

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020216\
 Data File : BF084754.D
 Acq On : 2 Feb 2016 19:08
 Operator : SJ/IZ
 Sample : PB88135BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88135BL

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	4.156	178	181	189	rVB	402363	513318	9.41%	1.158%
2	4.864	239	243	245	rBV	2421858	3603383	66.08%	8.127%
3	5.299	278	281	283	rBV	4165249	4081834	74.86%	9.206%
4	5.699	314	316	318	rBV	256374	219156	4.02%	0.494%
5	6.350	370	373	375	rBV	4082834	4445496	81.53%	10.026%
6	6.465	380	383	386	rBV	4158634	3854106	70.68%	8.692%
7	6.693	401	403	406	rVB	1192398	1052823	19.31%	2.374%
8	6.853	414	417	419	rBV	3778008	3310961	60.72%	7.467%
9	7.265	450	453	455	rBV	2615180	2552587	46.81%	5.757%
10	7.985	513	516	518	rBV	1548374	1484227	27.22%	3.347%
11	9.059	607	610	613	rBV	3402768	4752518	87.16%	10.719%
12	9.733	666	669	672	rBV	1695443	1596818	29.28%	3.601%
13	10.522	735	738	741	rBV	3119783	3076595	56.42%	6.939%
14	11.208	796	798	801	rBV	1214564	1616894	29.65%	3.647%
15	12.808	935	938	940	rBV	4426983	5452776	100.00%	12.298%
16	13.848	1026	1029	1031	rBV	1258156	1575332	28.89%	3.553%
17	15.220	1146	1149	1152	rBV	993847	1150461	21.10%	2.595%

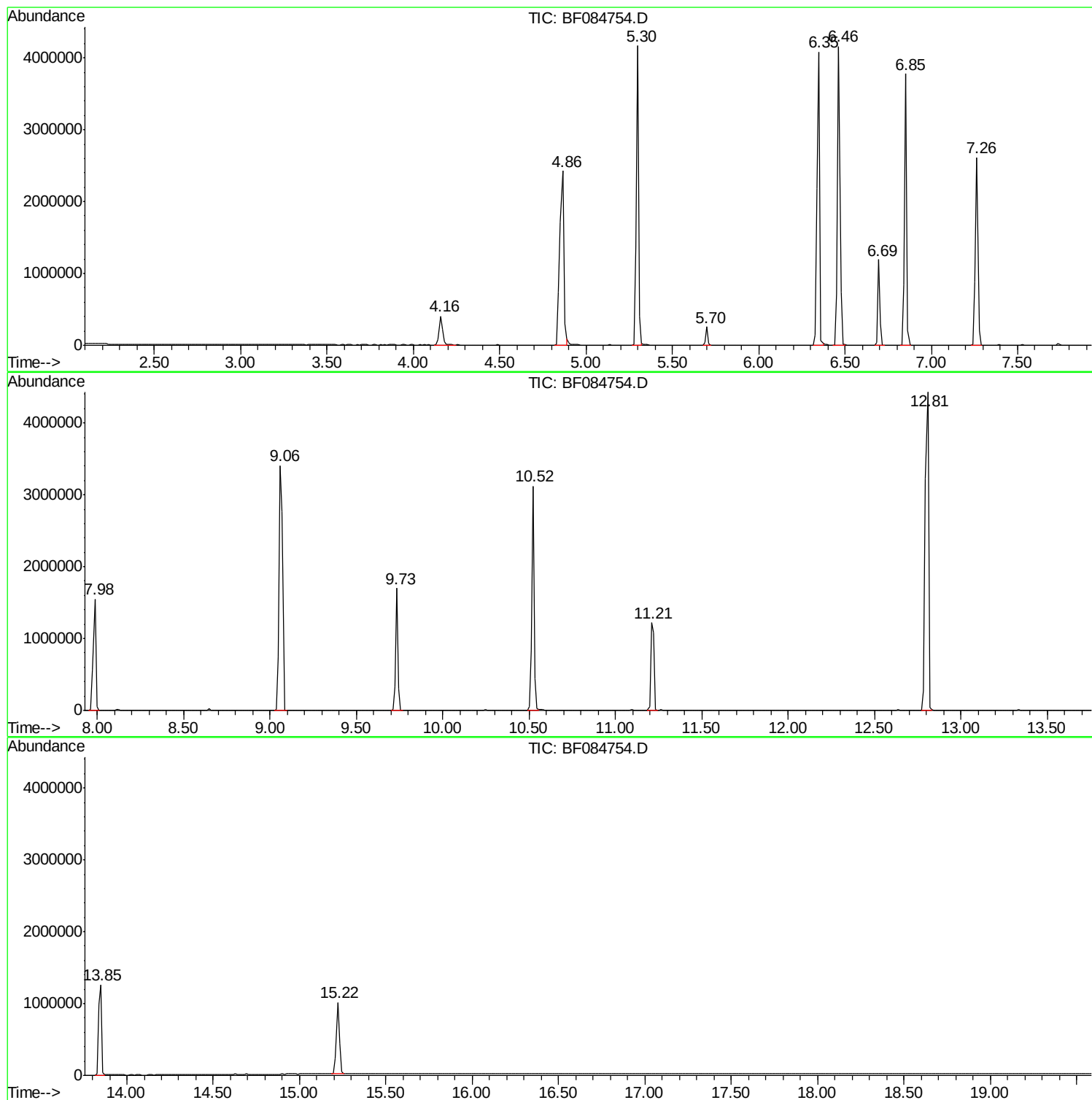
Sum of corrected areas: 44339285

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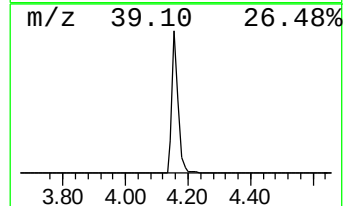
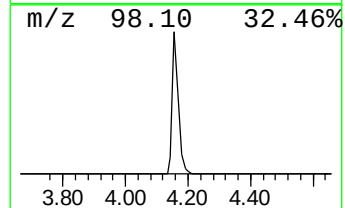
