

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032317\
 Data File : BF093878.D
 Acq On : 23 Mar 2017 14:56
 Operator : SJ/MA
 Sample : PB97768BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97768BL

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-BF032217.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	2.110	34	38	45	rVB	106532	127348	2.48%	0.304%
2	4.128	375	381	391	rBV	549536	757636	14.74%	1.810%
3	4.504	439	445	448	rBV	3883137	4307235	83.81%	10.288%
4	4.898	509	512	516	rVB	60821	54282	1.06%	0.130%
5	5.557	617	624	627	rBV	3415710	4357671	84.79%	10.409%
6	5.716	645	651	654	rBV	4080447	4438788	86.37%	10.603%
7	5.975	690	695	698	rBV	1099507	1049519	20.42%	2.507%
8	6.151	720	725	729	rVB	3259276	3494508	68.00%	8.347%
9	6.622	798	805	808	rBV	2394546	2818174	54.84%	6.732%
10	7.475	945	950	954	rBV	1401510	1433062	27.88%	3.423%
11	8.804	1169	1176	1179	rBV	4332475	5139354	100.00%	12.276%
12	9.522	1291	1298	1309	rVB3	119433	292262	5.69%	0.698%
13	9.622	1309	1315	1319	rVB2	1445638	1565587	30.46%	3.740%
14	10.592	1472	1480	1484	rBV	2410598	2953139	57.46%	7.054%
15	11.445	1619	1625	1629	rBV2	1504351	1561006	30.37%	3.729%
16	13.433	1952	1963	1966	rBV2	3927483	4844602	94.26%	11.572%
17	14.698	2173	2178	2182	rBV	1287110	1471760	28.64%	3.515%
18	16.339	2452	2457	2465	rBV	1008864	1199298	23.34%	2.865%

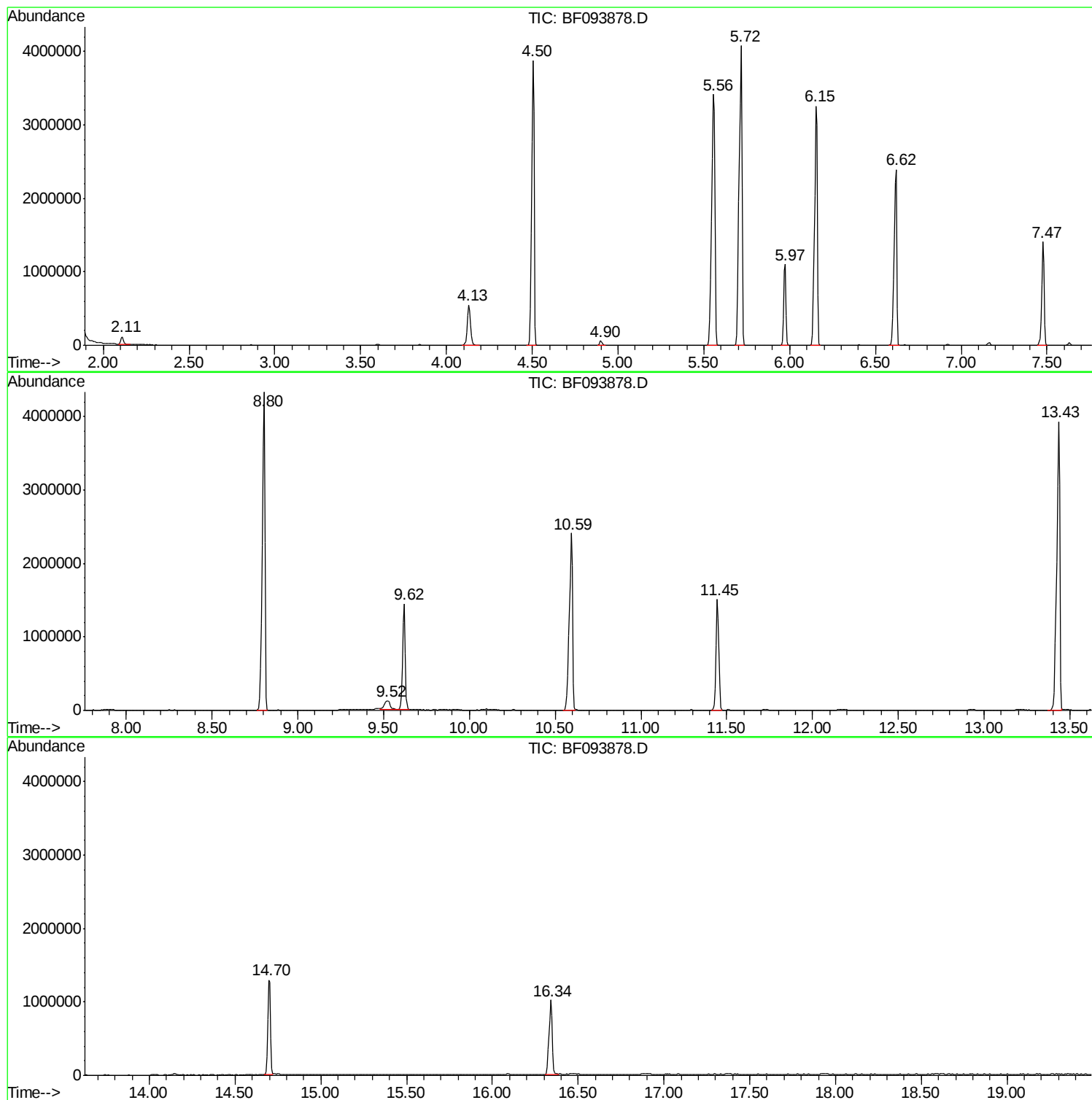
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampled :
