

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020216\
 Data File : BF084769.D
 Acq On : 3 Feb 2016 3:26
 Operator : SJ/IZ
 Sample : H1287-03
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B013(16-18)

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-BF020116.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	2.327	11	21	26	rVB3	21620	101137	1.30%	0.153%
2	2.453	30	32	36	rVB	130253	168971	2.17%	0.256%
3	4.190	181	184	189	rVB	548574	940602	12.08%	1.424%
4	4.898	241	246	252	rVB	2486778	5575488	71.60%	8.438%
5	5.321	280	283	285	rBV	4491854	6129218	78.72%	9.276%
6	5.710	315	317	321	rVB	350672	365538	4.69%	0.553%
7	6.361	370	374	376	rBV	4876369	5915461	75.97%	8.953%
8	6.476	381	384	386	rVV	6063204	6496693	83.44%	9.832%
9	6.693	401	403	406	rBV	1304567	1218182	15.64%	1.844%
10	6.853	415	417	419	rBV	5148876	4571523	58.71%	6.919%
11	6.956	424	426	428	rBV	91632	87081	1.12%	0.132%
12	7.264	450	453	455	rBV	3479115	3750309	48.16%	5.676%
13	7.733	490	494	499	rBV2	83956	135746	1.74%	0.205%
14	7.984	513	516	520	rBV2	1534606	3419427	43.91%	5.175%
15	8.693	576	578	580	rBV	242838	282026	3.62%	0.427%
16	8.796	584	587	589	rVB	154061	170112	2.18%	0.257%
17	9.070	607	611	613	rBV	4749114	7786487	100.00%	11.784%
18	9.733	666	669	671	rBV	1743005	1956002	25.12%	2.960%
19	9.768	671	672	674	rVB	305019	217916	2.80%	0.330%
20	9.939	684	687	689	rBV	154346	154722	1.99%	0.234%
