

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060615\
 Data File : BF079772.D
 Acq On : 6 Jun 2015 16:46
 Operator : TP/IZ
 Sample : PB83864BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB83864BL

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	16360083	11438791	100.00%	38.313%
2	1.690	41	44	52	rVB2	87019	245957	2.15%	0.824%
3	2.433	106	109	112	rBV	865688	1170205	10.23%	3.919%
4	5.713	394	396	399	rVB	300648	292880	2.56%	0.981%
5	6.090	427	429	432	rBV	1326088	1535830	13.43%	5.144%
6	7.073	512	515	517	rBV	1952443	1708984	14.94%	5.724%
7	7.245	527	530	532	rBV	2060039	1733981	15.16%	5.808%
8	7.473	548	550	552	rVB	313721	343651	3.00%	1.151%
9	7.633	562	564	567	rBV	1216473	1280988	11.20%	4.291%
10	8.033	596	599	601	rBV	1100425	947709	8.29%	3.174%
11	8.765	661	663	665	rVB	452681	534260	4.67%	1.789%
12	9.839	755	757	760	rBV	2336567	2541053	22.21%	8.511%
13	10.548	817	819	821	rVB	599017	544607	4.76%	1.824%
14	11.336	886	888	891	rBV	1257533	1181613	10.33%	3.958%
15	12.057	948	951	953	rBV	582261	578514	5.06%	1.938%
16	13.714	1094	1096	1099	rBV	2846186	2509363	21.94%	8.405%
17	14.960	1202	1205	1208	rBV	664850	657429	5.75%	2.202%
18	16.868	1369	1372	1376	rBV	352432	610460	5.34%	2.045%

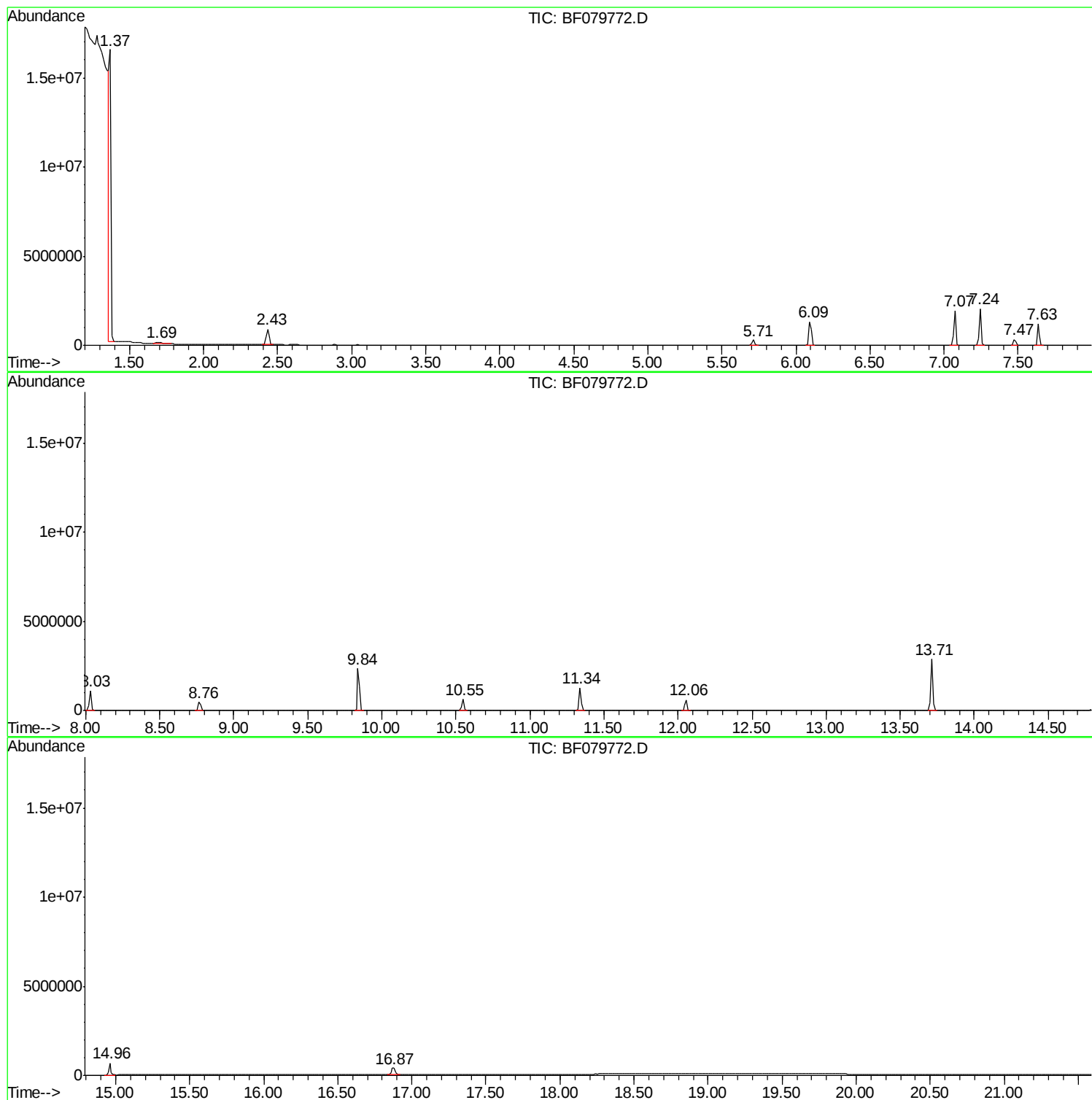
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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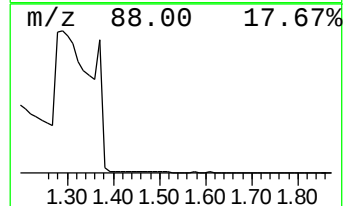
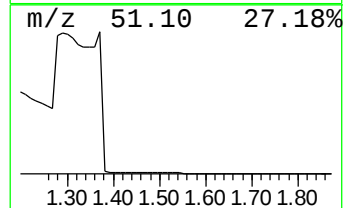
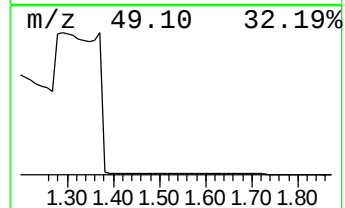
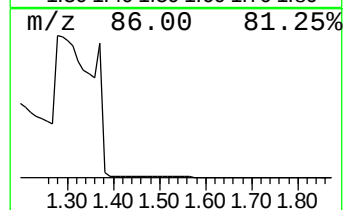
