

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020116\
 Data File : BF084711.D
 Acq On : 1 Feb 2016 16:06
 Operator : SJ/IZ
 Sample : PB88012BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88012BL

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	4.178	181	183	190	rVB	270466	348704	6.41%	0.788%
2	4.876	240	244	247	rBV	2077449	3142619	57.73%	7.104%
3	5.310	280	282	285	rBV	3684115	4024844	73.94%	9.098%
4	5.710	315	317	320	rBV	217188	192061	3.53%	0.434%
5	6.362	371	374	376	rBV	4245220	4419183	81.19%	9.989%
6	6.476	382	384	387	rBV	3685994	4042398	74.26%	9.138%
7	6.704	402	404	407	rBV	965684	1061662	19.50%	2.400%
8	6.864	416	418	421	rBV	3770564	3252245	59.75%	7.351%
9	7.276	451	454	457	rBV	2502084	2547838	46.81%	5.759%
10	7.996	514	517	519	rBV	1664544	1502007	27.59%	3.395%
11	9.082	608	612	614	rBV	3625756	5097095	93.64%	11.522%
12	9.745	667	670	673	rVB	1628036	1618556	29.74%	3.659%
13	10.533	736	739	742	rBV	2938537	3066827	56.34%	6.932%
14	11.231	797	800	802	rBV	1550747	1687972	31.01%	3.816%
15	12.819	936	939	941	rBV	5096456	5443234	100.00%	12.304%
16	13.859	1027	1030	1032	rBV	1664792	1602218	29.44%	3.622%
17	15.242	1148	1151	1153	rBV	918762	1189962	21.86%	2.690%

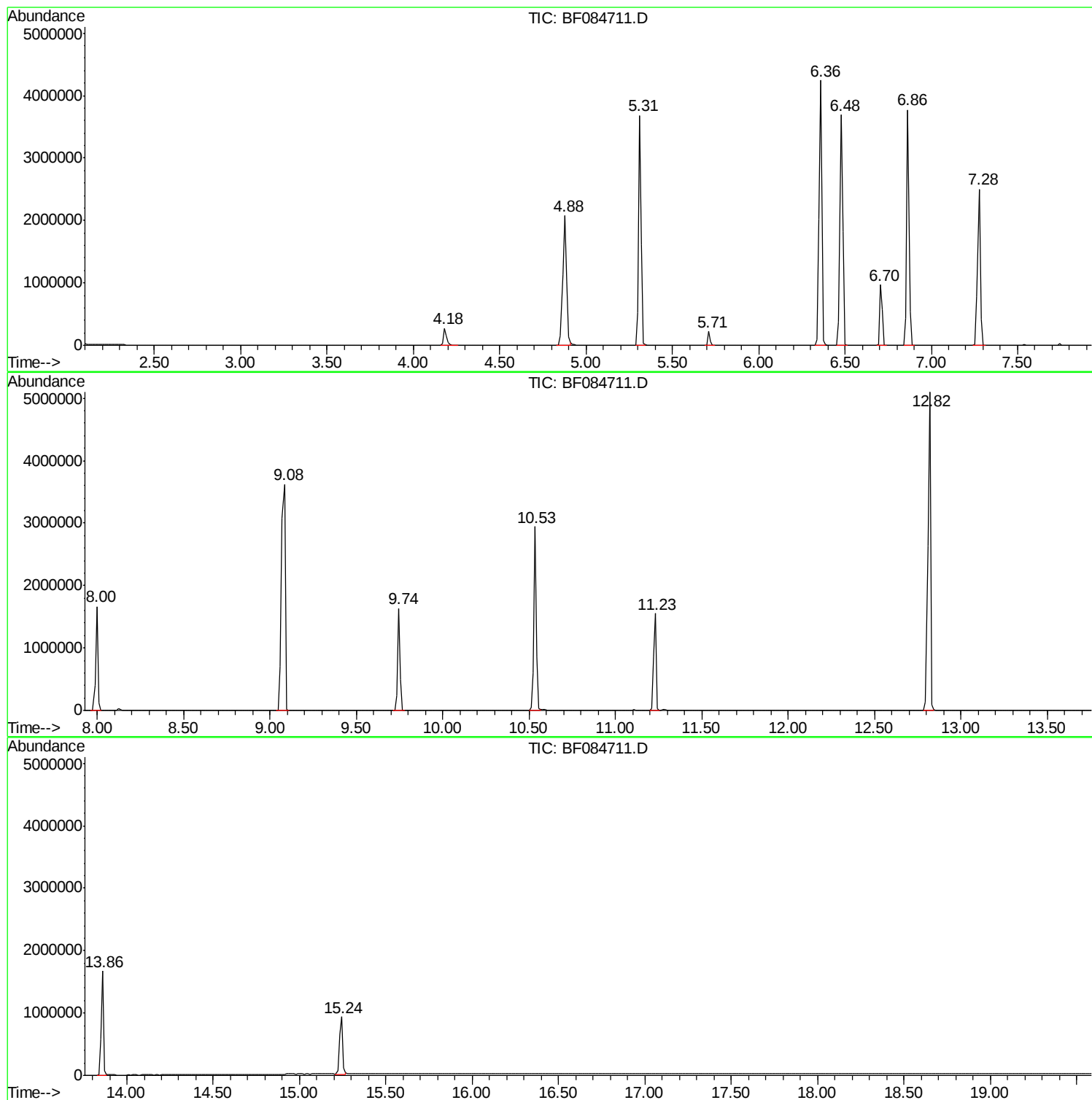
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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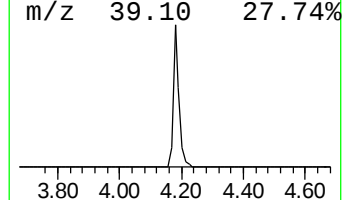
