

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
 Data File : BF091629.D
 Acq On : 15 Dec 2016 15:38
 Operator : UM/SJ
 Sample : PB95351BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB95351BL

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-BF120916.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	3.287	102	105	114	rVB	117562	218295	2.76%	0.304%
2	4.293	191	193	197	rVB	298172	361261	4.57%	0.503%
3	4.624	219	222	230	rVB2	28891	81457	1.03%	0.113%
4	4.967	249	252	261	rBV	2237863	3173539	40.15%	4.419%
5	5.390	286	289	292	rBV	5628607	6604880	83.55%	9.196%
6	6.430	377	380	382	rBV	6549017	7474568	94.55%	10.407%
7	6.556	388	391	393	rBV	6941829	7126659	90.15%	9.923%
8	6.784	408	411	413	rBV	2171316	1886012	23.86%	2.626%
9	6.944	422	425	427	rBV	4648946	5551686	70.23%	7.730%
10	7.344	457	460	463	rBV	3731708	4265503	53.96%	5.939%
11	8.064	521	523	526	rBV	2077038	2391844	30.26%	3.330%
12	9.150	614	618	620	rBV	7563500	7855274	99.37%	10.937%
13	9.745	666	670	674	rBV	243782	347591	4.40%	0.484%
14	9.825	674	677	679	rVB	2879943	2872037	36.33%	3.999%
15	10.613	743	746	748	rBV	4455109	4923517	62.28%	6.855%
16	11.299	804	806	809	rVB2	2427380	2691535	34.05%	3.748%
17	12.899	942	946	948	rBV	5367854	7905030	100.00%	11.007%
18	13.939	1034	1037	1039	rBV	2114245	2639490	33.39%	3.675%
19	15.208	1145	1148	1151	rBV	68694	101794	1.29%	0.142%
20	15.345	1157	1160	1162	rBV	1654494	2136117	27.02%	2.974%
21	15.391	1162	1164	1168	rVB	94954	139247	1.76%	0.194%
22	15.677	1186	1189	1191	rBV	92303	171131	2.16%	0.238%
23	15.791	1197	1199	1204	rVB	109796	161624	2.04%	0.225%
