

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032817\
 Data File : BF093993.D
 Acq On : 28 Mar 2017 15:31
 Operator : SJ/MA
 Sample : PB97829BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97829BL

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	2.022	18	23	29	rVB	79953	101127	2.28%	0.283%
2	4.075	368	372	380	rBV	417318	536338	12.09%	1.502%
3	4.463	433	438	441	rBV	3429700	3583219	80.78%	10.036%
4	4.851	501	504	509	rVB	51471	44923	1.01%	0.126%
5	5.522	612	618	621	rBV	2929842	3594323	81.03%	10.067%
6	5.669	638	643	647	rBV	3286312	3737379	84.26%	10.468%
7	5.928	683	687	690	rBV	898060	846591	19.09%	2.371%
8	6.104	712	717	721	rBV	2880982	2962358	66.78%	8.297%
9	6.575	790	797	800	rBV	2088066	2377321	53.59%	6.659%
10	7.428	937	942	946	rBV	1164511	1148821	25.90%	3.218%
11	8.751	1161	1167	1171	rBV	3745412	4435736	100.00%	12.424%
12	9.475	1285	1290	1300	rVB2	69384	155902	3.51%	0.437%
13	9.569	1300	1306	1310	rVB2	1201191	1262053	28.45%	3.535%
14	10.539	1463	1471	1475	rBV	2126633	2552946	57.55%	7.150%
15	11.392	1610	1616	1620	rBV	1296068	1287124	29.02%	3.605%
16	13.374	1947	1953	1956	rBV	3629504	4422572	99.70%	12.387%
17	14.639	2163	2168	2172	rBV	1261942	1298445	29.27%	3.637%
18	16.274	2440	2446	2453	rBV	943728	1151550	25.96%	3.225%
19	16.392	2462	2466	2471	rBV	37935	47151	1.06%	0.132%
20	16.804	2531	2536	2543	rBV	36597	59079	1.33%	0.165%
21	17.268	2610	2615	2621	rBV	33071	51449	1.16%	0.144%
22	18.451	2810	2816	2824	rVB7	16385	46926	1.06%	0.131%