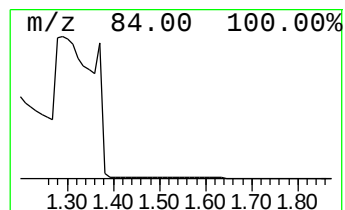
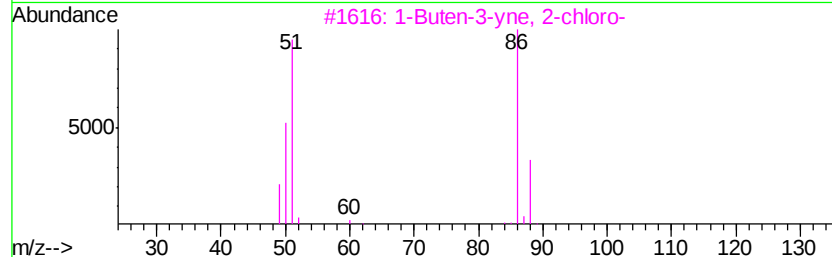
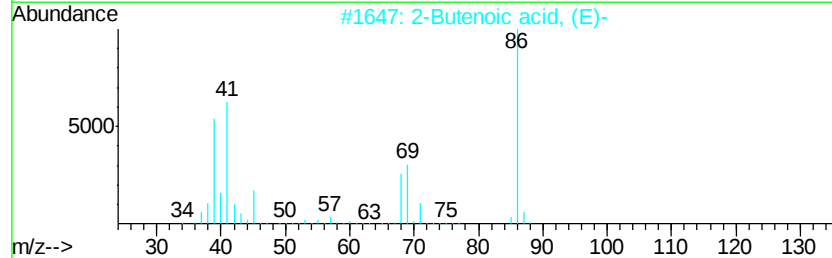
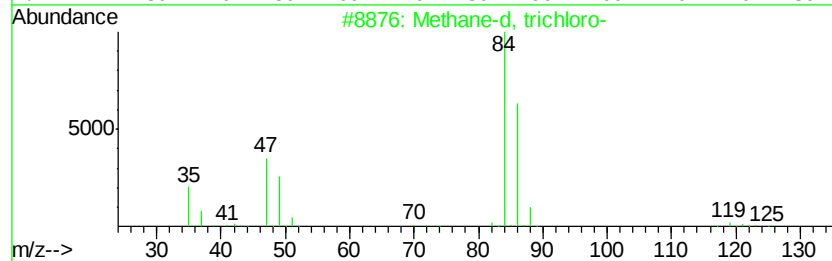
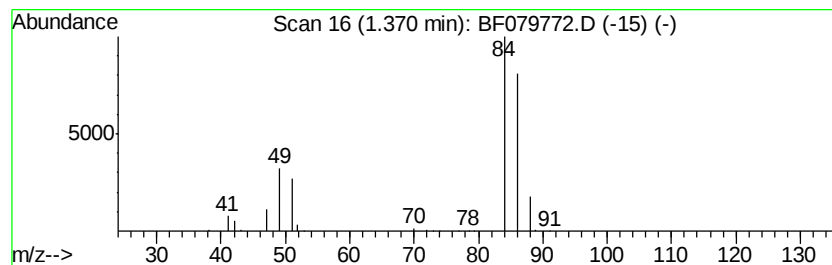
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	665.72 ng	11438800	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methane-d, trichloro-	119	CDCl3	000865-49-6	9
2		2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	5
3		1-Buten-3-yne, 2-chloro-	86	C4H3Cl	017712-36-6	5
4		Phosphonic difluoride	86	F2HOP	014939-34-5	5
5		4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	5



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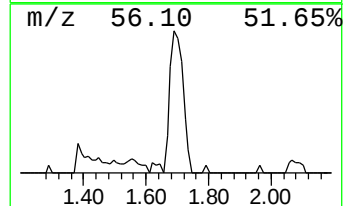
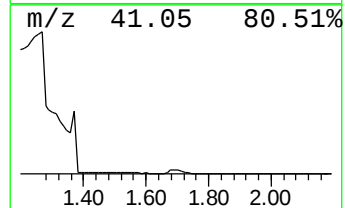