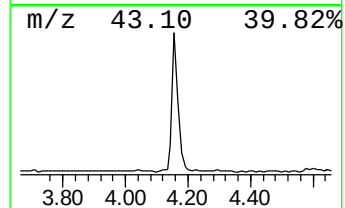
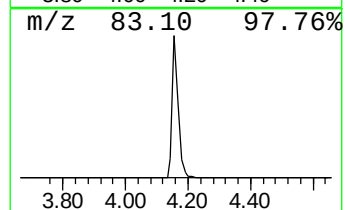
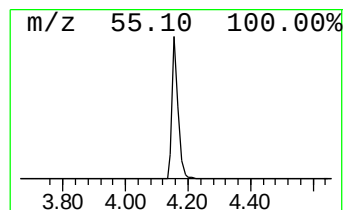
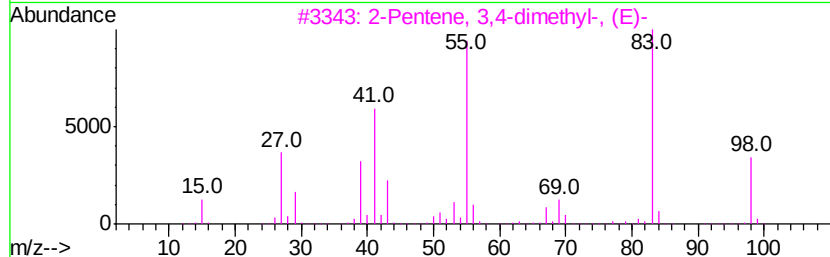
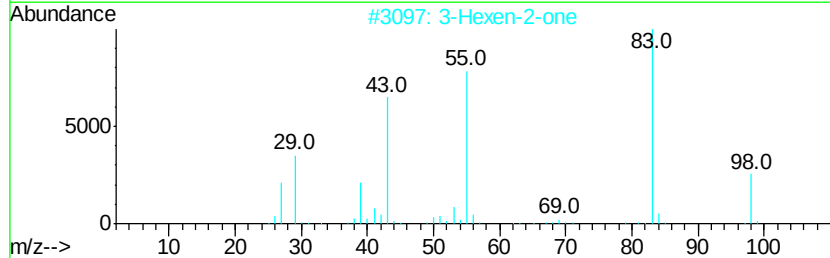
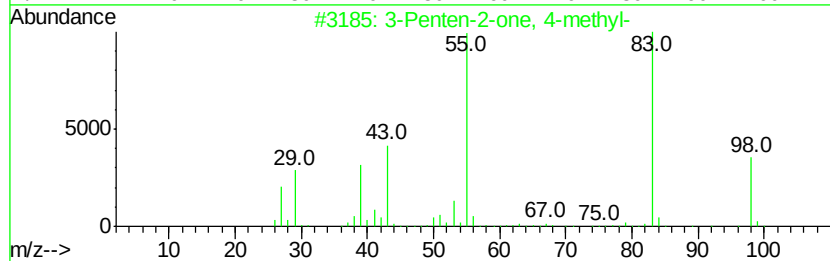
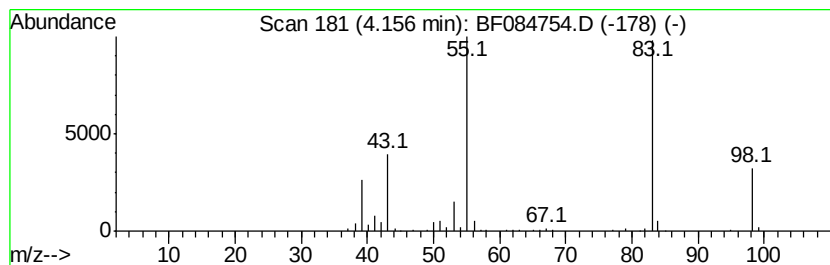
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	9.75 ng	513318	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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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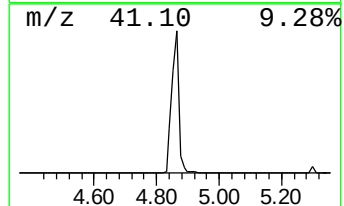
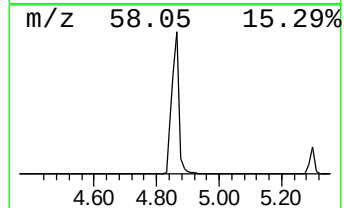
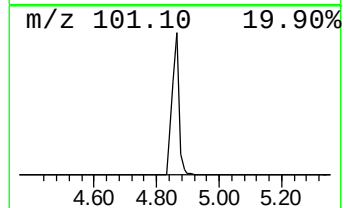
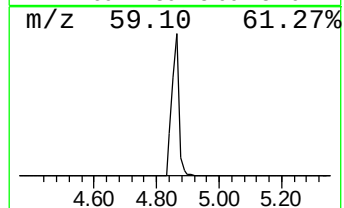
