

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
 Data File : BF084632.D
 Acq On : 29 Jan 2016 13:26
 Operator : SJ/IZ
 Sample : PB88038BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88038BL

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-BF012916.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	4.201	182	185	193	rVB	681626	974050	16.99%	1.920%
2	4.899	242	246	249	rBV	2968162	5608522	97.83%	11.057%
3	5.333	281	284	286	rBV	3958895	4893182	85.35%	9.647%
4	5.733	316	319	321	rBV	272999	363228	6.34%	0.716%
5	6.373	372	375	377	rBV	4573273	4556266	79.48%	8.983%
6	6.499	383	386	388	rBV	3843849	4804252	83.80%	9.472%
7	6.727	403	406	408	rBV	877498	1034151	18.04%	2.039%
8	6.876	417	419	422	rBV	3379675	3446821	60.12%	6.796%
9	7.287	452	455	458	rBV	2601772	2729026	47.60%	5.380%
10	8.007	516	518	521	rBV	1594173	1391324	24.27%	2.743%
11	9.093	610	613	615	rBV	5056105	5676358	99.01%	11.191%
12	9.756	669	671	674	rBV	1386213	1488371	25.96%	2.934%
13	10.545	737	740	743	rBV	3146717	3468444	60.50%	6.838%
14	11.242	798	801	803	rBV	1721300	1606873	28.03%	3.168%
15	12.831	937	940	942	rBV	5922704	5732929	100.00%	11.303%
16	13.871	1029	1031	1033	rBV	1807280	1615429	28.18%	3.185%
17	15.254	1149	1152	1155	rBV	1155725	1332599	23.24%	2.627%

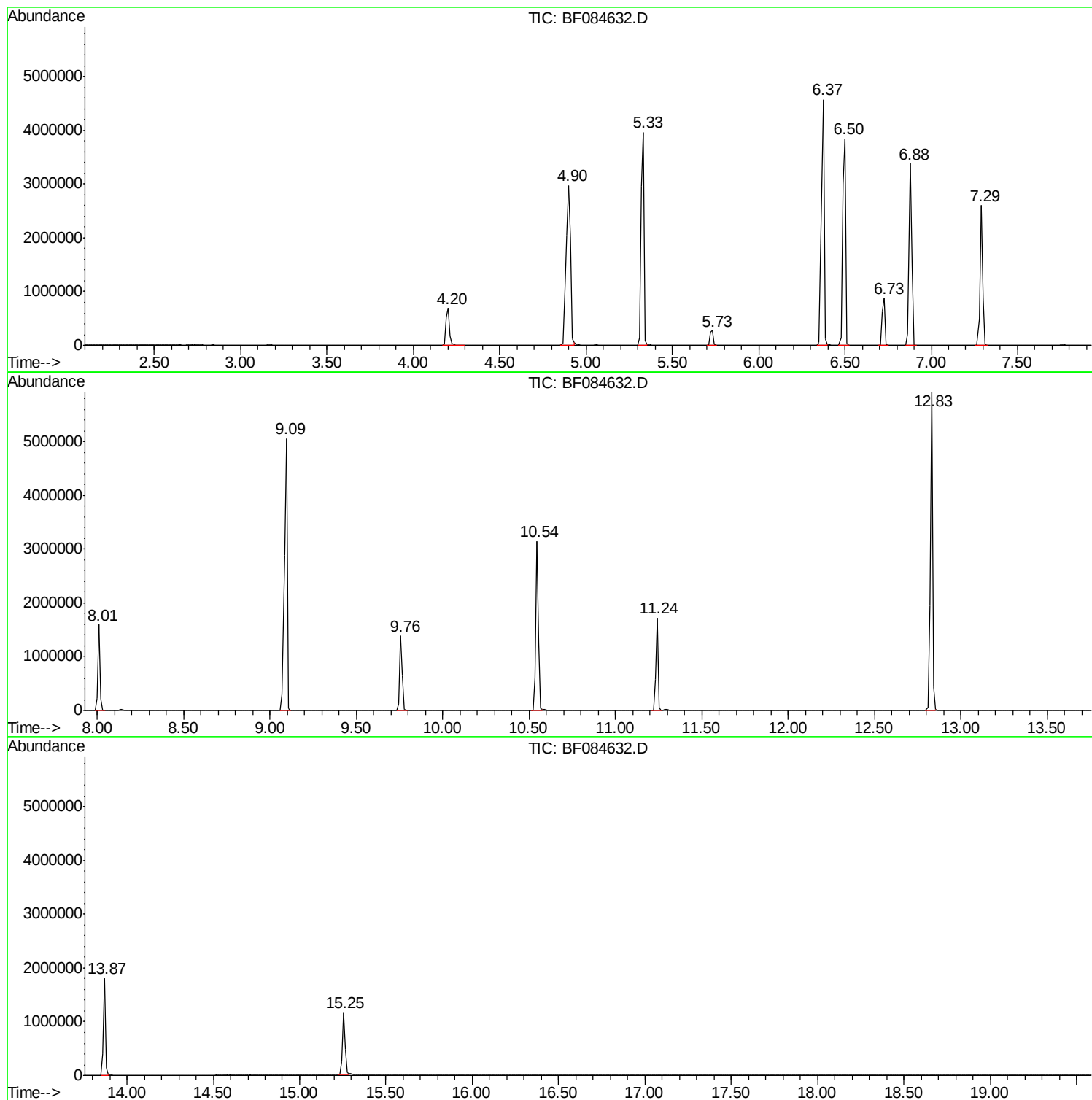
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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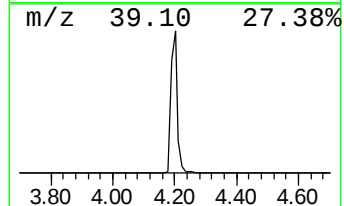
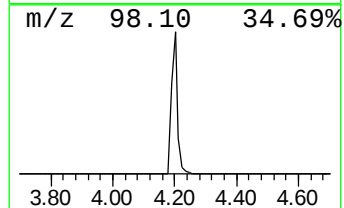
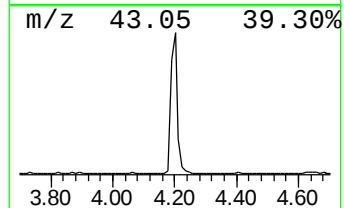