21	10.282	712	717	719	rVB	155662	158707	2.04%	0.240%
22	10.522	734	738	741	rBV2	3348290	4957792	63.67%	7.503%
23	11.219	795	799	801	rBV	1446672	2024077	25.99%	3.063%
24	12.808	935	938	940	rVB	6567860	6895482	88.56%	10.436%
25	13.848	1026	1029	1031	rBV	1309869	1529186	19.64%	2.314%
26	15.219	1146	1149	1152	rBV	806930	1066364	13.70%	1.614%

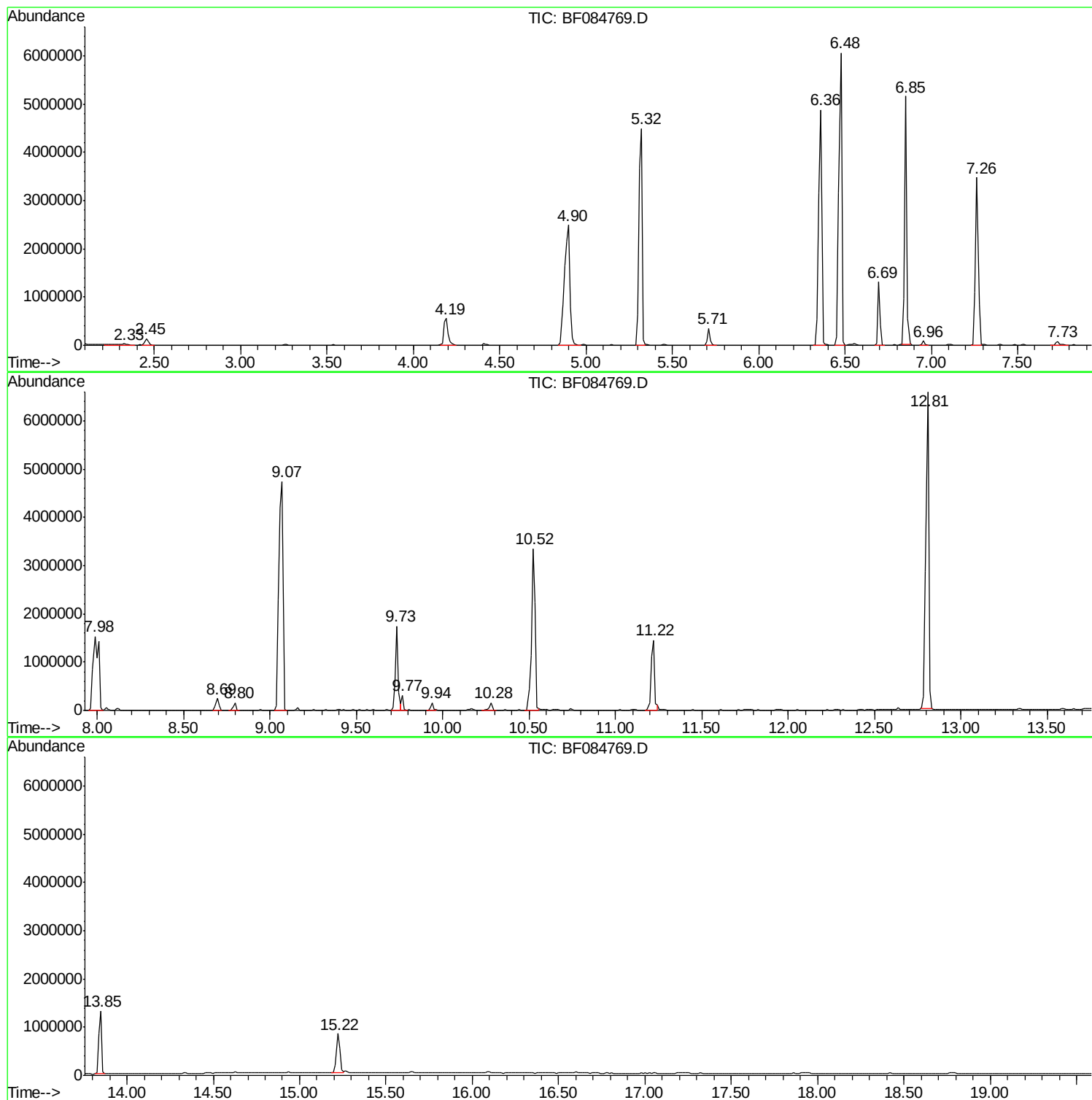
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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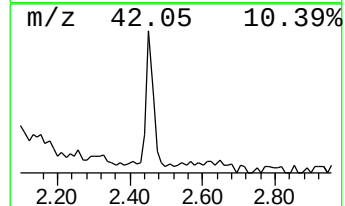
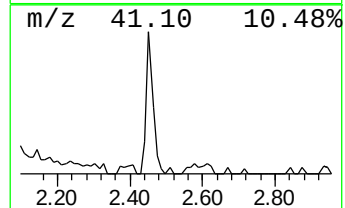
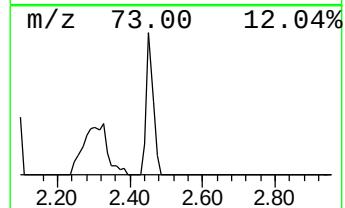
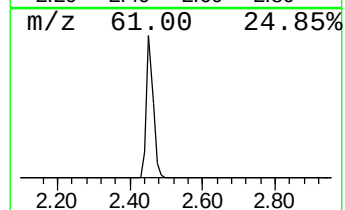
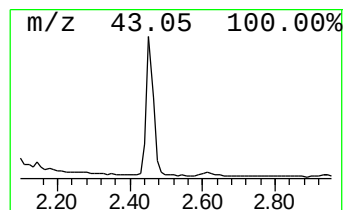
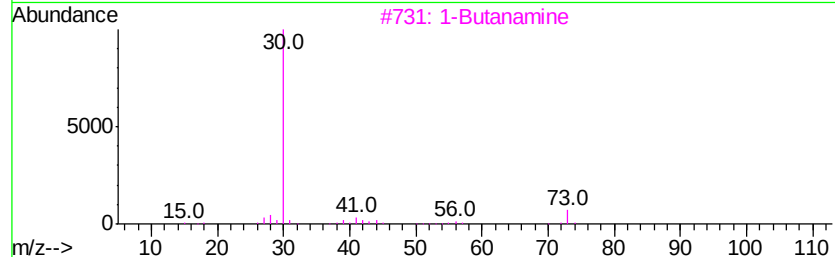
