

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020216\
 Data File : BF084751.D
 Acq On : 2 Feb 2016 17:44
 Operator : SJ/IZ
 Sample : PB88120BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88120BL

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-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	4.156	178	181	189	rBV	373623	464623	8.52%	1.047%
2	4.864	239	243	252	rBV	2506300	3692874	67.69%	8.320%
3	5.299	278	281	283	rBV	4078779	3944256	72.30%	8.887%
4	5.699	314	316	318	rBV	279177	235813	4.32%	0.531%
5	6.350	370	373	375	rBV	4134391	4412745	80.88%	9.942%
6	6.464	380	383	386	rBV	3984489	3793194	69.53%	8.546%
7	6.693	401	403	406	rBV	1132268	1048193	19.21%	2.362%
8	6.853	414	417	419	rBV	3672871	3213068	58.89%	7.239%
9	7.265	450	453	455	rBV	2581473	2531253	46.40%	5.703%
10	7.985	513	516	518	rBV	1519481	1438305	26.36%	3.241%
11	9.070	607	611	613	rBV	3266157	4897919	89.78%	11.035%
12	9.733	666	669	672	rBV	1592268	1570779	28.79%	3.539%
13	10.522	735	738	741	rBV	2847728	3010225	55.18%	6.782%
14	11.219	796	799	801	rBV	1304673	1642668	30.11%	3.701%
15	12.808	935	938	940	rBV	5197193	5455739	100.00%	12.292%
16	13.848	1026	1029	1031	rBV	1772894	1726750	31.65%	3.890%
17	15.231	1147	1150	1152	rBV	931969	1306131	23.94%	2.943%

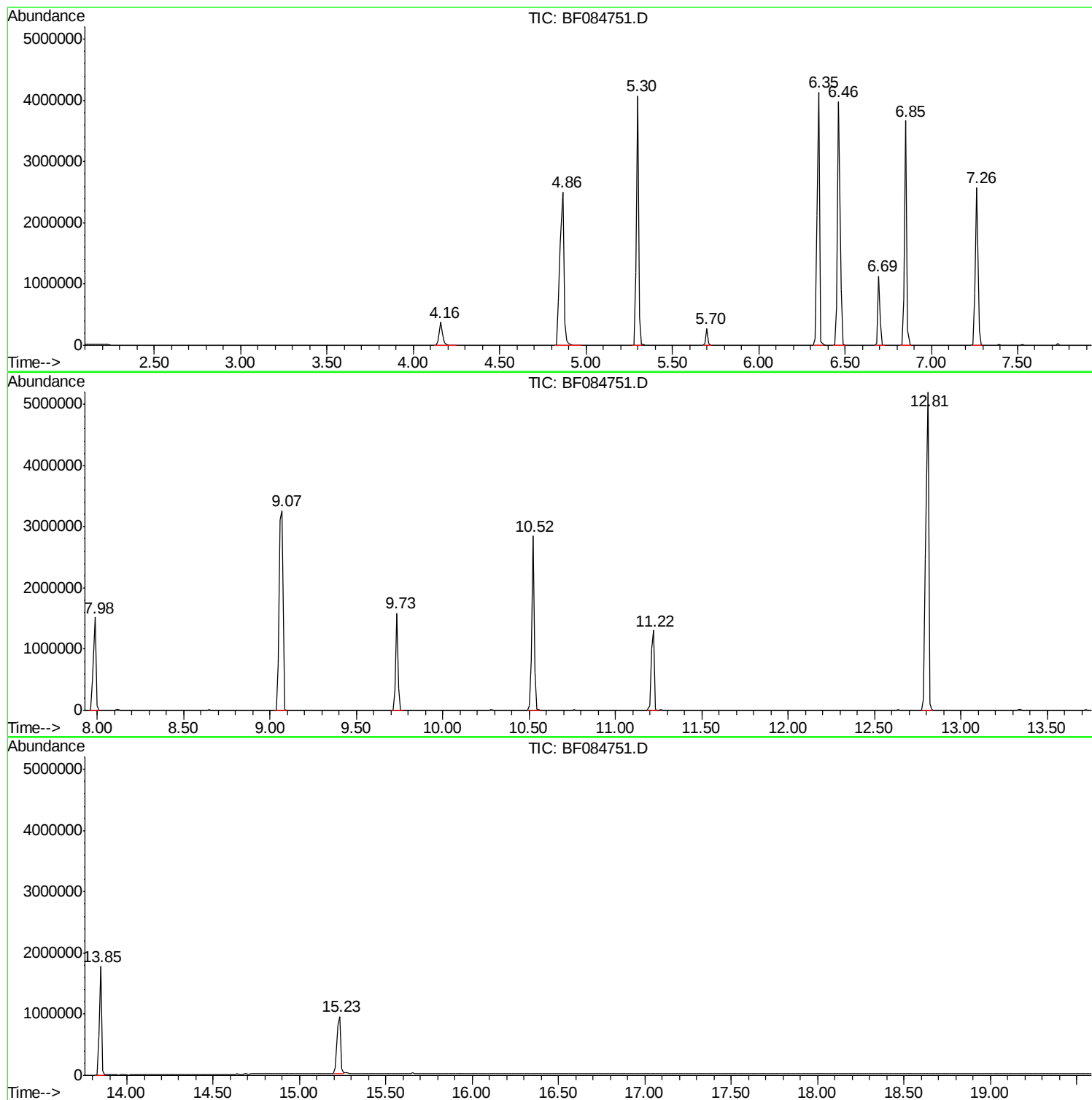