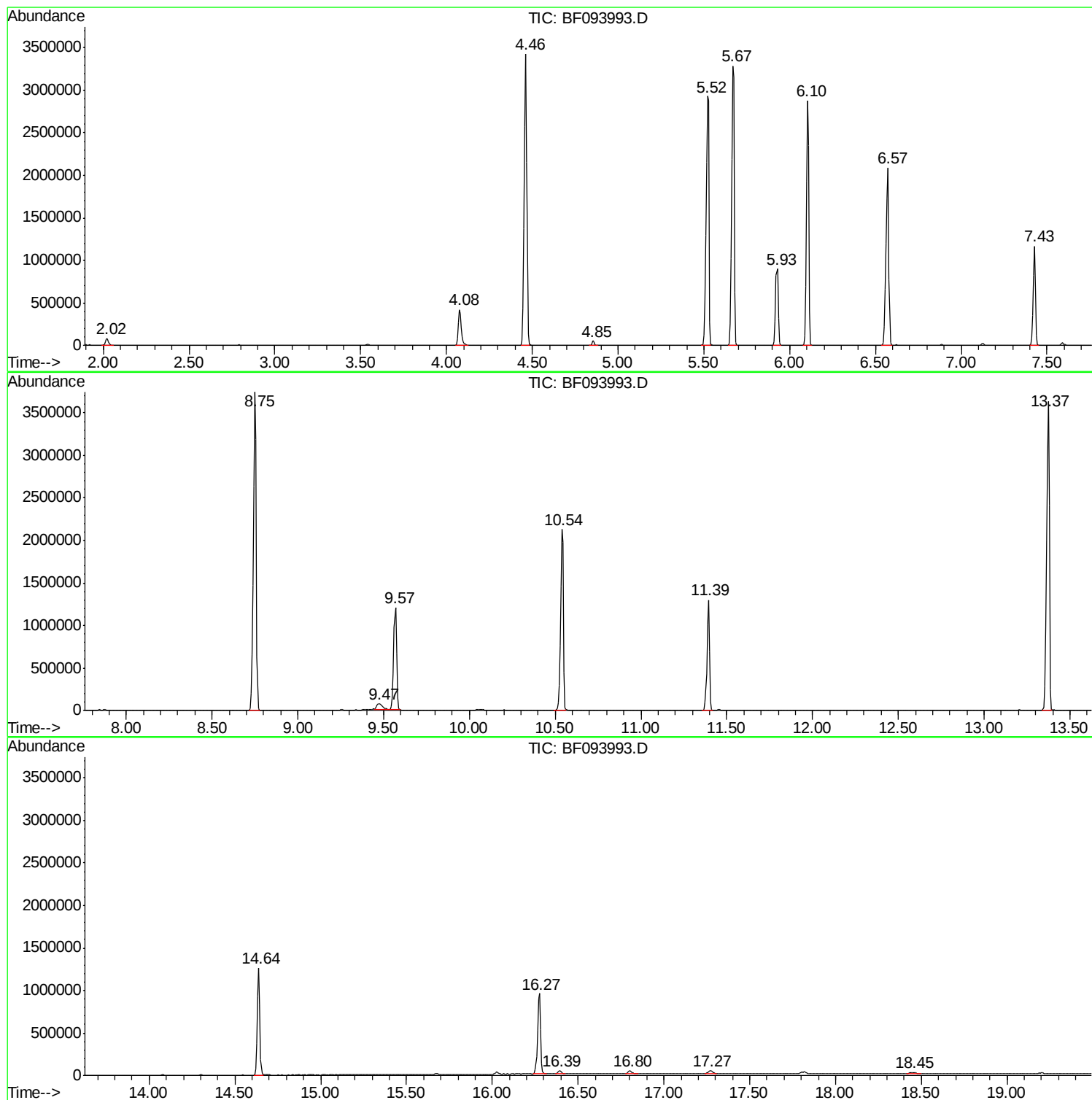
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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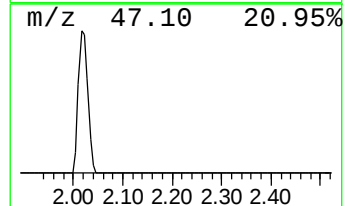
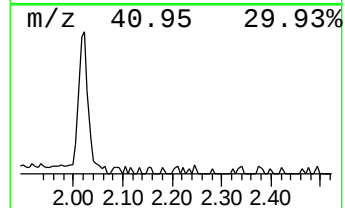
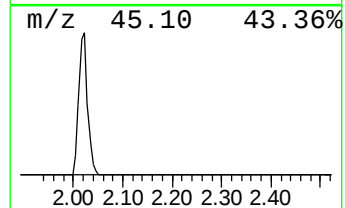
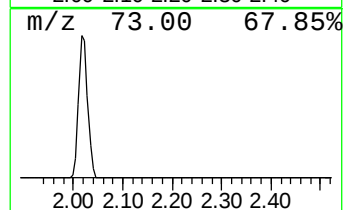
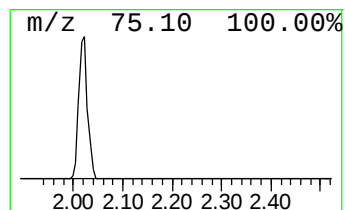
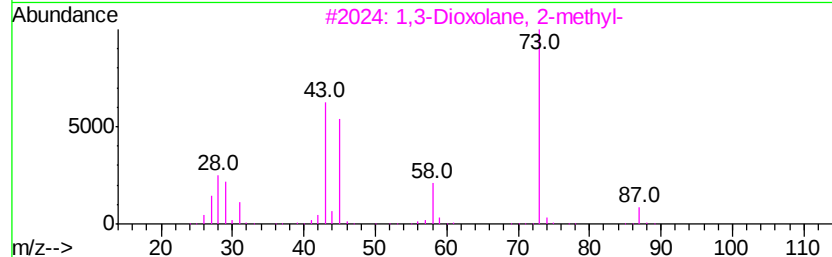
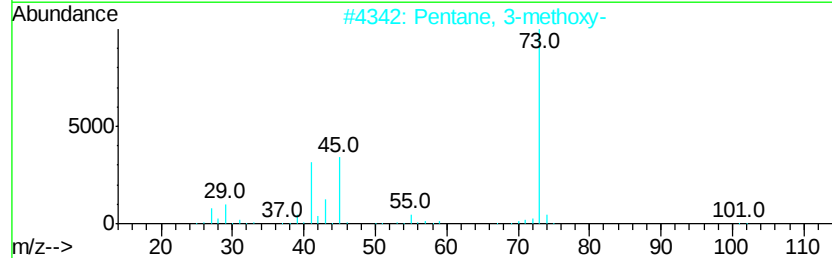
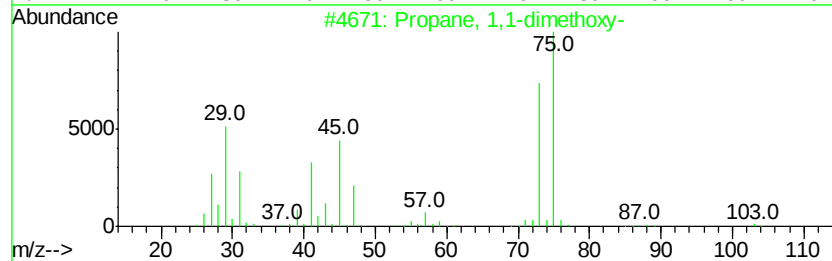
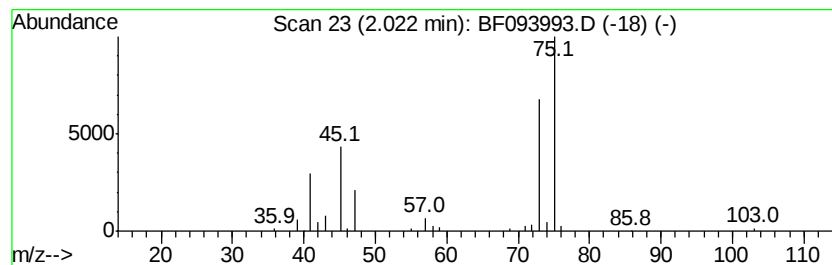
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.02	2.39 ng	101127	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	10
4		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5		2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	9