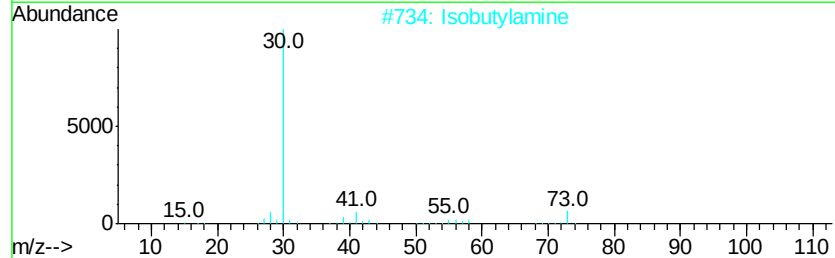
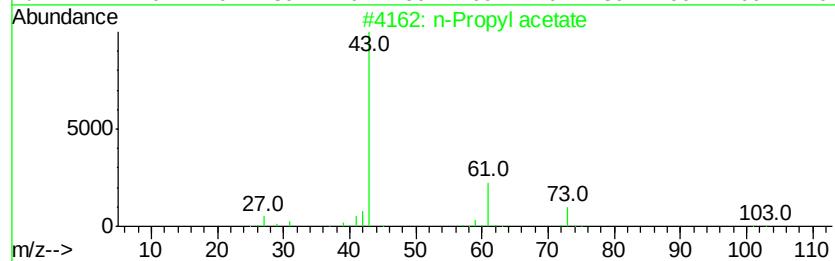
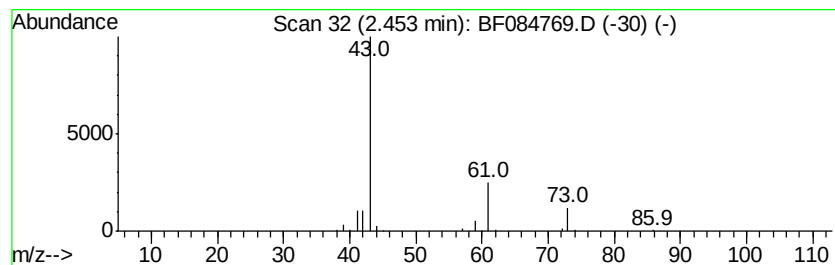
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.77 ng	168971	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	78
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
5			Pentane	72	C5H12	000109-66-0	4



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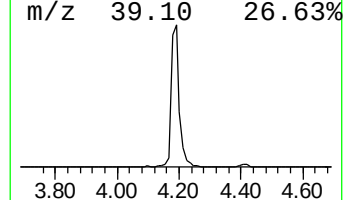
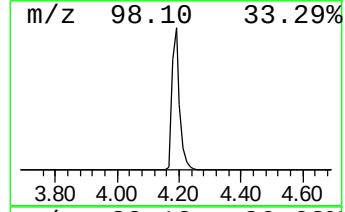
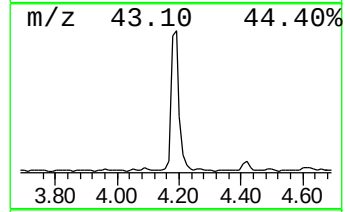
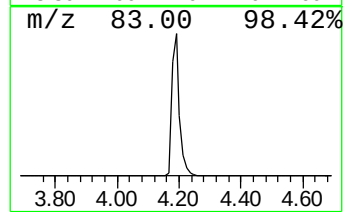
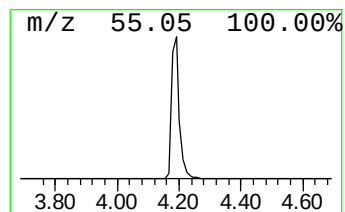
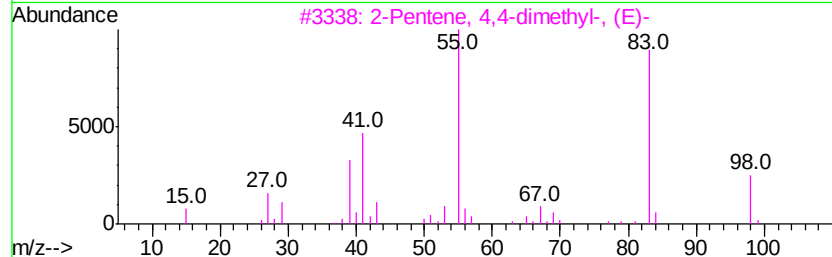
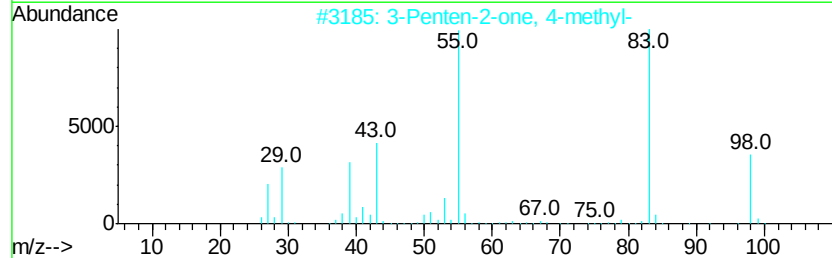
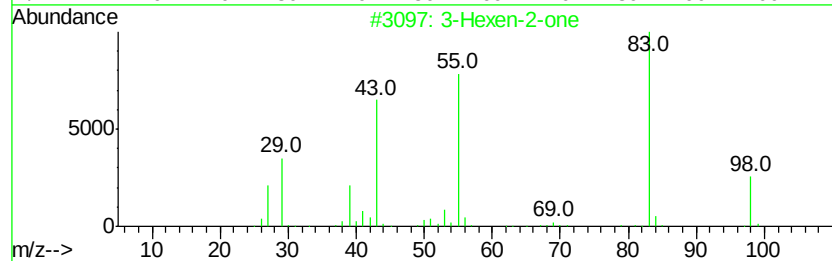