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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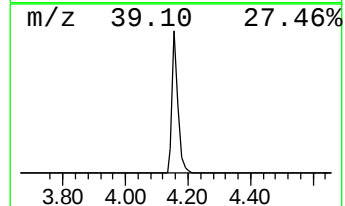
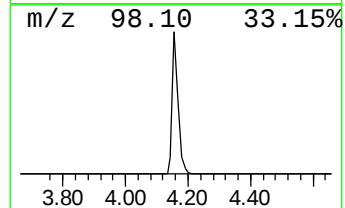
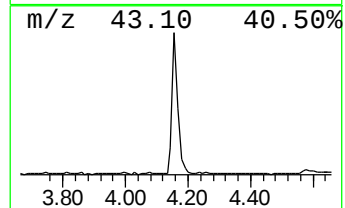
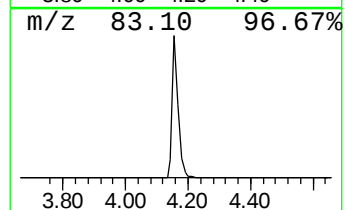
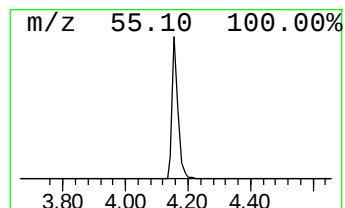
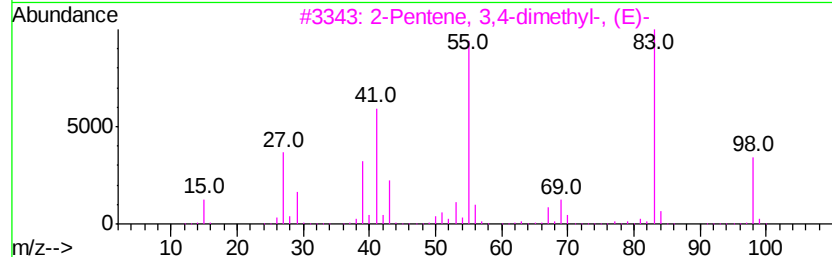
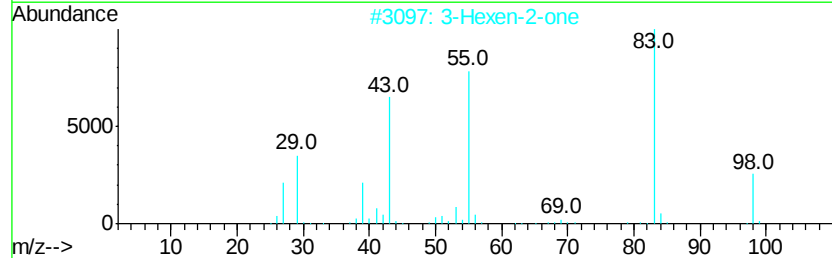
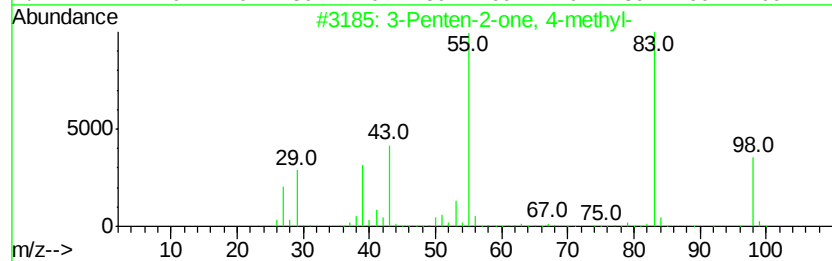
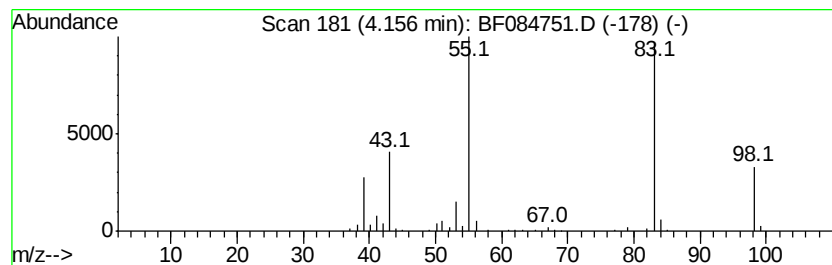
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	8.87 ng	464623	1,4-Dichlorobenzene-d4	6.69

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	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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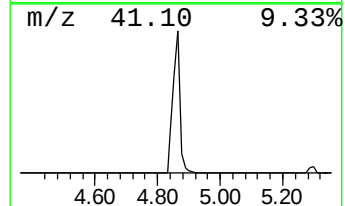