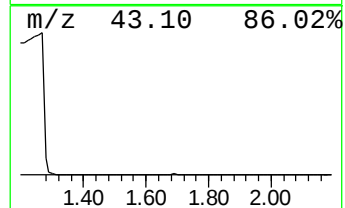
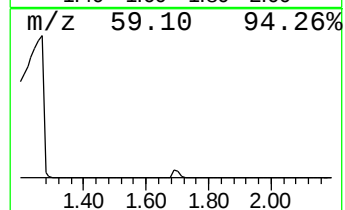
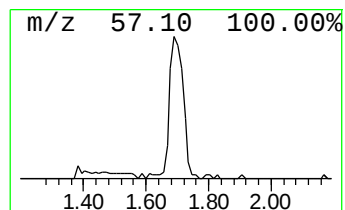
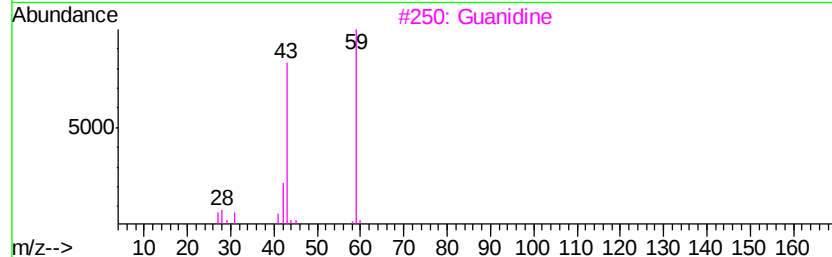
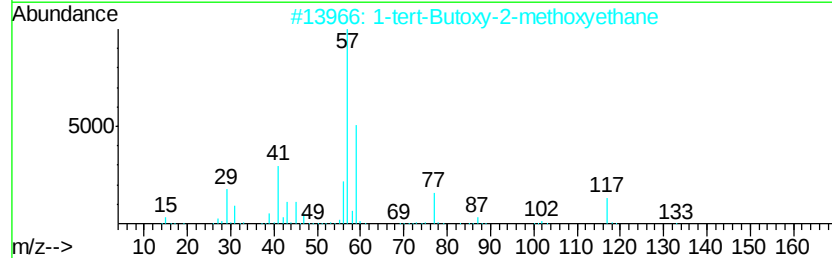
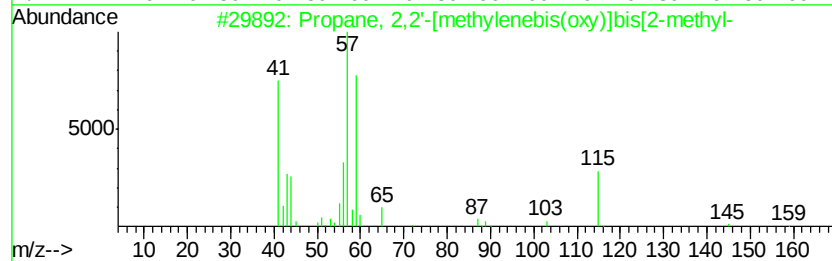
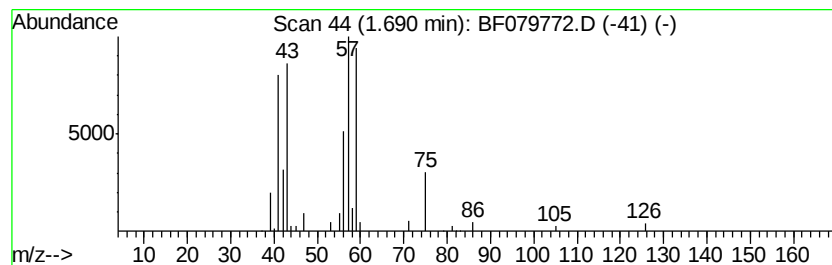
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown1.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	14.31 ng	245957	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2'-[methylenebis(oxy)]...	160	C9H20O2	002568-93-6	40
2		1-tert-Butoxy-2-methoxyethane	132	C7H16O2	066728-50-5	36
3		Guanidine	59	CH5N3	000113-00-8	35
4		Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	33
5		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	25



