.71	9.2	ng	219795	1	7.47	477636	20.0
unknown7.24	7.24	84.0	ng	2007080	1	7.47	477636	20.0