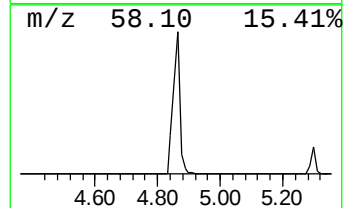
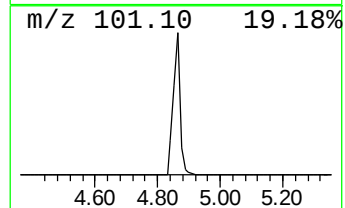
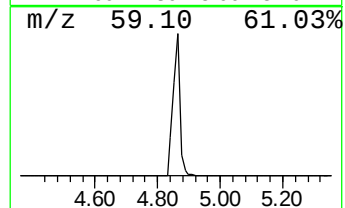
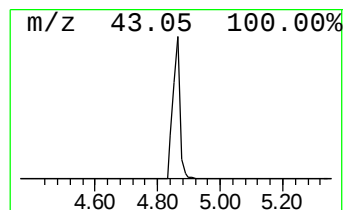
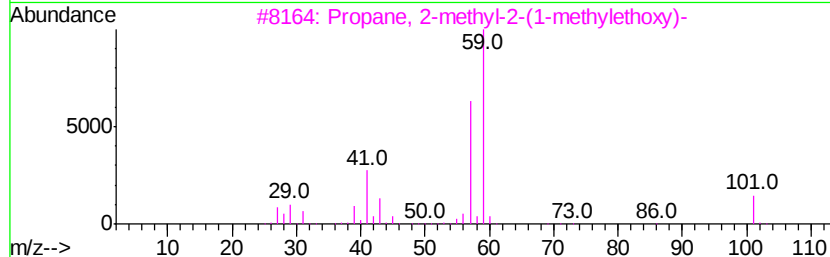
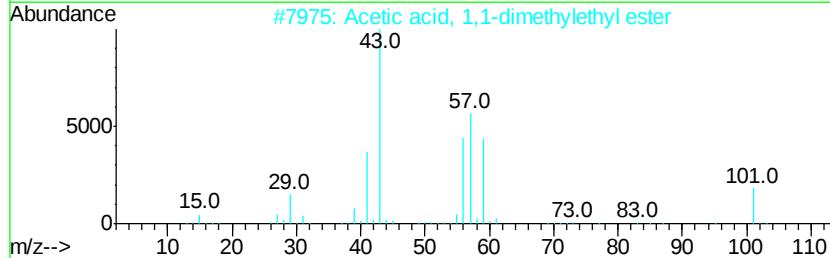
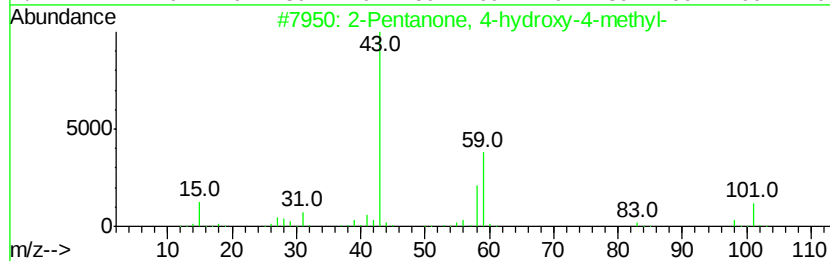
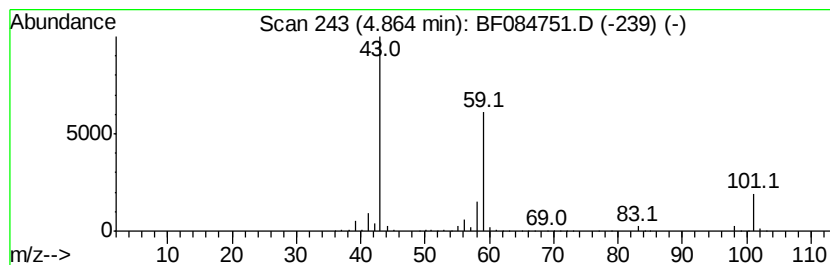
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	70.46 ng	3692870	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	59
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	36
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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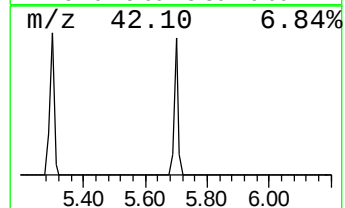