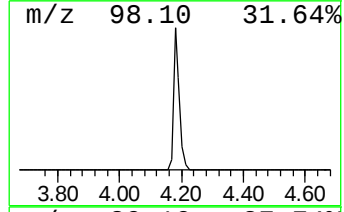
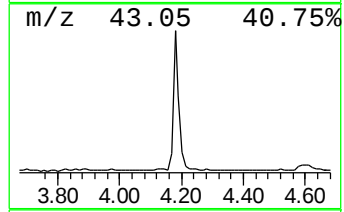
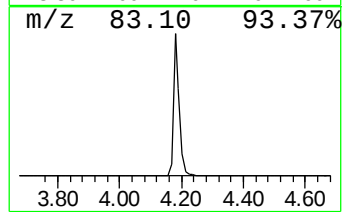
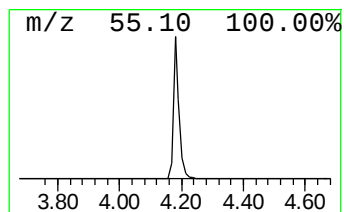
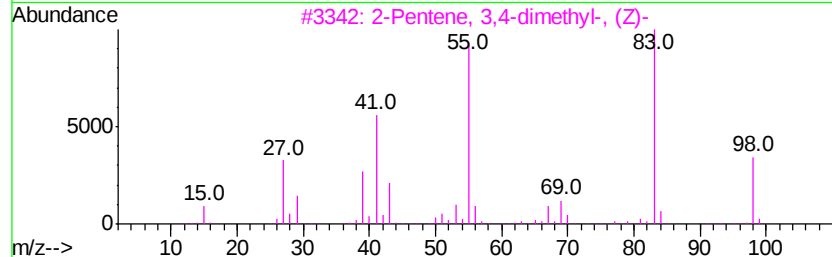
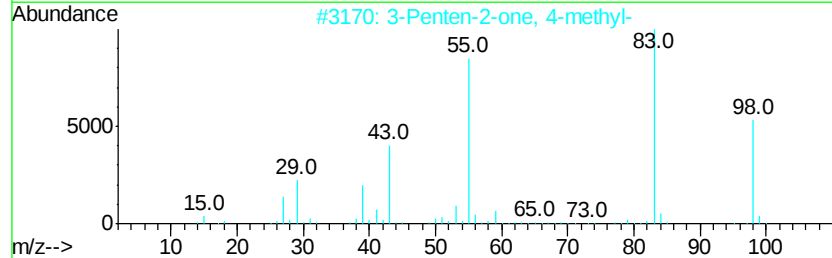
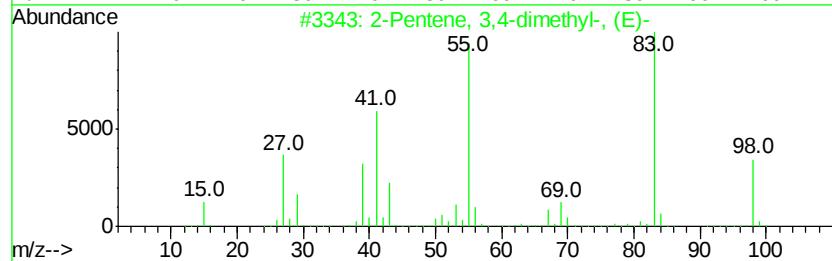
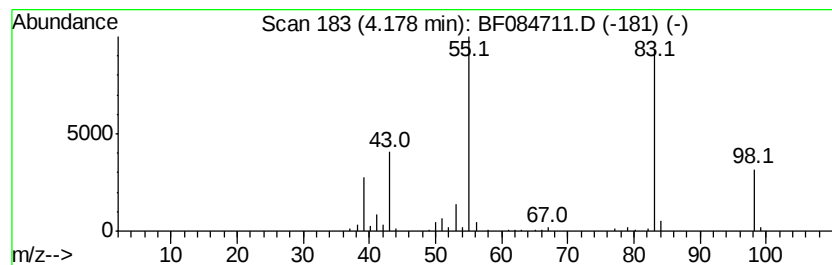
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentene, 3,4-dimethyl-, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	6.57 ng	348704	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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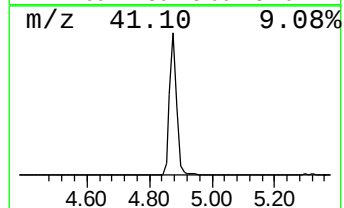