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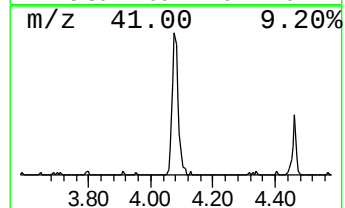
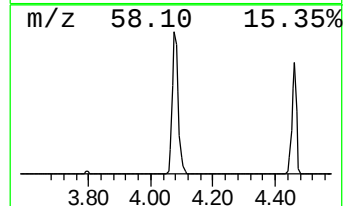
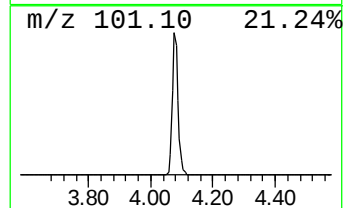
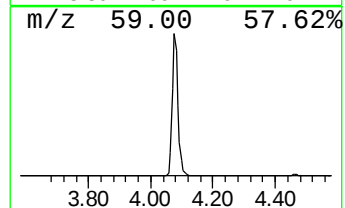
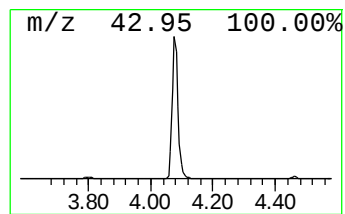
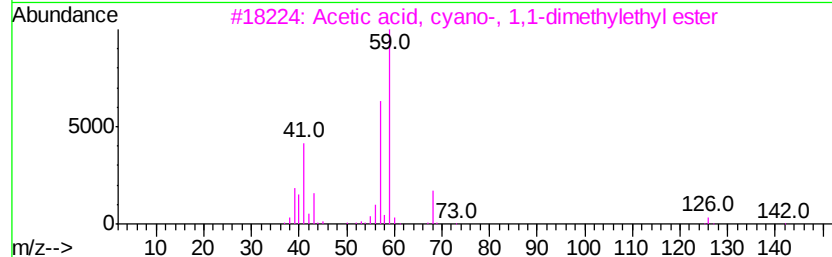
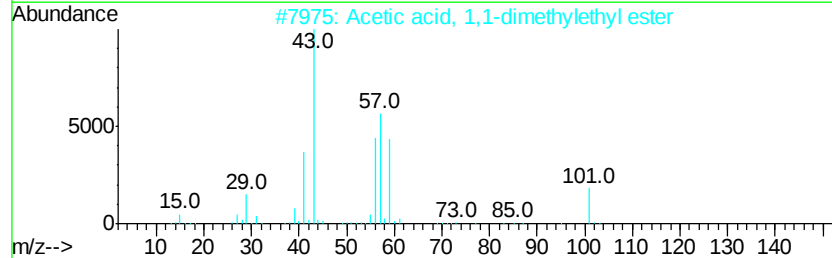
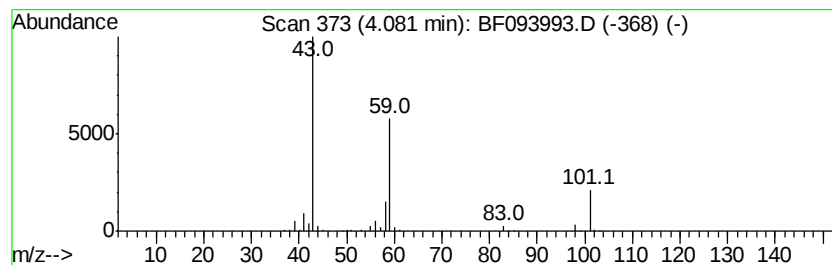
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	12.67 ng	536338	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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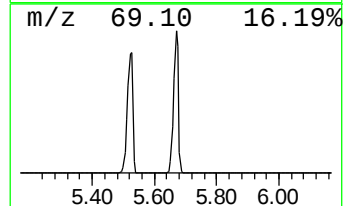
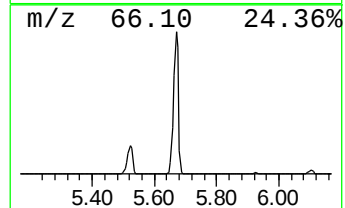
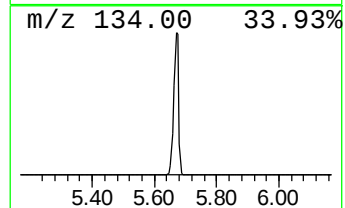