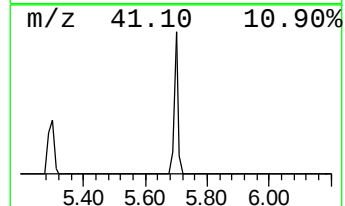
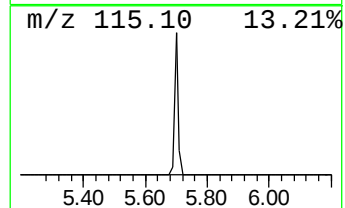
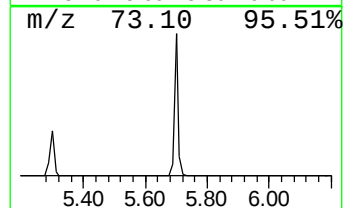
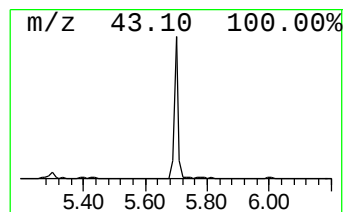
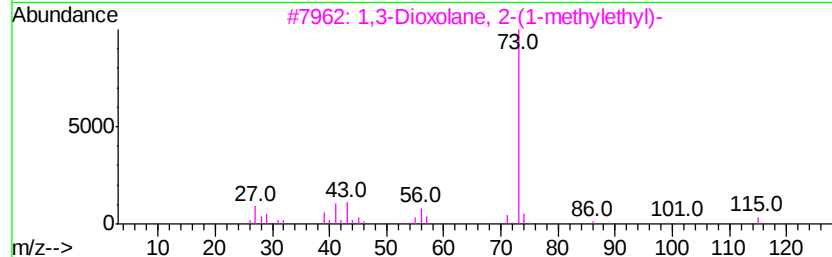
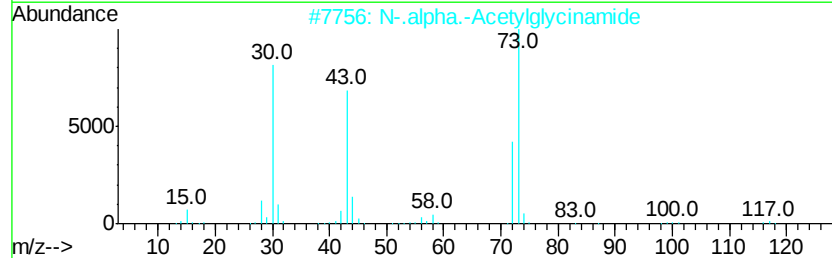
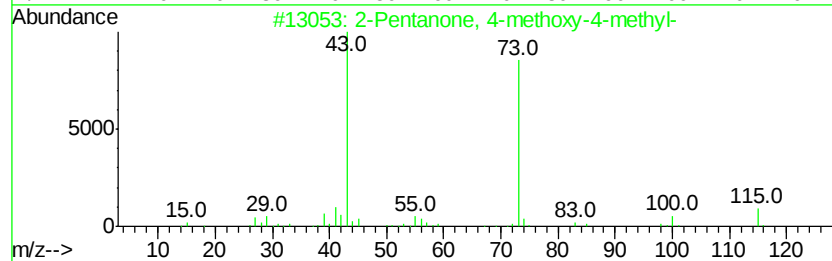
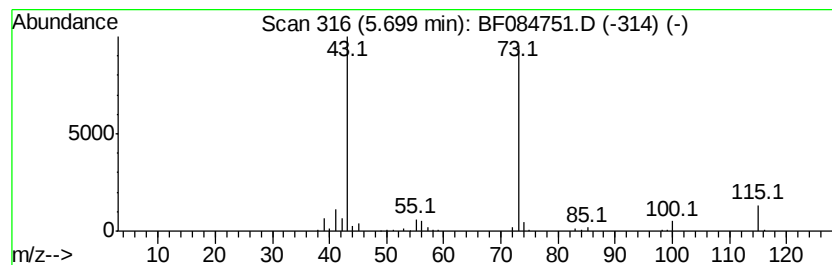
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	4.50 ng	235813	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-.alpha.-Acetylglucosamine	116	C4H8N2O2	002620-63-5	43
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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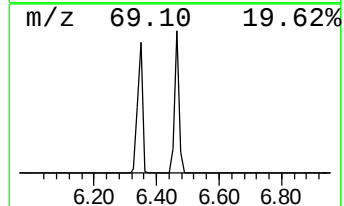
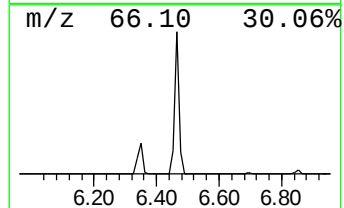