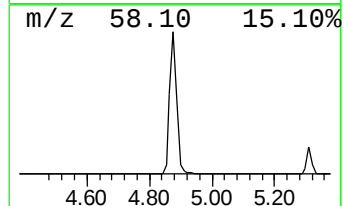
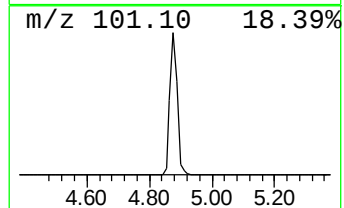
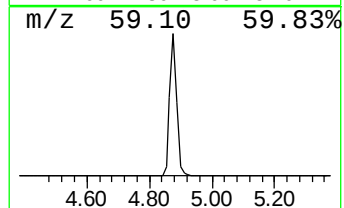
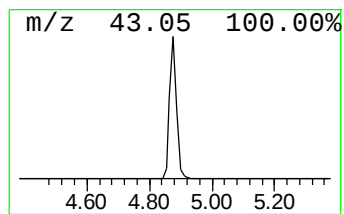
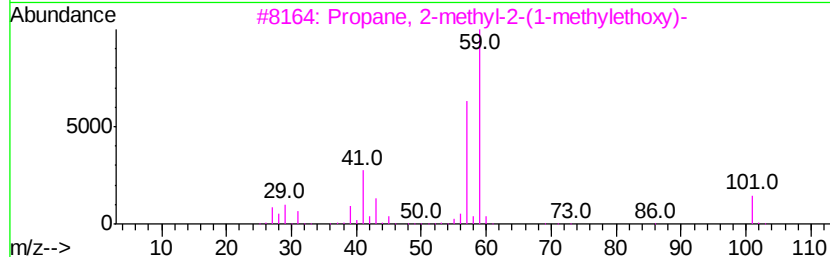
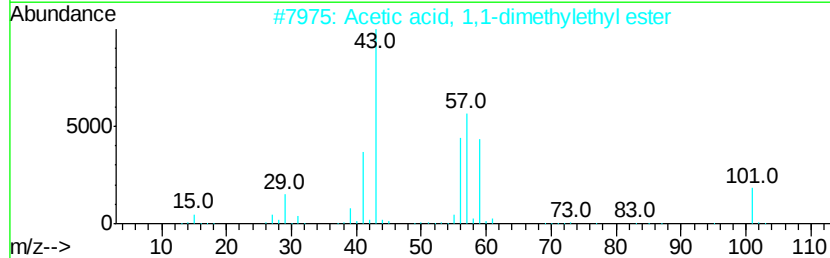
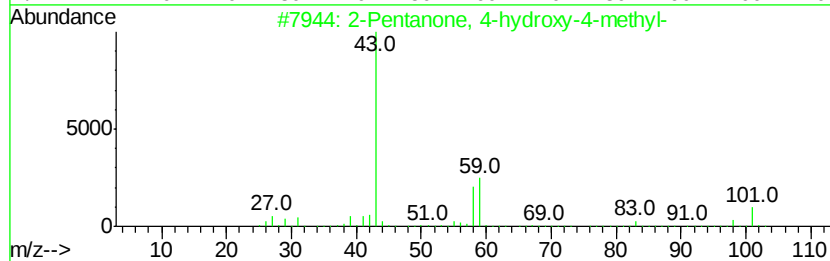
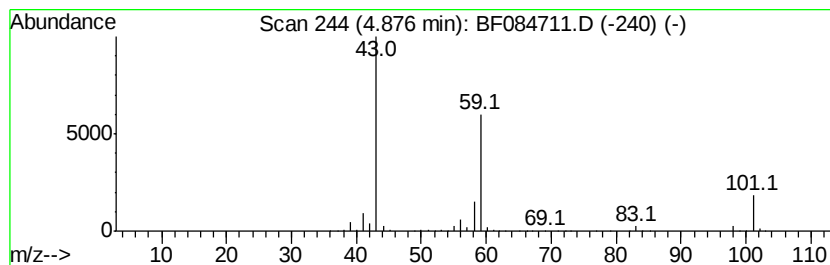
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	59.20 ng	3142620	1,4-Dichlorobenzene-d4	6.70

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	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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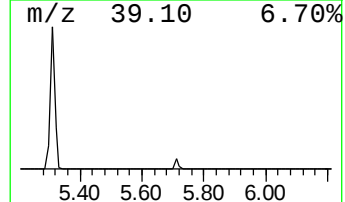
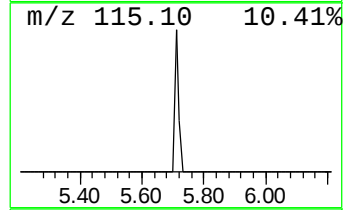