24	16.225	1233	1237	1238	rBV	71270	154566	1.96%	0.215%
25	16.260	1238	1240	1245	rVB	90563	156577	1.98%	0.218%
26	16.808	1285	1288	1291	rBV	49816	102160	1.29%	0.142%
27	16.888	1291	1295	1299	rVB2	49541	135247	1.71%	0.188%
28	17.448	1341	1344	1348	rBV	37396	87154	1.10%	0.121%
29	17.688	1361	1365	1370	rVB2	32490	104526	1.32%	0.146%

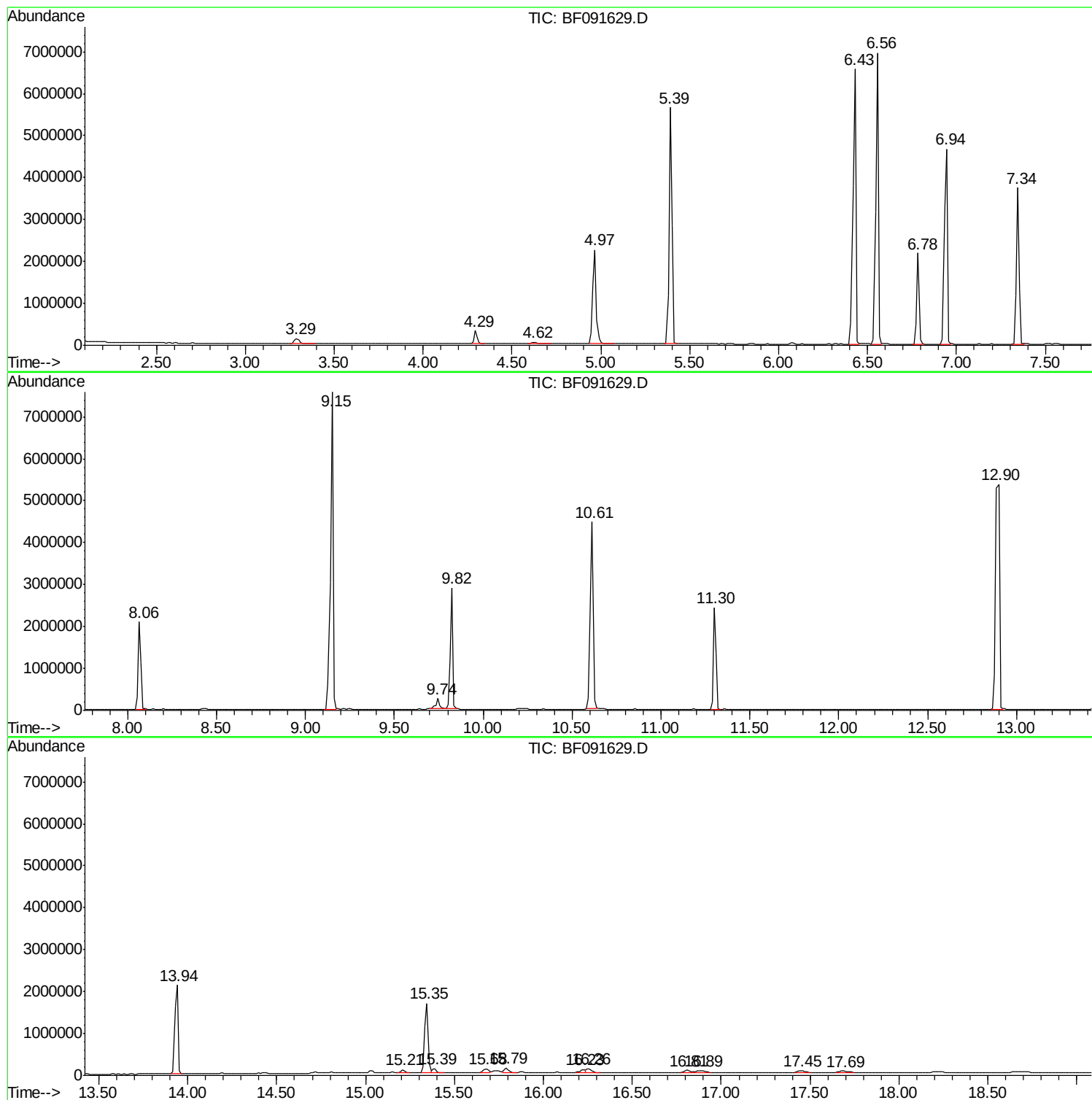
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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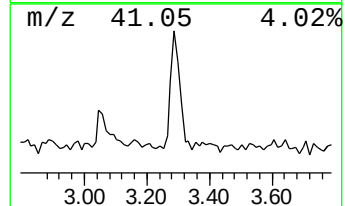
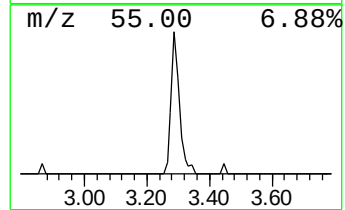
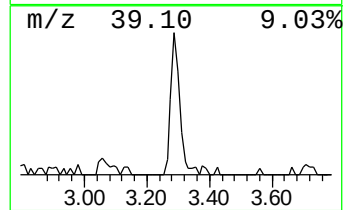
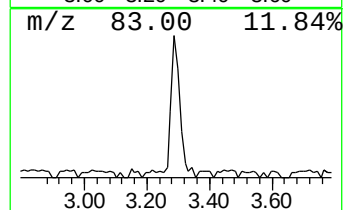
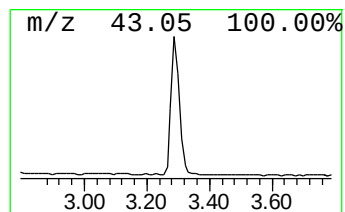
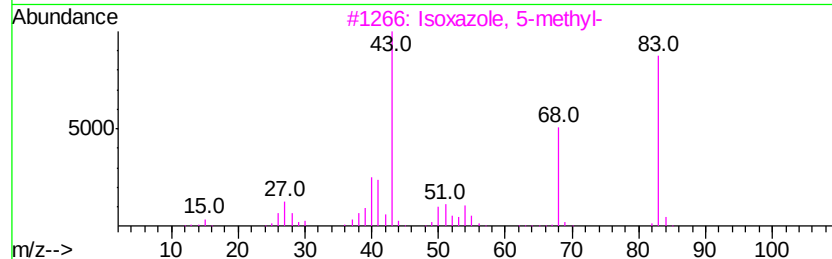
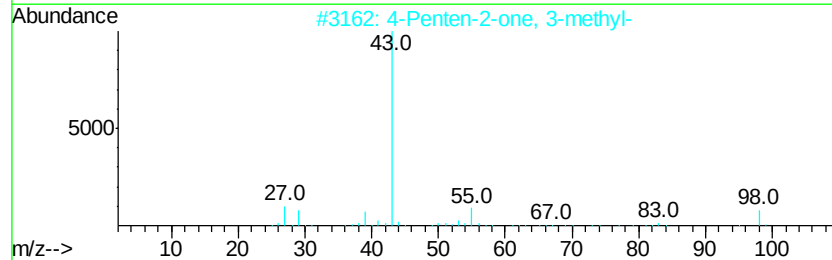