PB97768BL

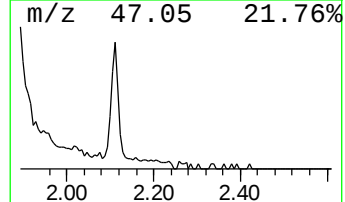
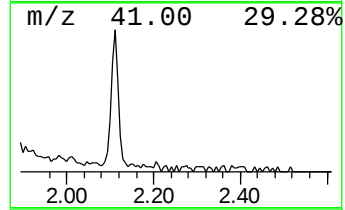
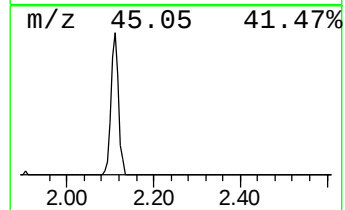
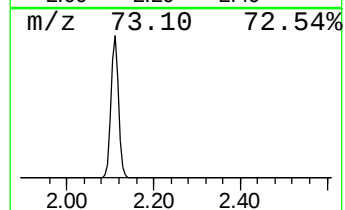
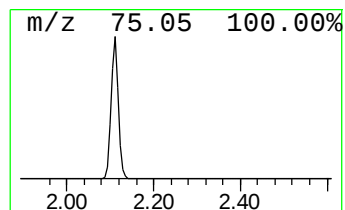
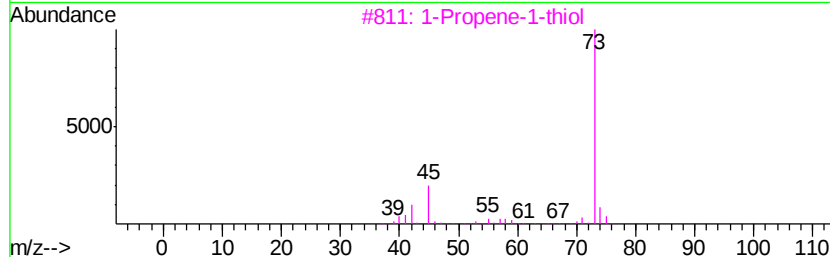
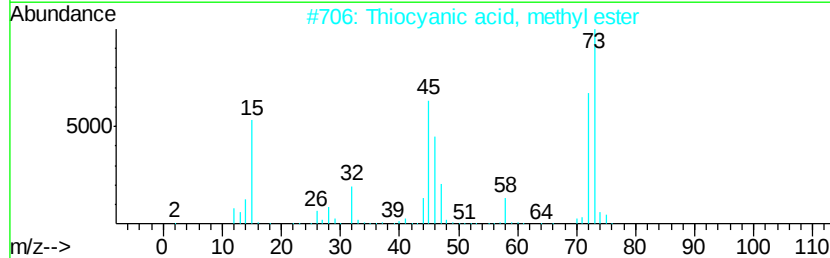
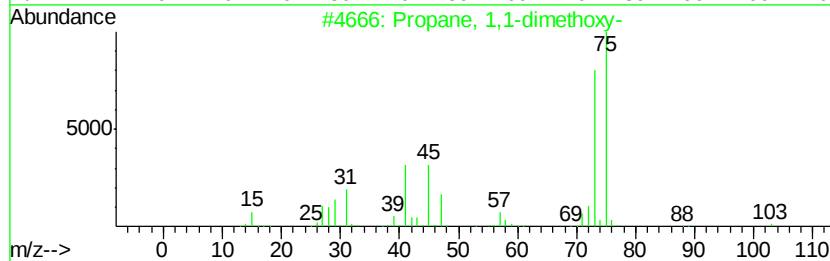
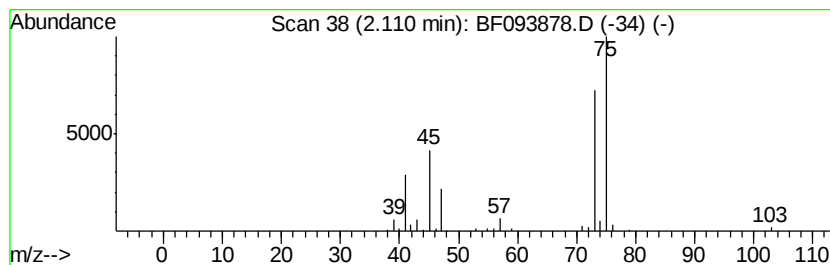
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	2.43 ng	127348	1,4-Dichlorobenzene-d4	5.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5		Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9



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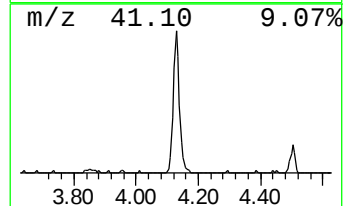