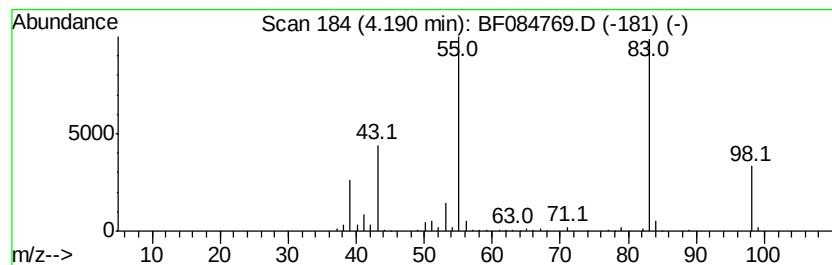
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	15.44 ng	940602	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72



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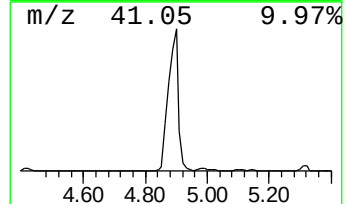
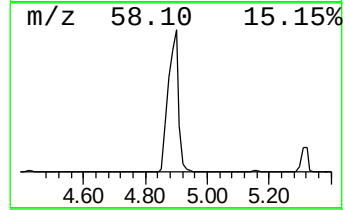
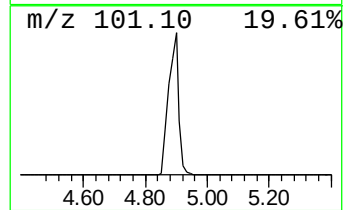
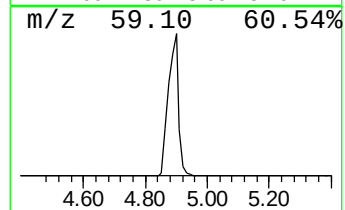
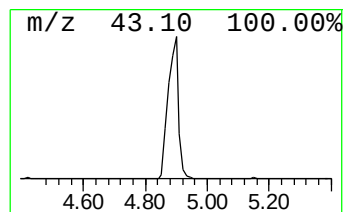
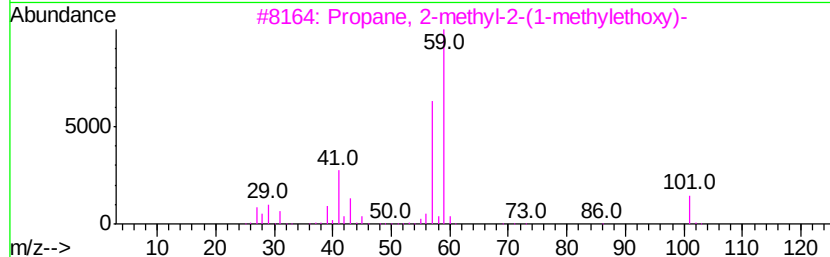
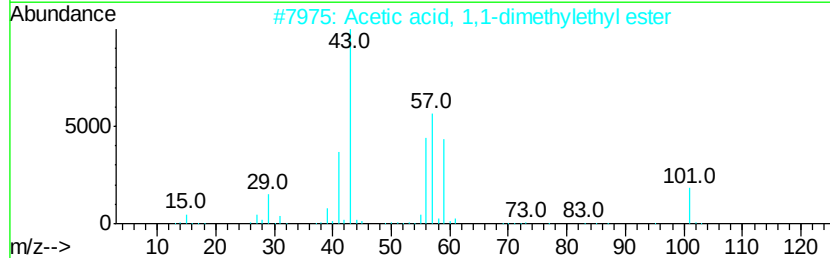
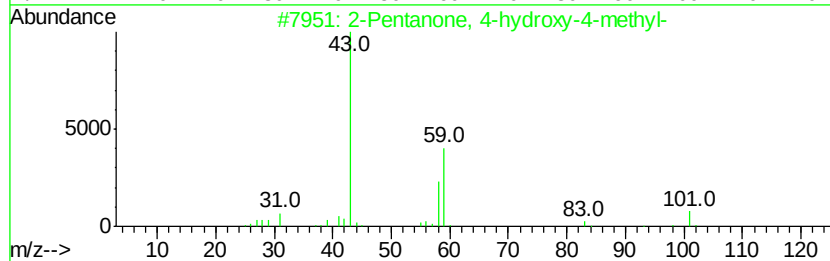
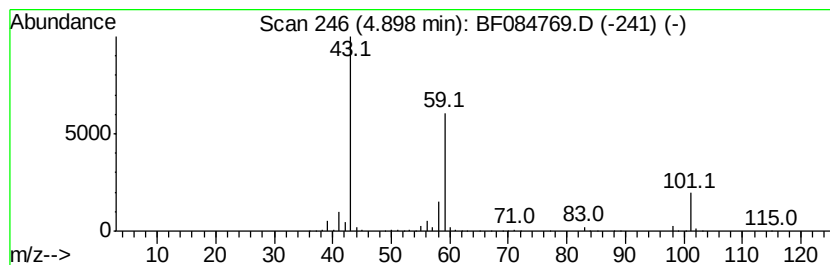
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	91.54 ng	5575490	1,4-Dichlorobenzene-d4	6.69