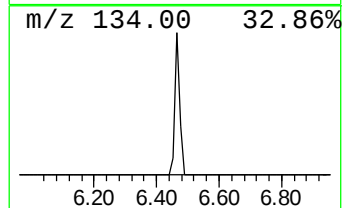
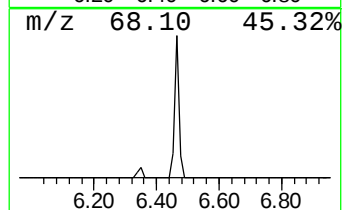
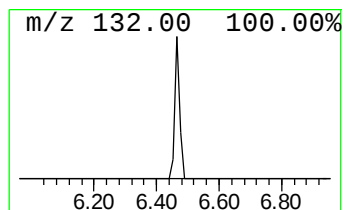
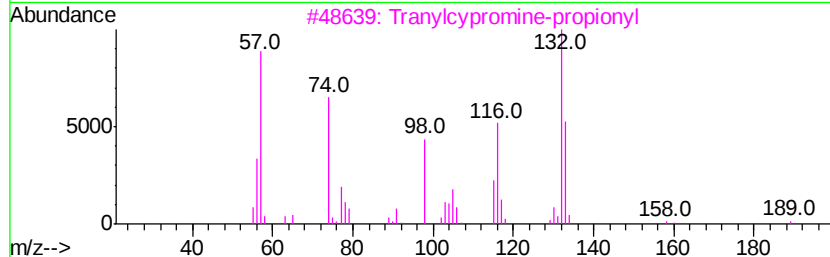
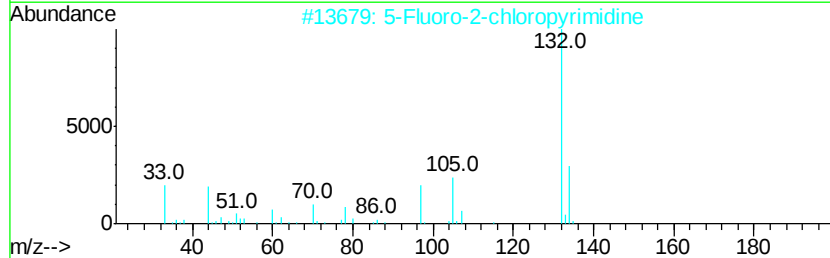
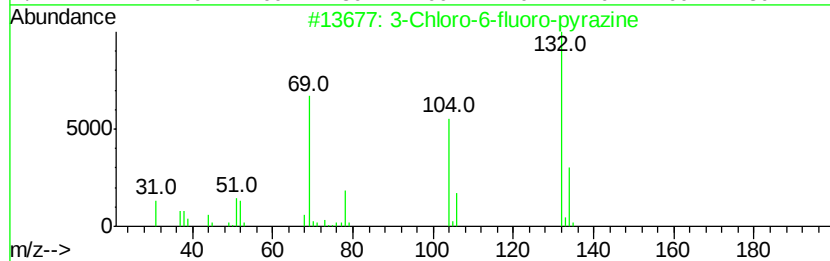
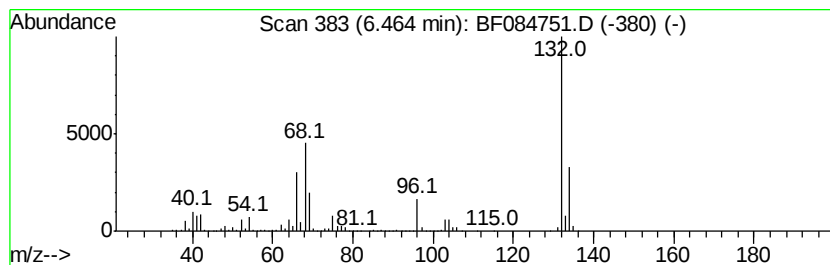
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Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	72.38 ng	3793190	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.16	8.9	ng	464623	1	6.69	1048190	20.0
2-Pentanone, 4-hy...	4.86	70.5	ng	3692870	1	6.69	1048190	20.0
2-Pentanone, 4-me...	5.70	4.5	ng	235813	1	6.69	1048190	20.0
unknown6.46	6.46	72.4	ng	3793190	1	6.69	1048190	20.0