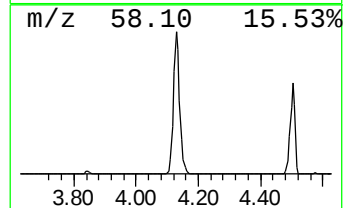
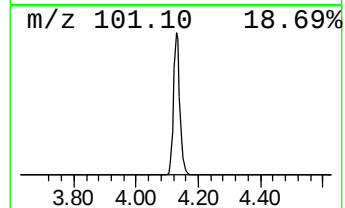
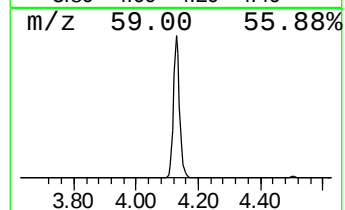
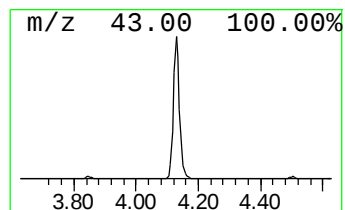
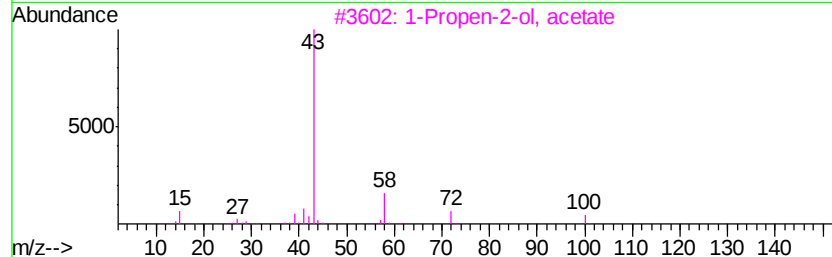
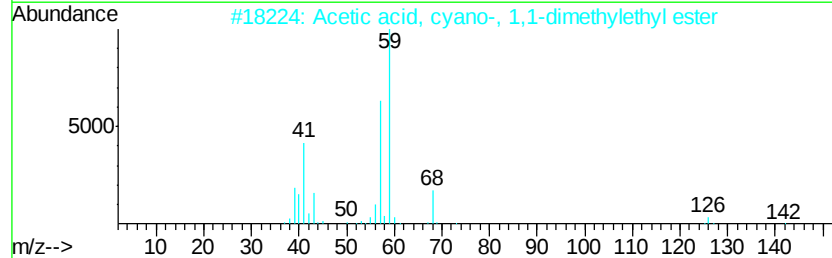
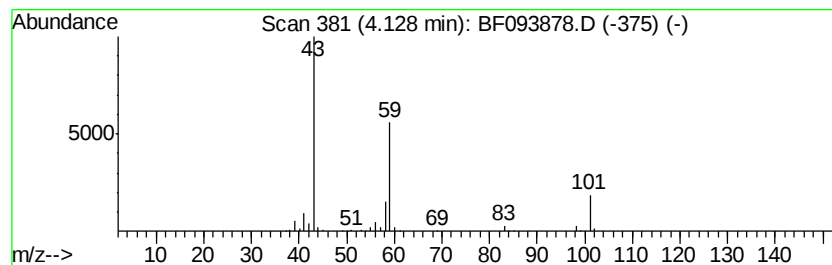
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.13	14.44 ng	757636	1,4-Dichlorobenzene-d4	5.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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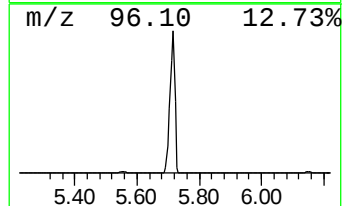
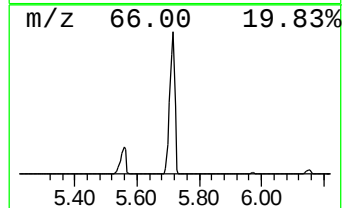
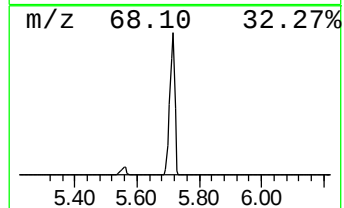
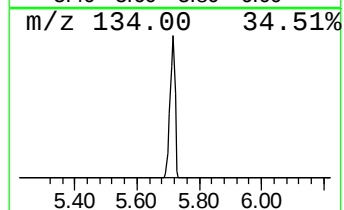
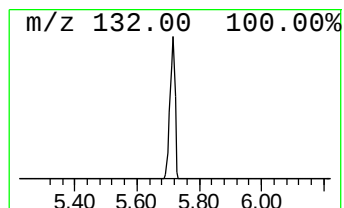