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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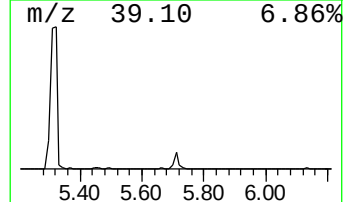
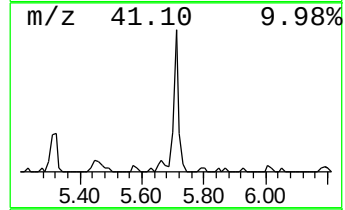
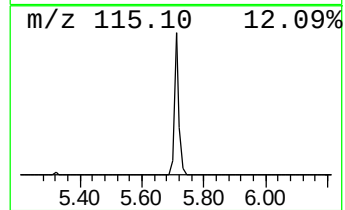
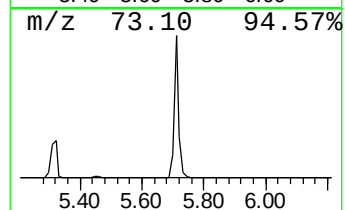
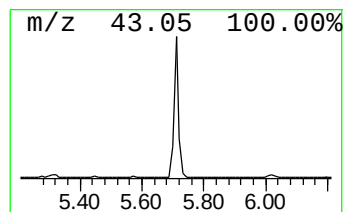
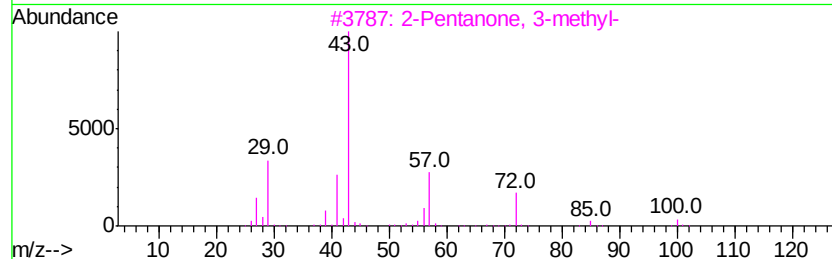
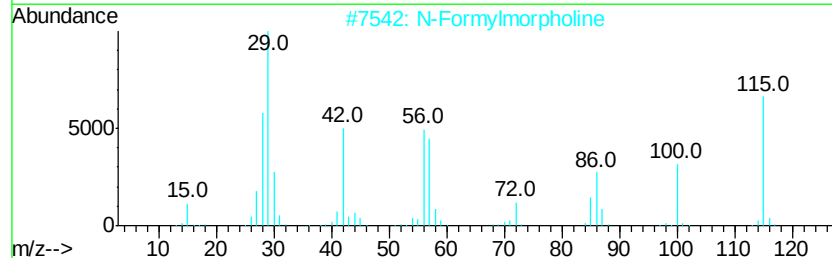
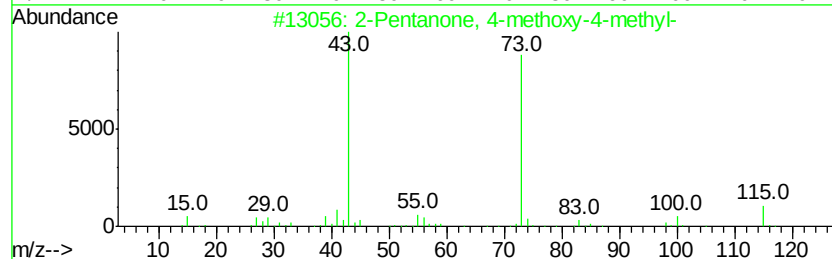
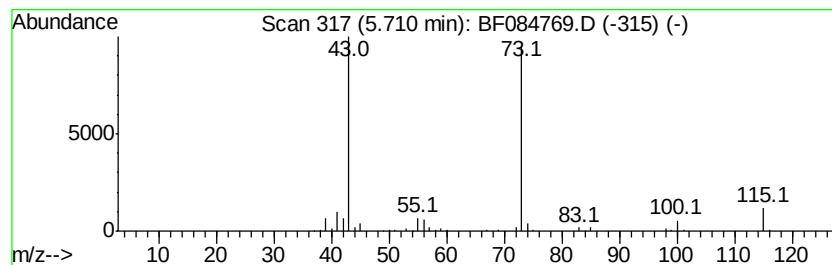
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	6.00 ng	365538	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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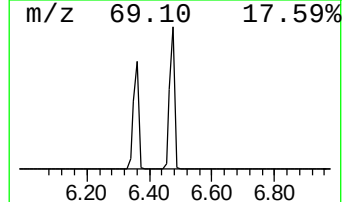