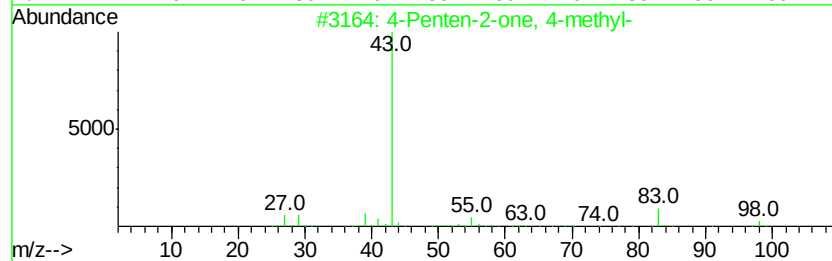
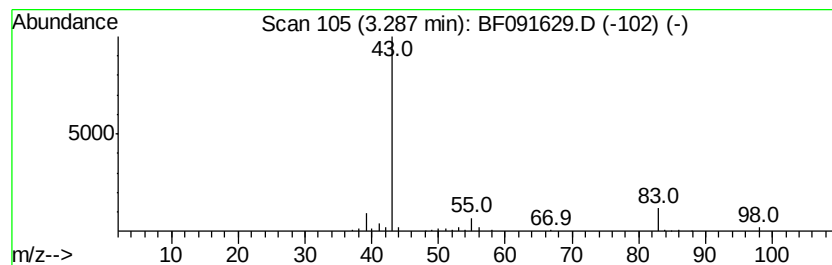
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	2.31 ng	218295	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	23
3			Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9
4			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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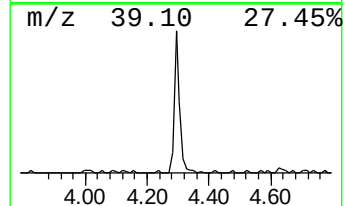
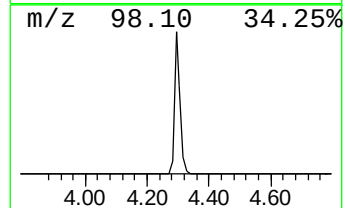
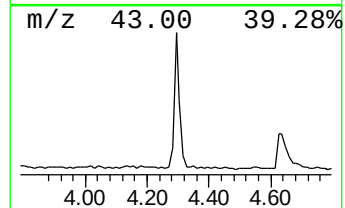
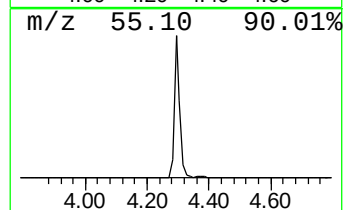
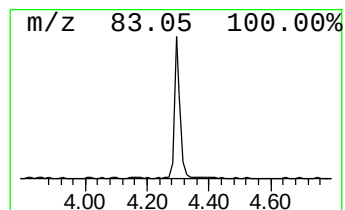
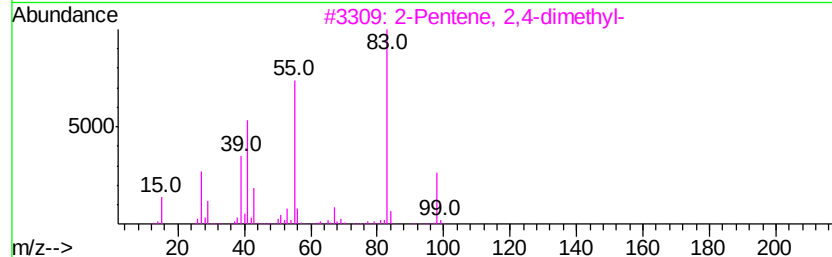
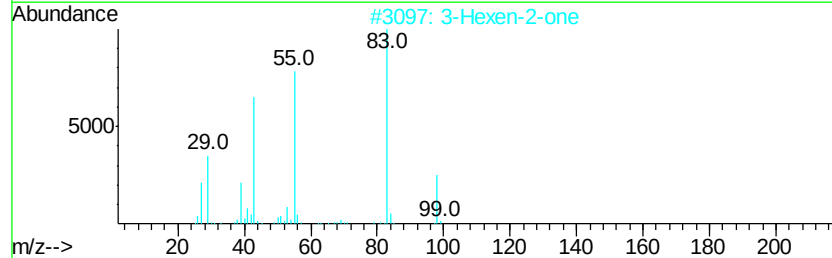
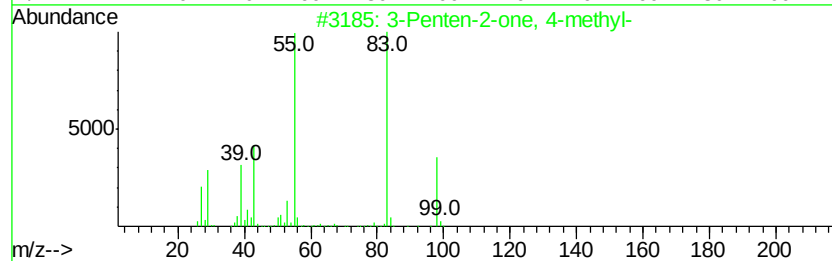
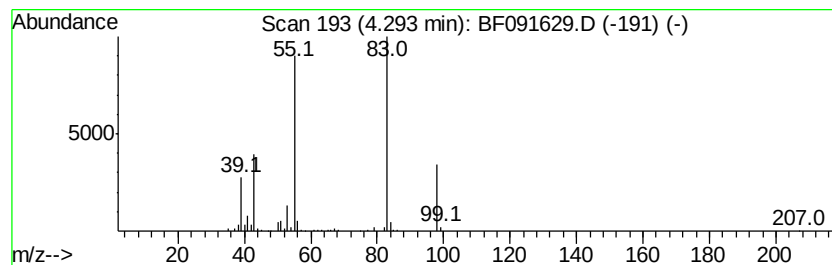