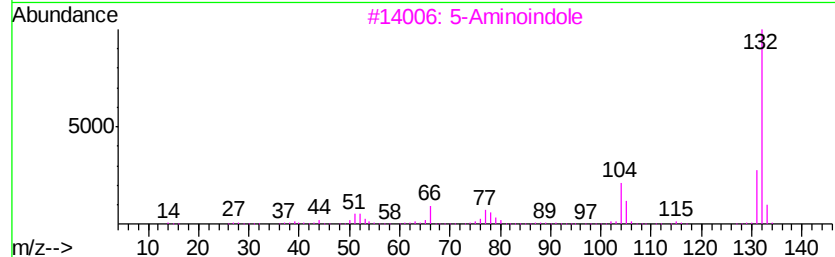
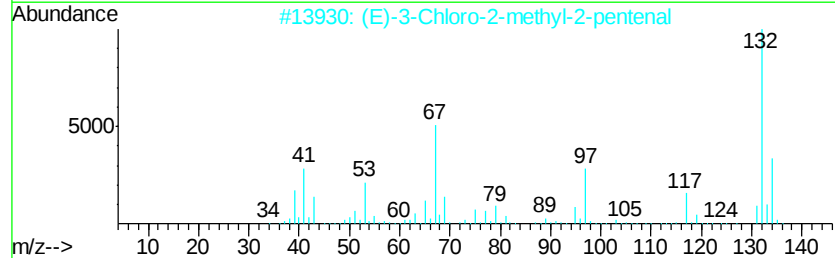
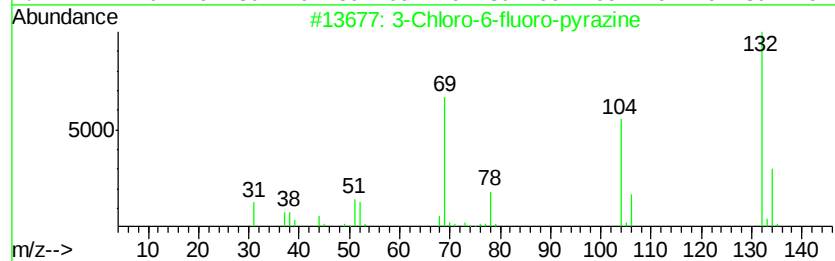
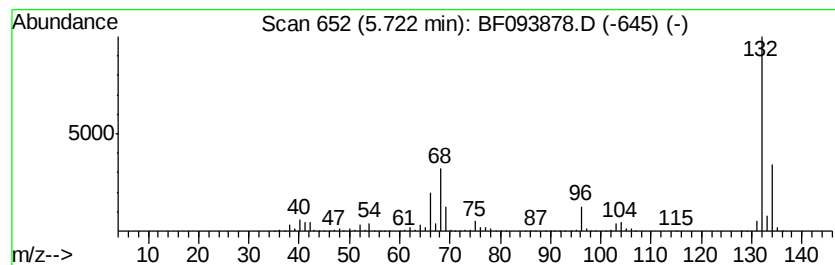
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Peak Number 3 unknown5.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	84.59 ng	4438790	1,4-Dichlorobenzene-d4	5.97

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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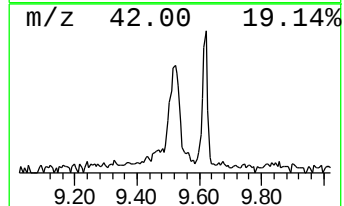
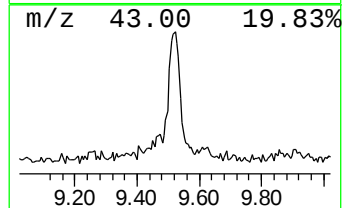
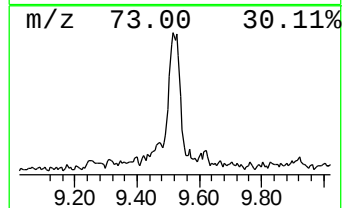
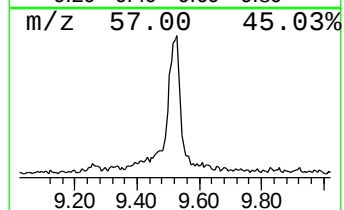
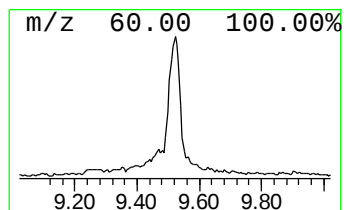
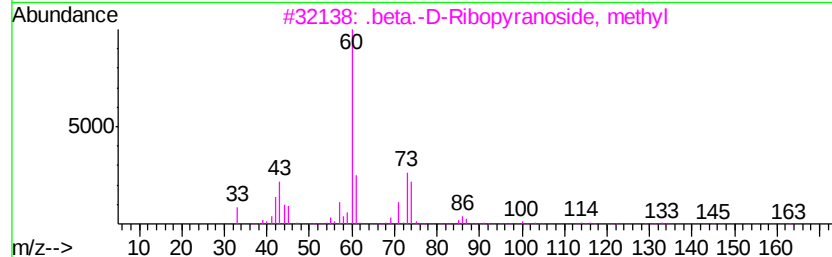