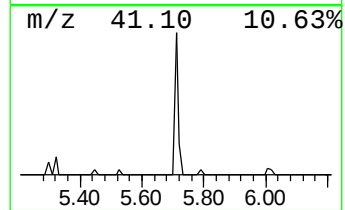
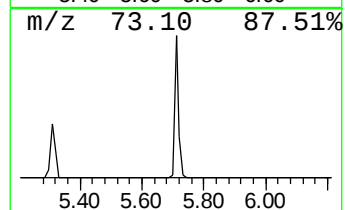
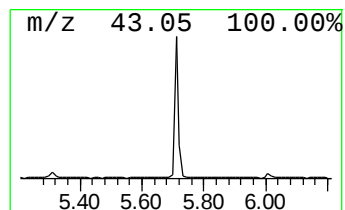
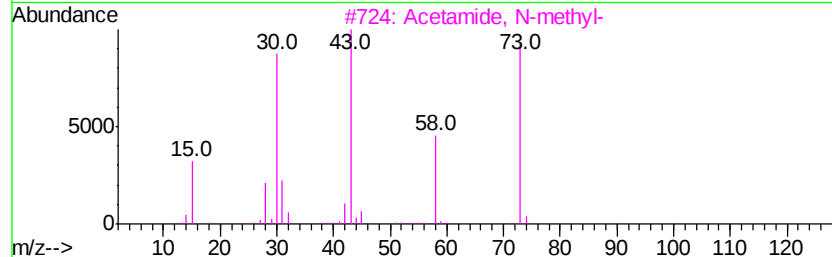
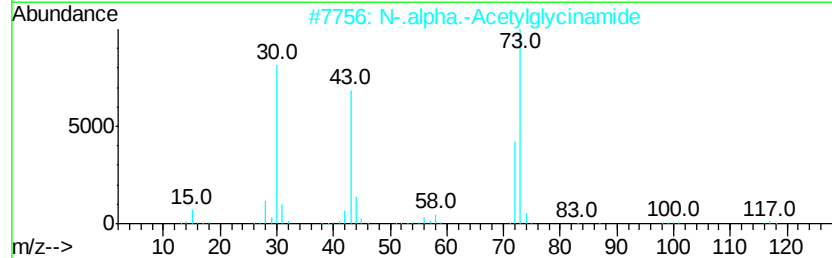
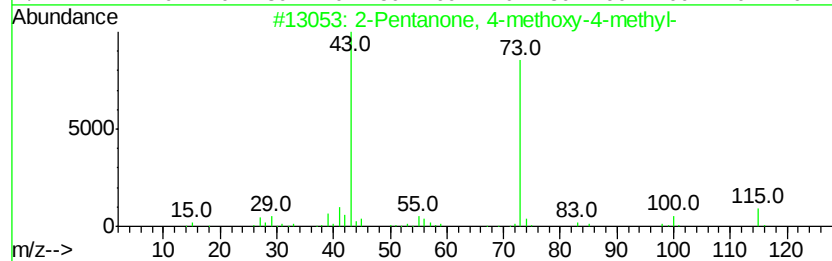
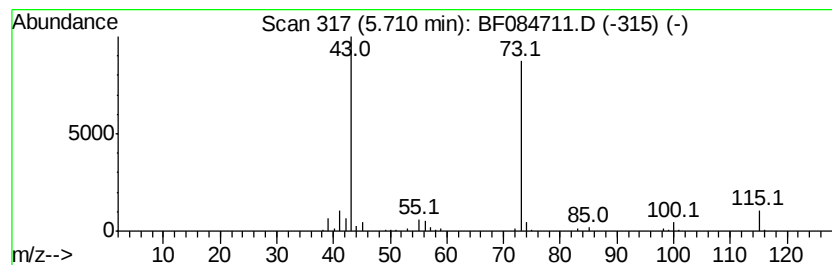
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	3.62 ng	192061	1,4-Dichlorobenzene-d4	6.70

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.-Acetylglucynamide	116	C4H8N2O2	002620-63-5	38
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12



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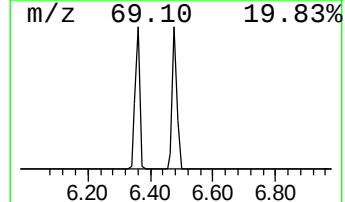
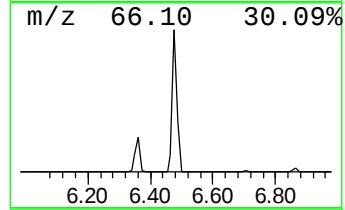