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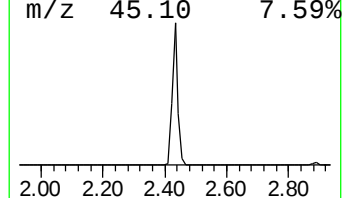
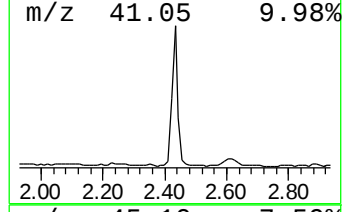
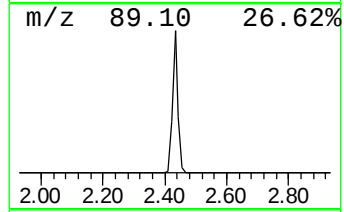
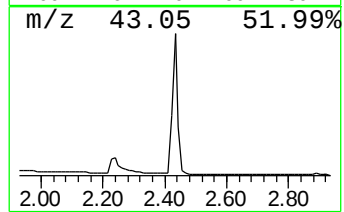
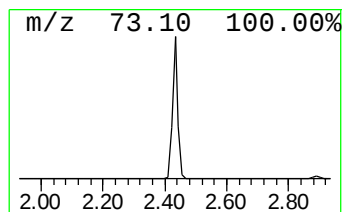
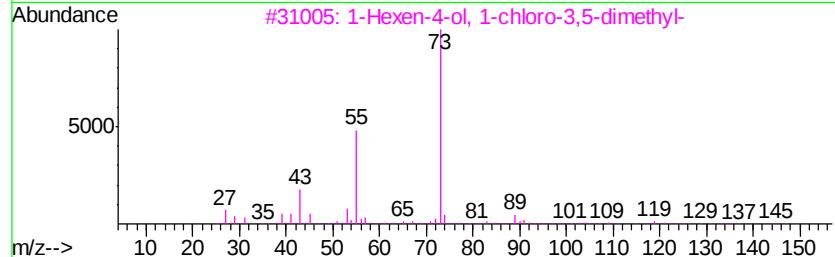
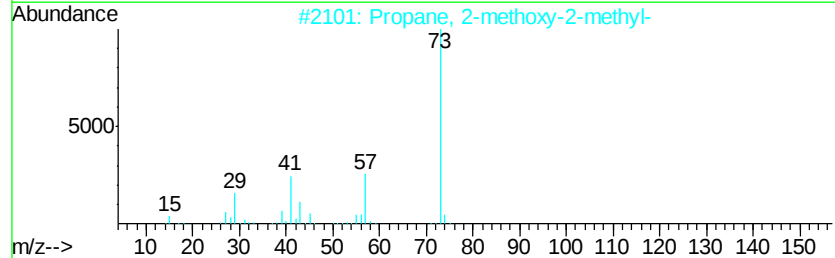
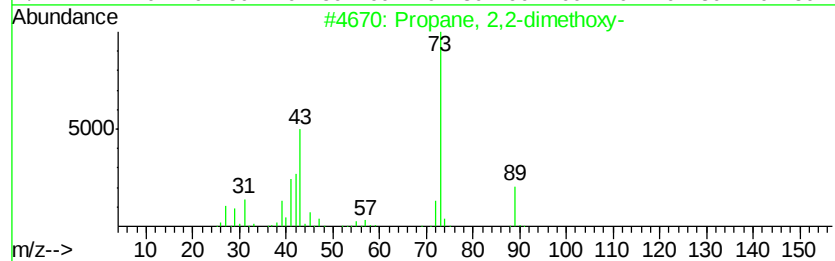
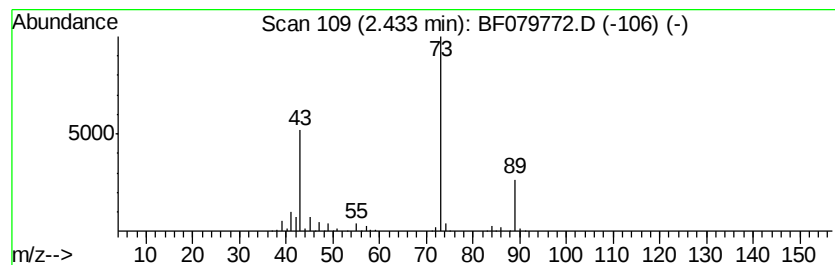
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Peak Number 3 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	68.10 ng	1170210	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		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4		1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9