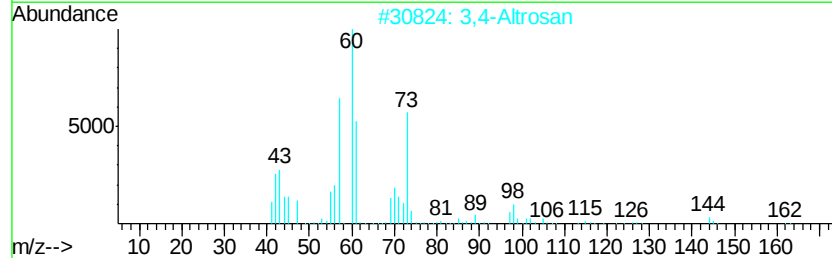
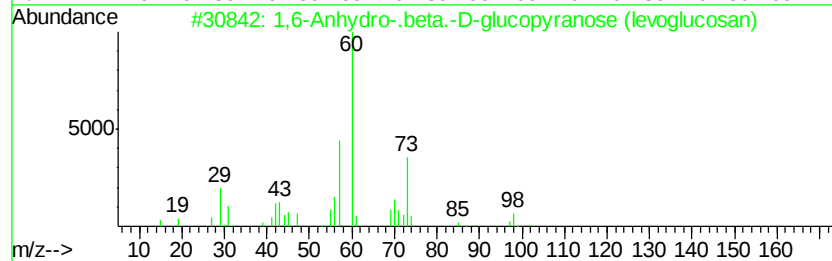
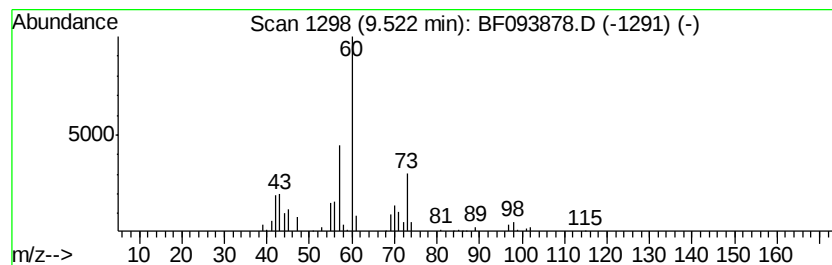
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	3.73 ng	292262	Acenaphthene-d10	9.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2		3,4-Altrosan	162	C6H10O5	1000129-76-4	59
3		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	59
4		Pentanoic acid	102	C5H10O2	000109-52-4	50
5		Hexanoic acid	116	C6H12O2	000142-62-1	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.11	2.4	ng	127348	1	5.97	1049520	20.0
2-Pentanone, 4-hy...	4.13	14.4	ng	757636	1	5.97	1049520	20.0
unknown5.72	5.72	84.6	ng	4438790	1	5.97	1049520	20.0
1,6-Anhydro-.beta...	9.52	3.7	ng	292262	3	9.62	1565590	20.0