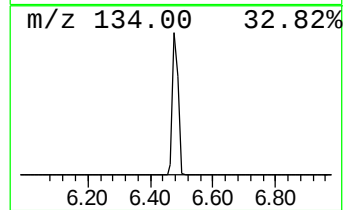
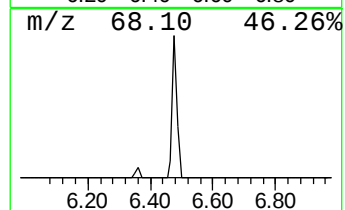
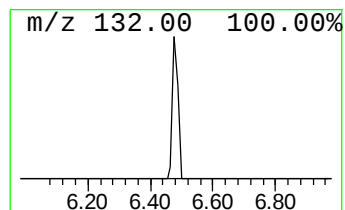
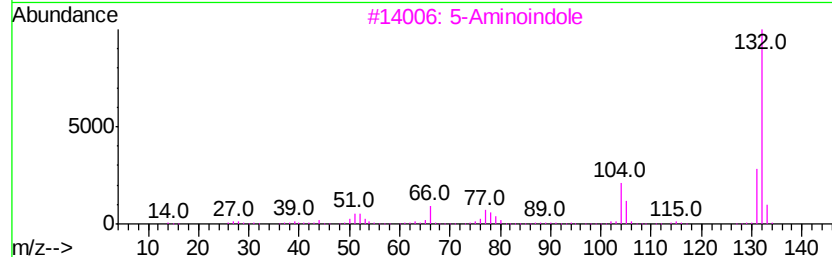
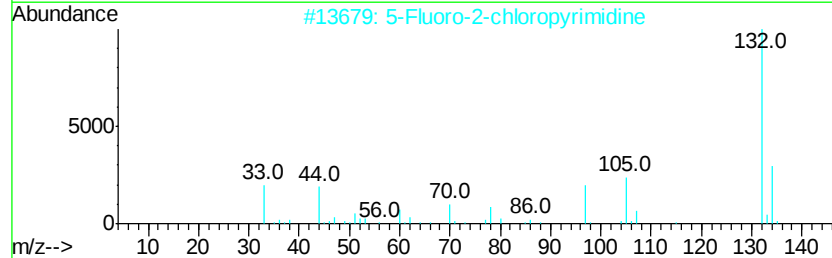
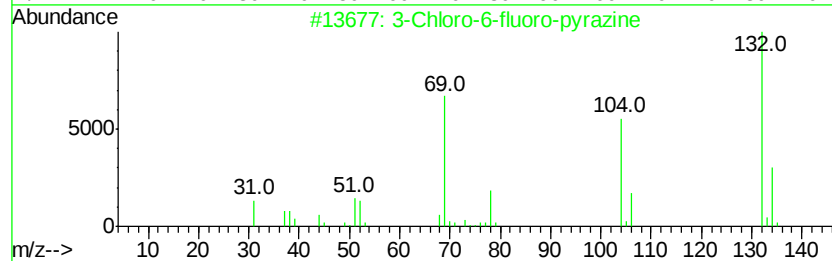
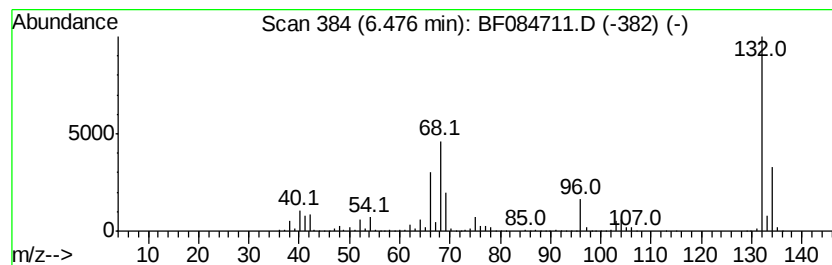
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	76.15 ng	4042400	1,4-Dichlorobenzene-d4	6.70

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentene, 3,4-di...	4.18	6.6	ng	348704	1	6.70	1061660	20.0
2-Pentanone, 4-hy...	4.88	59.2	ng	3142620	1	6.70	1061660	20.0
2-Pentanone, 4-me...	5.71	3.6	ng	192061	1	6.70	1061660	20.0
unknown6.48	6.48	76.2	ng	4042400	1	6.70	1061660	20.0