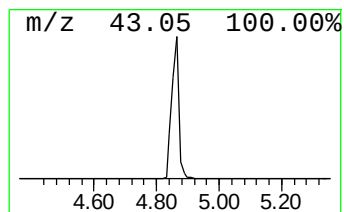
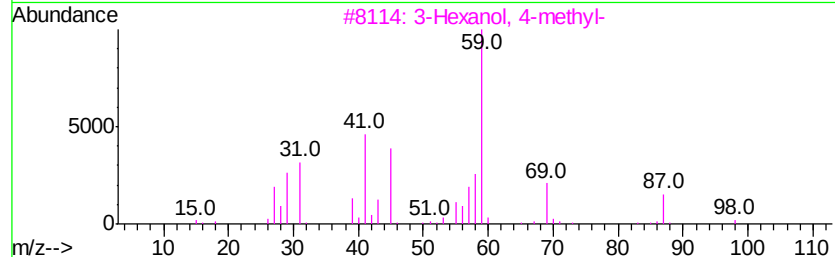
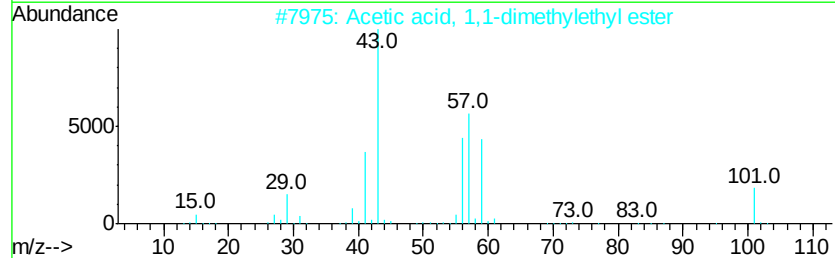
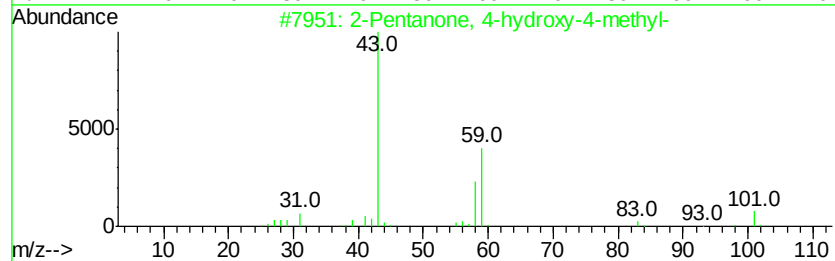
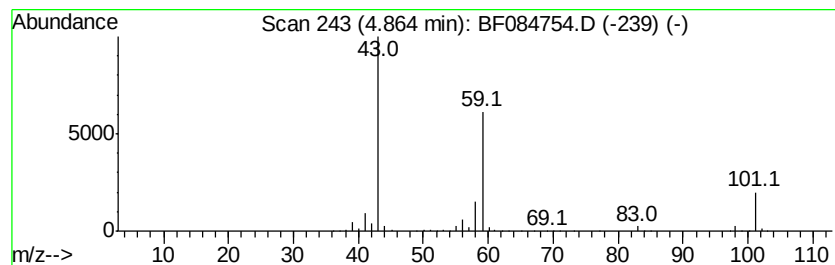
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	68.45 ng	3603380	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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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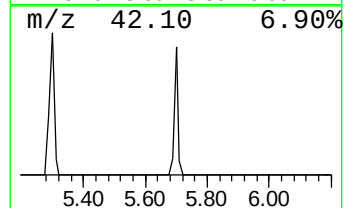
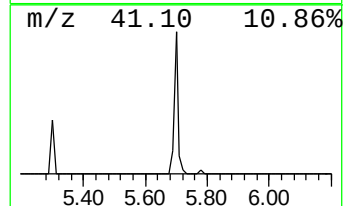
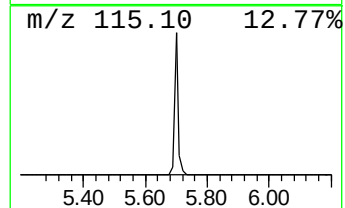
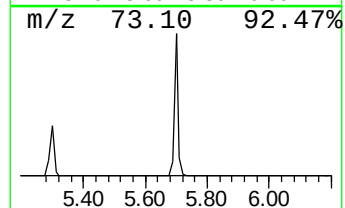
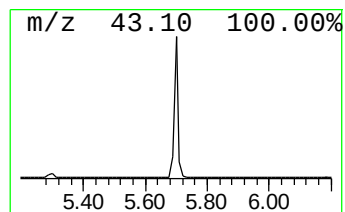
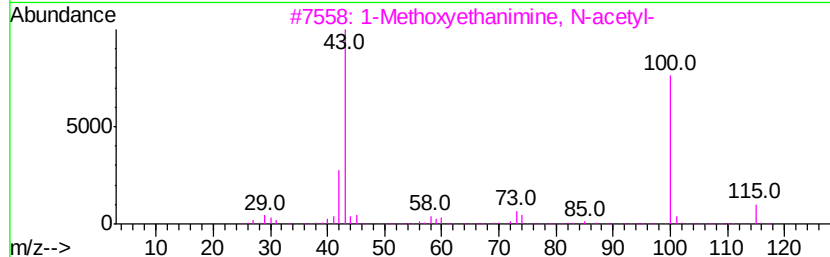