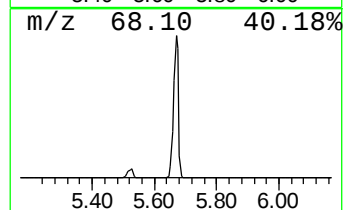
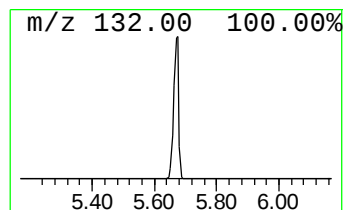
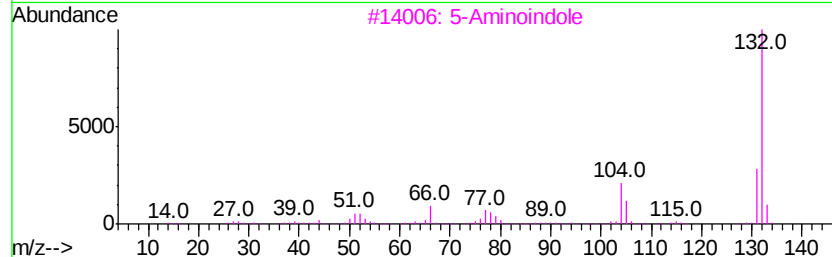
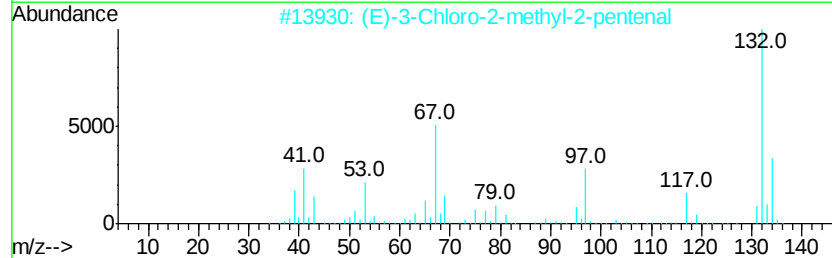
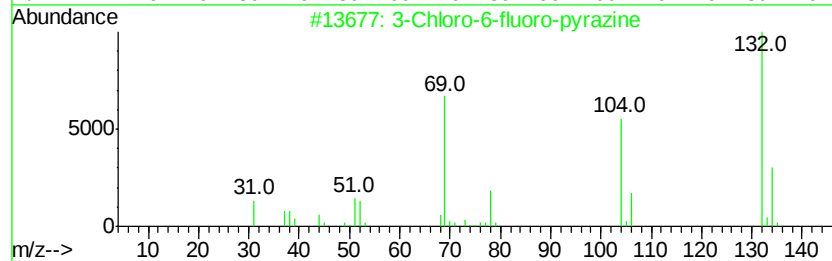
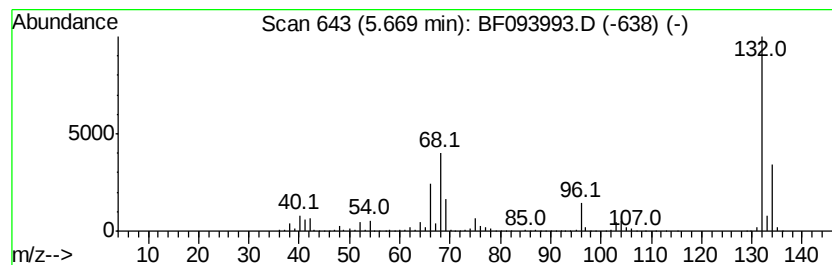
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Peak Number 3 unknown5.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	88.29 ng	3737380	1,4-Dichlorobenzene-d4	5.93

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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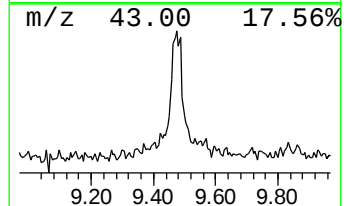
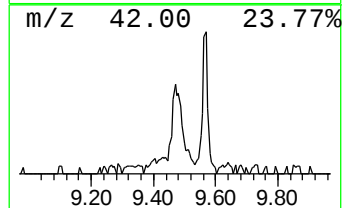
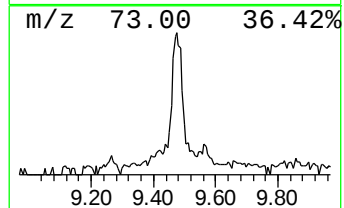
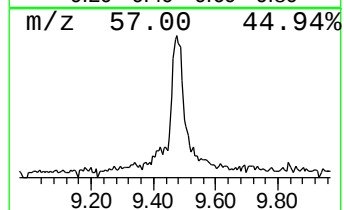
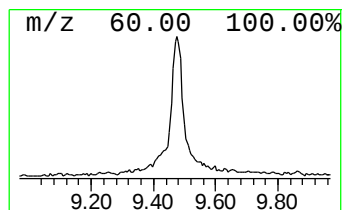