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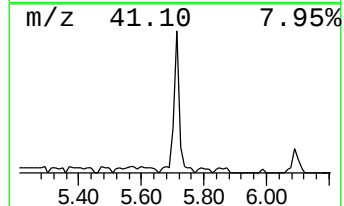
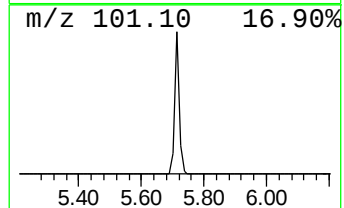
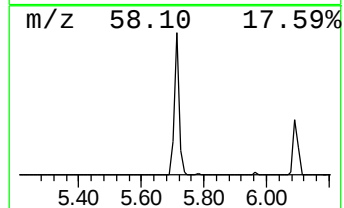
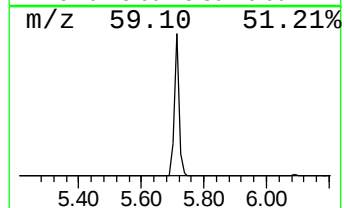
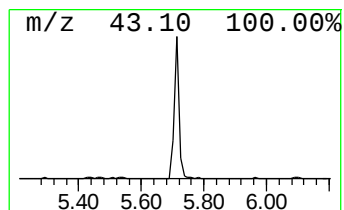
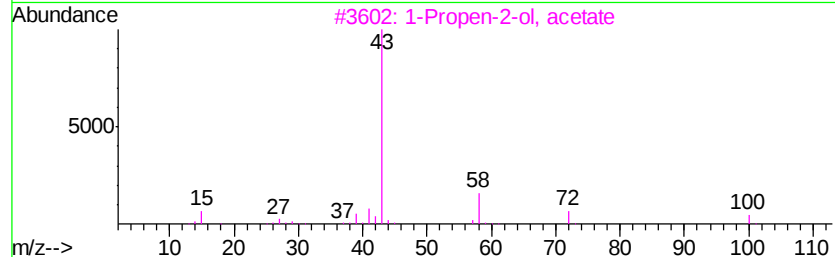
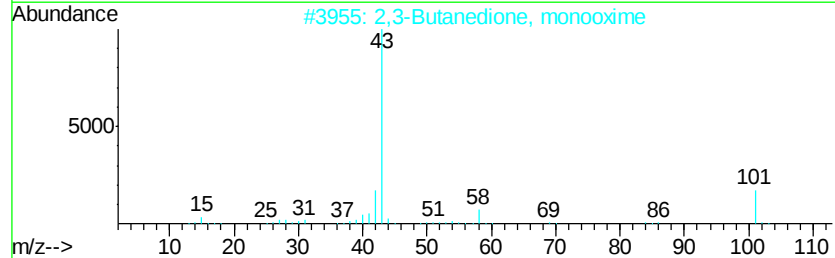
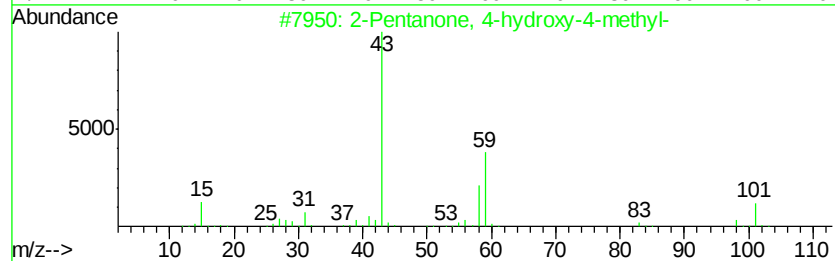
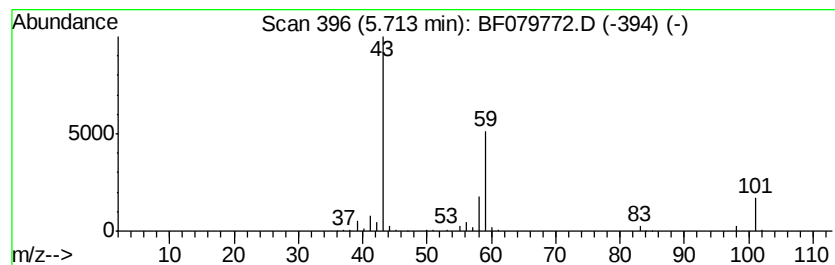
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	17.05 ng	292880	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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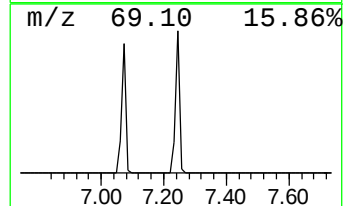
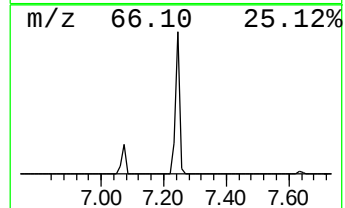
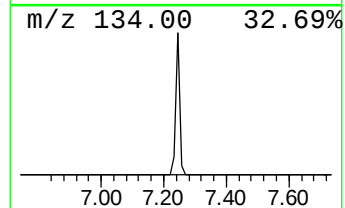
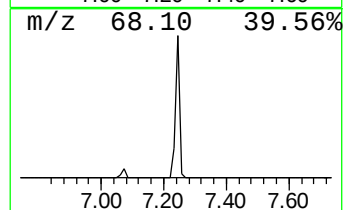
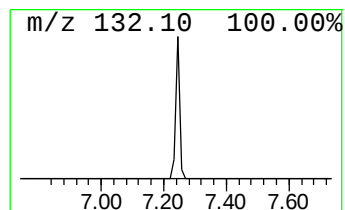