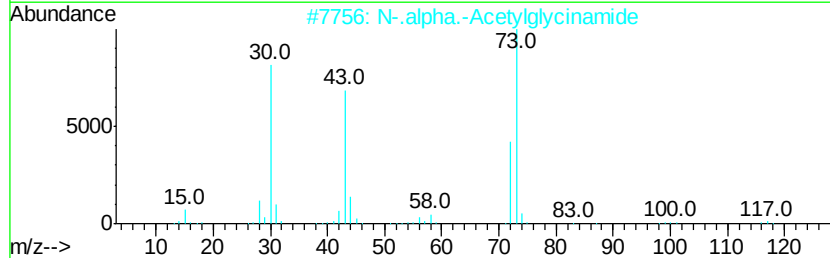
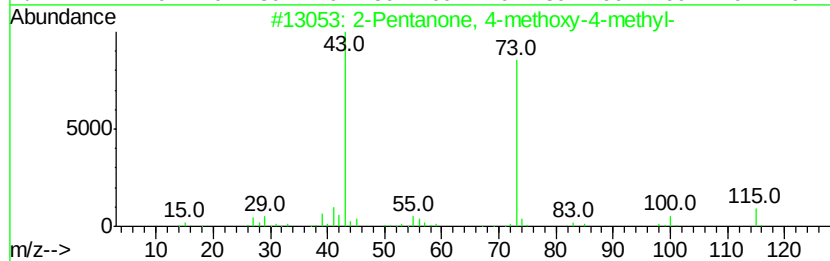
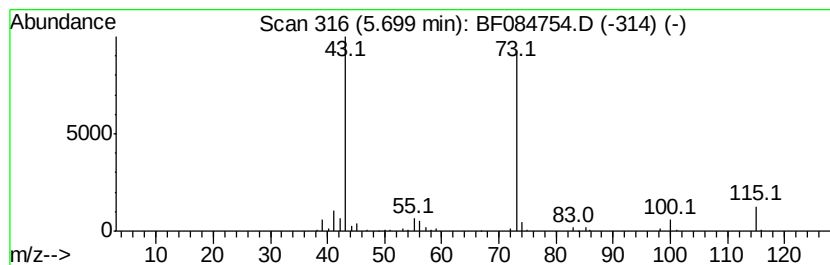
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	4.16 ng	219156	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	90
2		N-.alpha.-Acetylglucinamide	116	C4H8N2O2	002620-63-5	38
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	38
4		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	12
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12



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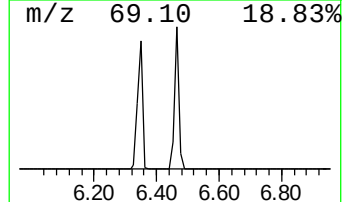
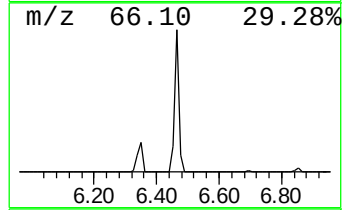
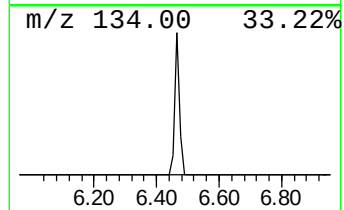
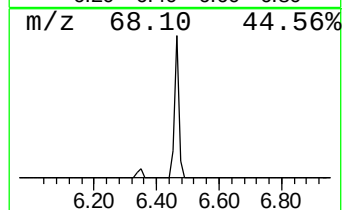