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	3.83 ng	361261	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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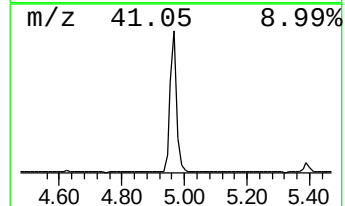
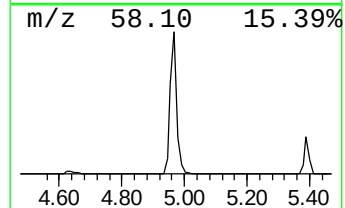
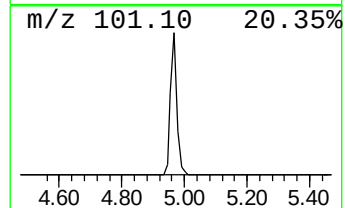
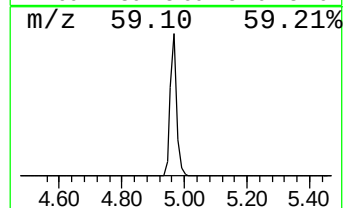
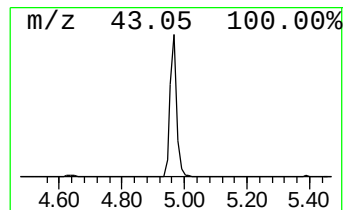
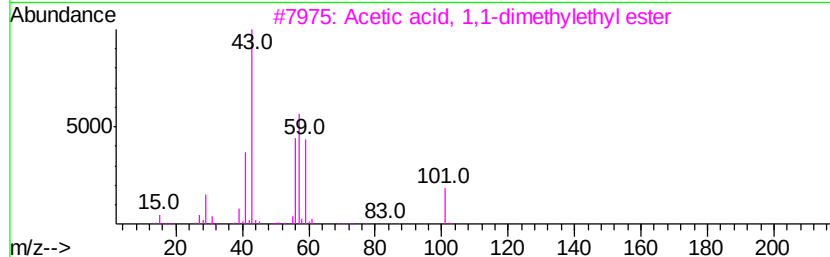
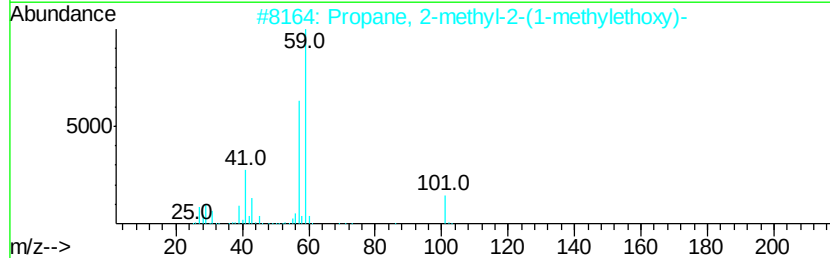
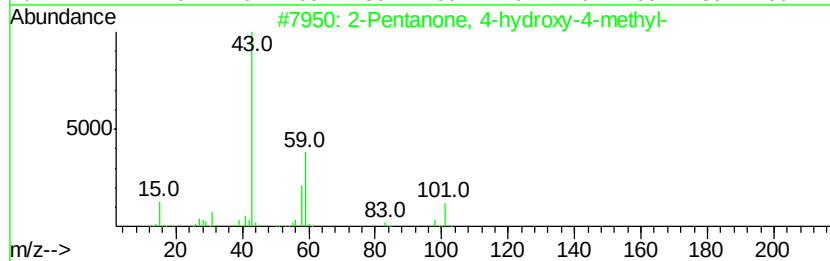
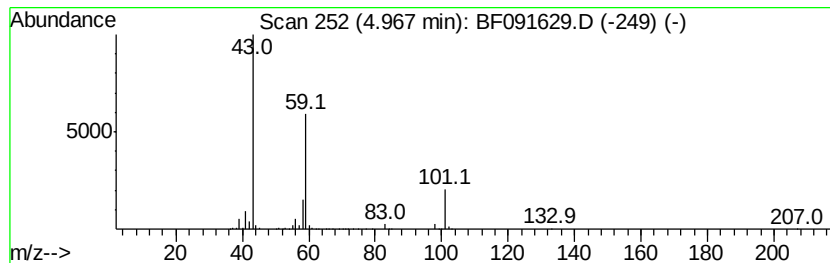
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	33.65 ng	3173540	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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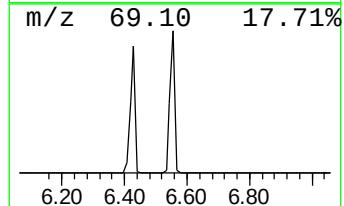
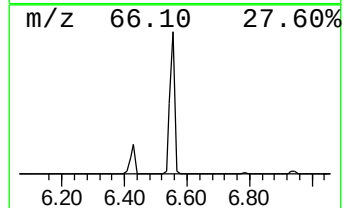