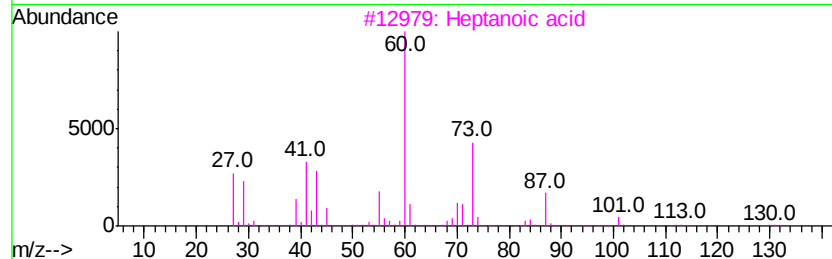
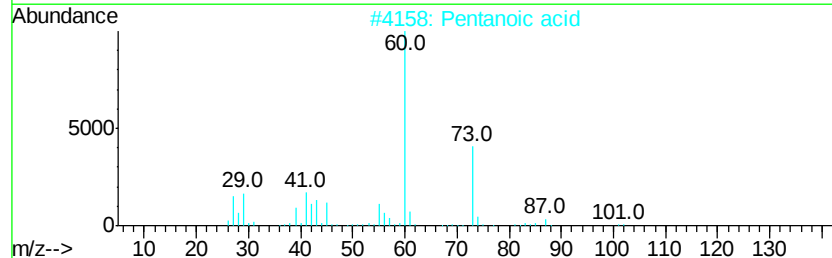
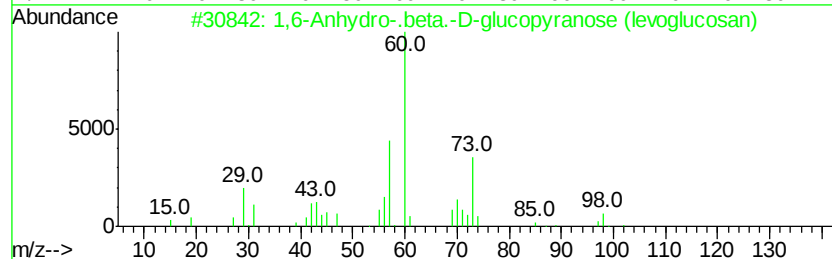
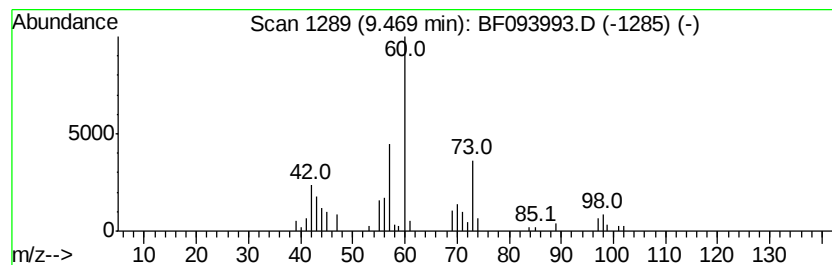
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	2.47 ng	155902	Acenaphthene-d10	9.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	80
2		Pentanoic acid	102	C5H10O2	000109-52-4	50
3		Heptanoic acid	130	C7H14O2	000111-14-8	47
4		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	45
5		L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.02	2.4	ng	101127	1	5.93	846591	20.0
2-Pentanone, 4-hy...	4.08	12.7	ng	536338	1	5.93	846591	20.0
unknown5.67	5.67	88.3	ng	3737380	1	5.93	846591	20.0
1,6-Anhydro-.beta...	9.47	2.5	ng	155902	3	9.57	1262050	20.0