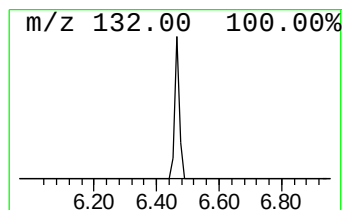
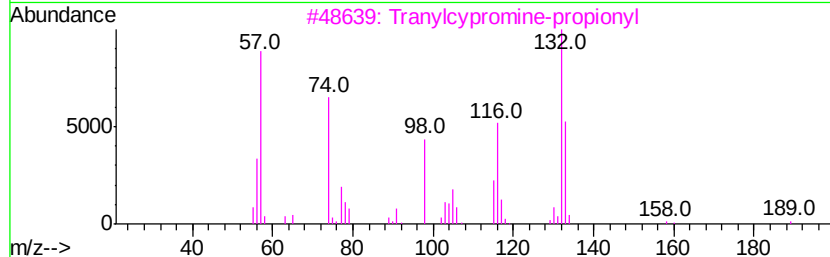
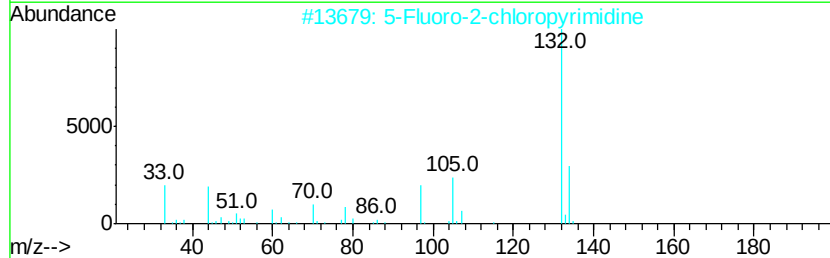
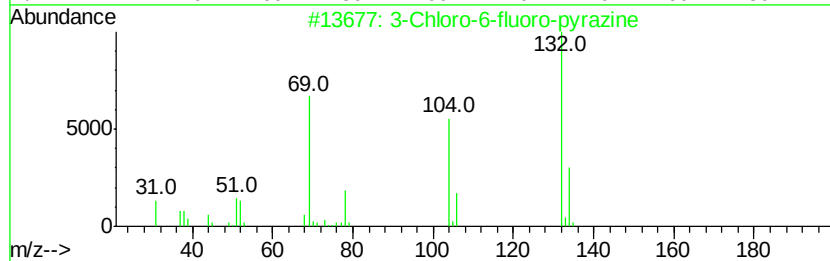
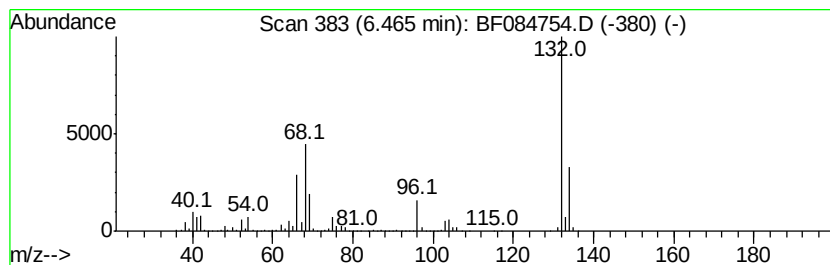
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Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	73.21 ng	3854110	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		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	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	9.8	ng	513318	1	6.69	1052820	20.0
2-Pentanone, 4-hy...	4.86	68.5	ng	3603380	1	6.69	1052820	20.0
2-Pentanone, 4-me...	5.70	4.2	ng	219156	1	6.69	1052820	20.0
unknown6.46	6.46	73.2	ng	3854110	1	6.69	1052820	20.0