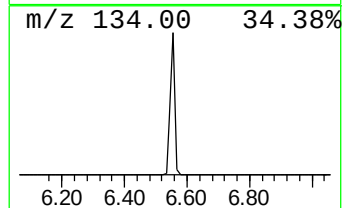
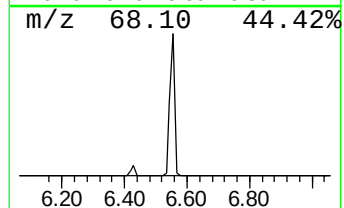
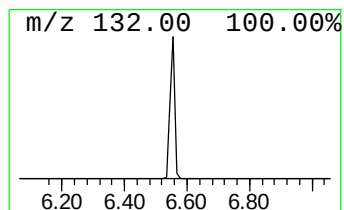
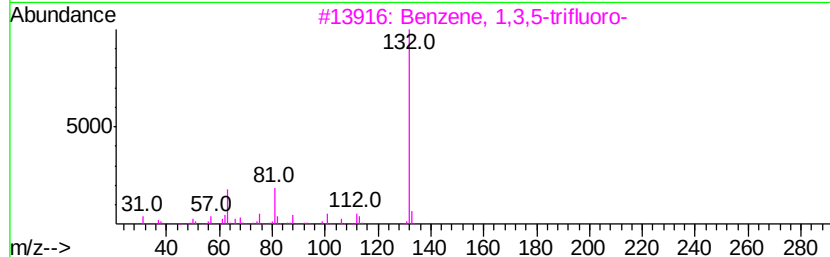
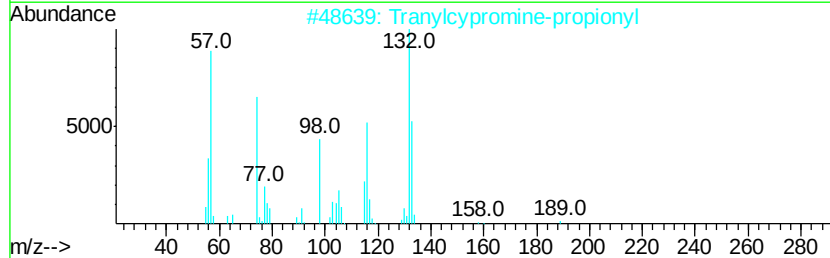
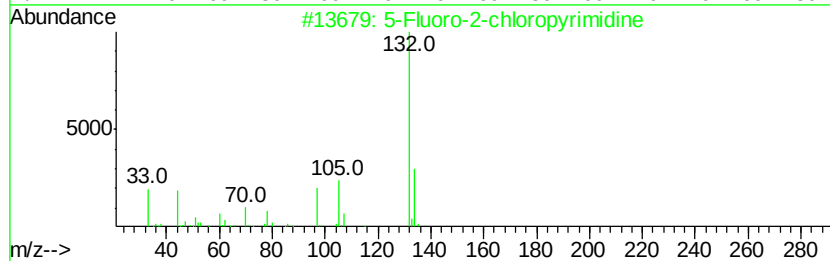
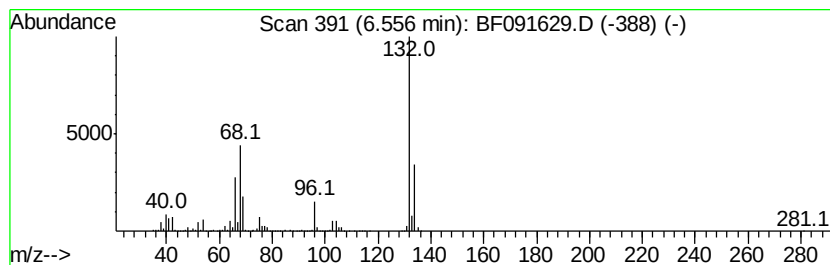
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	75.57 ng	7126660	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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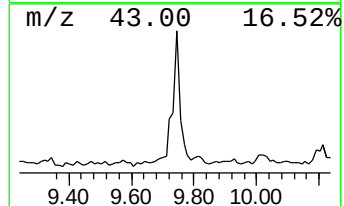
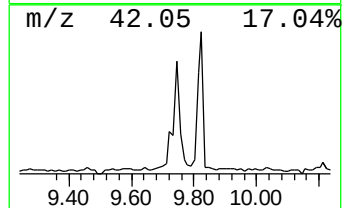
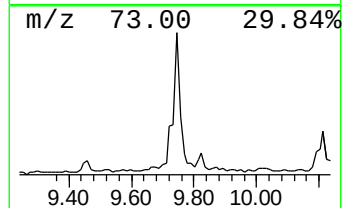
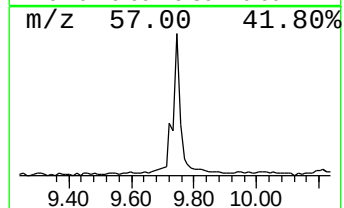
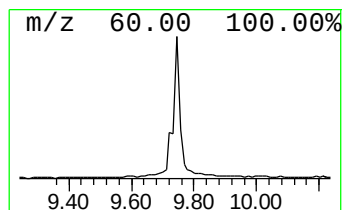
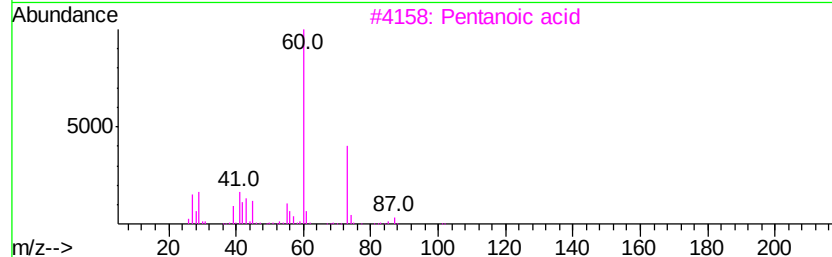
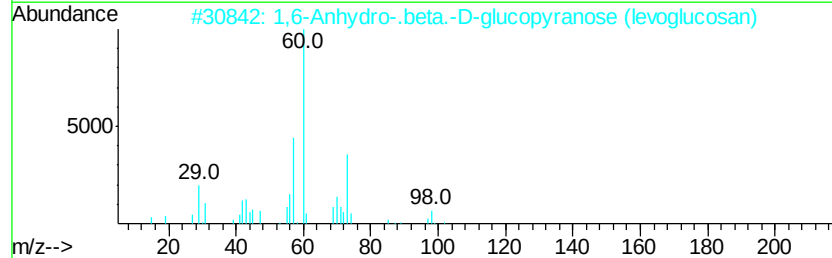
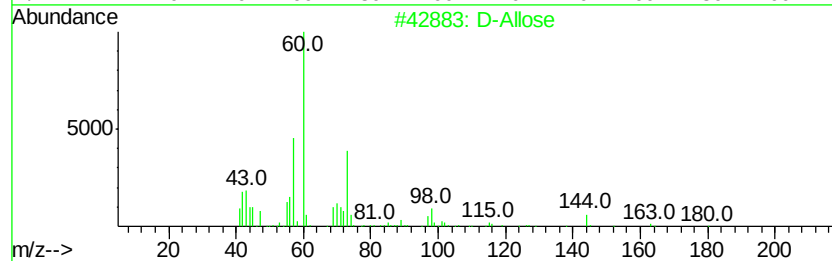