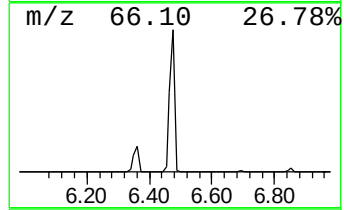
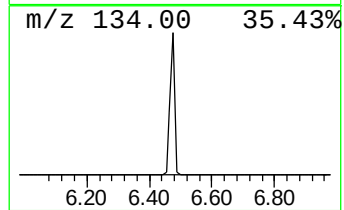
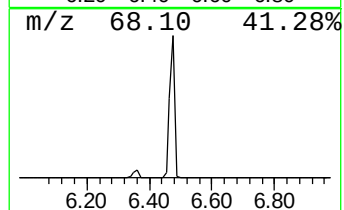
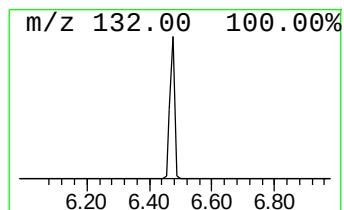
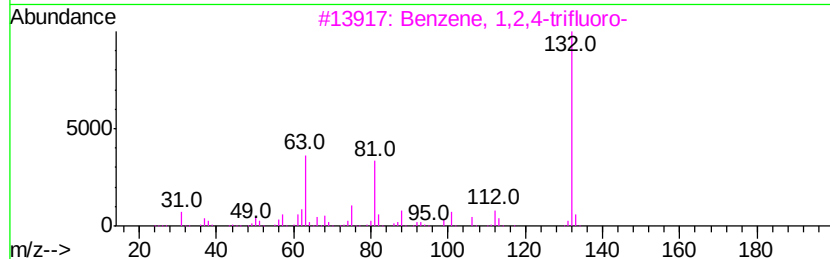
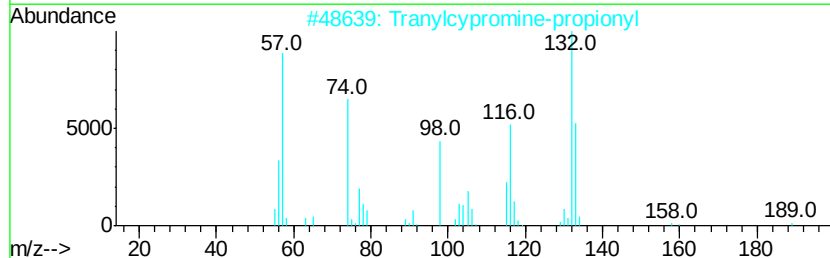
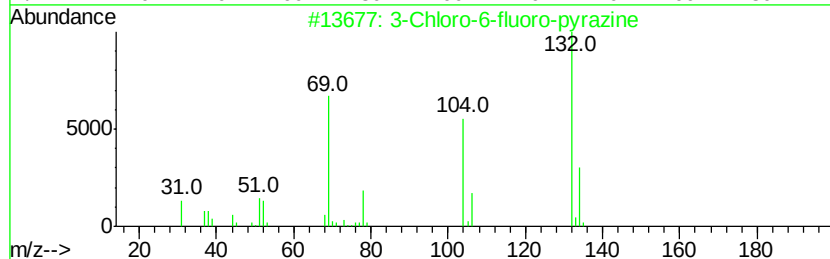
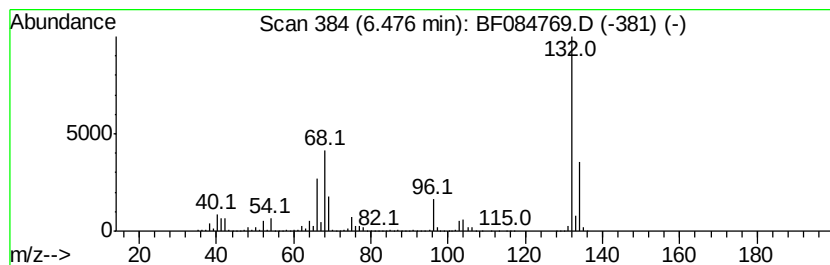
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	106.66 ng	6496690	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.45	2.8	ng	168971	1	6.69	1218180	20.0
3-Hexen-2-one	4.19	15.4	ng	940602	1	6.69	1218180	20.0
2-Pentanone, 4-hy...	4.90	91.5	ng	5575490	1	6.69	1218180	20.0
2-Pentanone, 4-me...	5.71	6.0	ng	365538	1	6.69	1218180	20.0
unknown6.48	6.48	106.7	ng	6496690	1	6.69	1218180	20.0