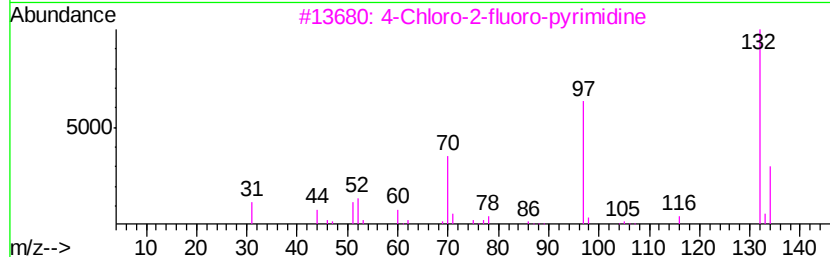
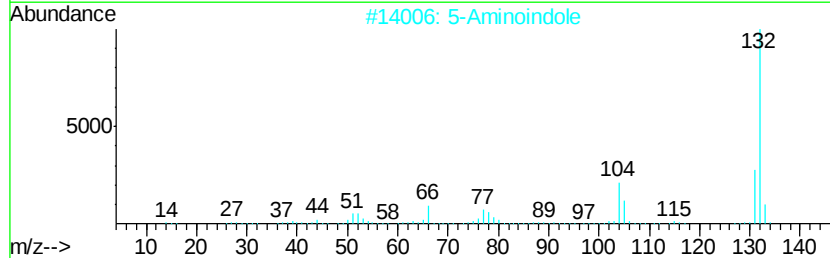
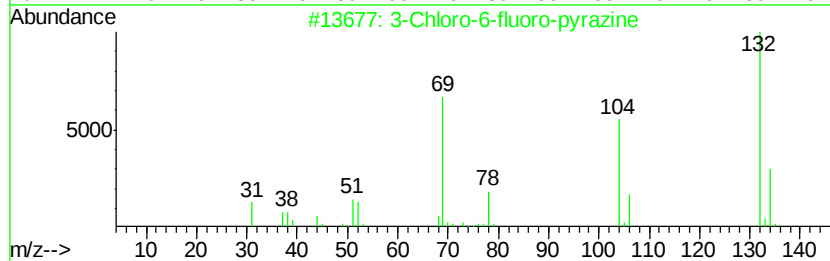
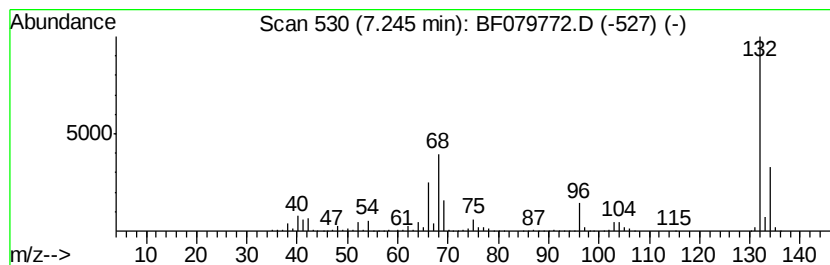
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TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	100.92 ng	1733980	1,4-Dichlorobenzene-d4	7.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	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	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.37	1.37	665.7	ng	11438800	1	7.47	343651	20.0
unknown1.69	1.69	14.3	ng	245957	1	7.47	343651	20.0
Propane, 2,2-dime...	2.43	68.1	ng	1170210	1	7.47	343651	20.0
2-Pentanone, 4-hy...	5.71	17.1	ng	292880	1	7.47	343651	20.0
unknown7.24	7.24	100.9	ng	1733980	1	7.47	343651	20.0