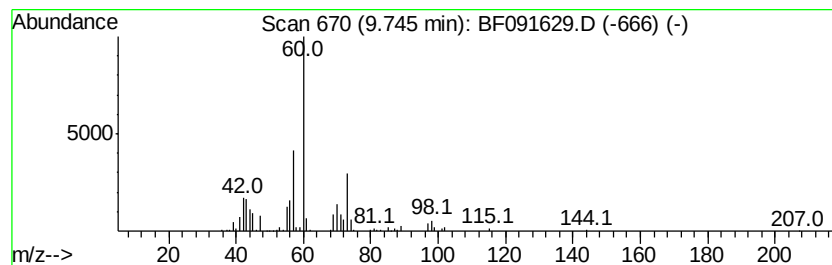
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 D-Allose Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	2.42 ng	347591	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Allose	180	C6H12O6	002595-97-3	90
2		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	90
3		Pentanoic acid	102	C5H10O2	000109-52-4	59
4		3,4-Altrosan	162	C6H10O5	1000129-76-4	53
5		Butanoic acid	88	C4H8O2	000107-92-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.29	2.3	ng	218295	1	6.78	1886010	20.0
3-Penten-2-one, 4...	4.29	3.8	ng	361261	1	6.78	1886010	20.0
2-Pentanone, 4-hy...	4.97	33.6	ng	3173540	1	6.78	1886010	20.0
unknown6.56	6.56	75.6	ng	7126660	1	6.78	1886010	20.0
D-Allose	9.74	2.4	ng	347591	3	9.82	2872040	20.0