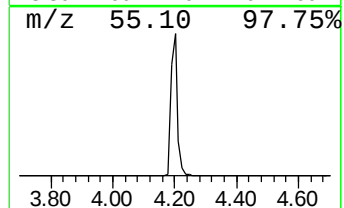
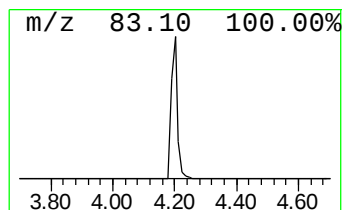
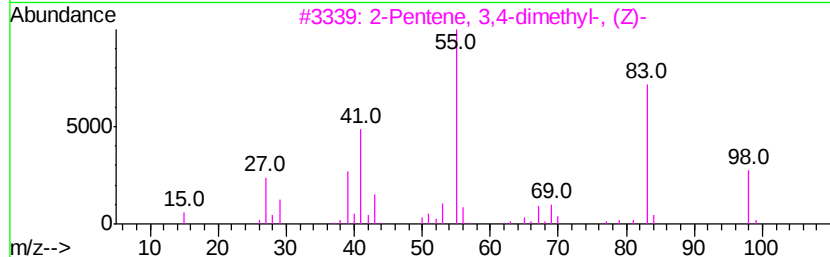
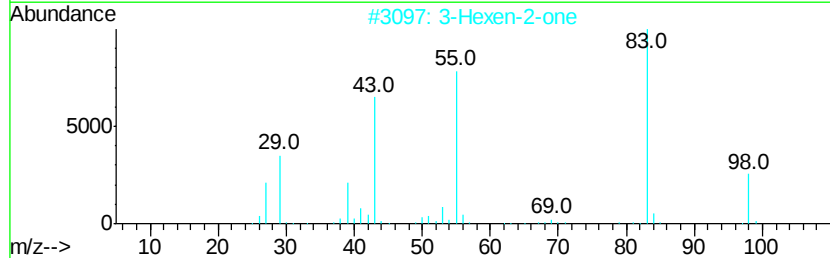
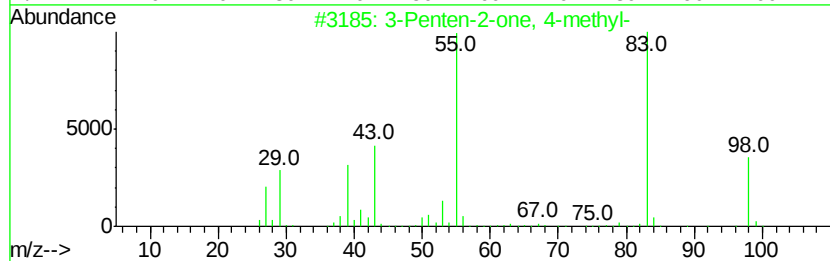
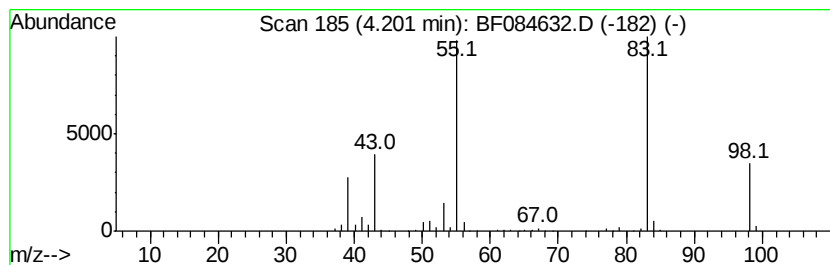
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	18.84 ng	974050	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
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, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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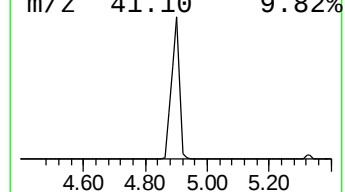
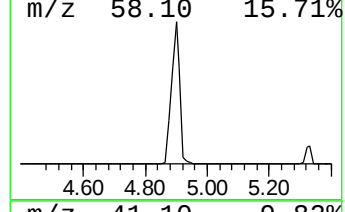
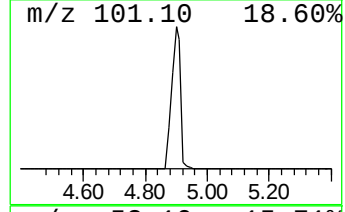
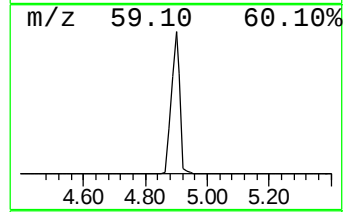
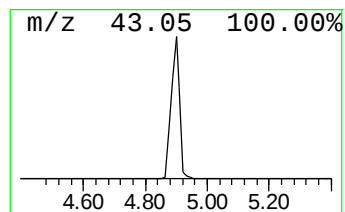
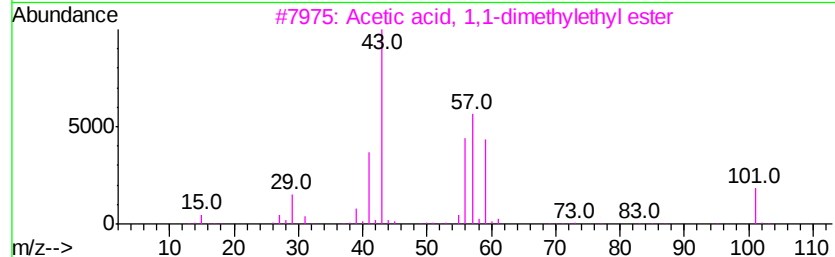
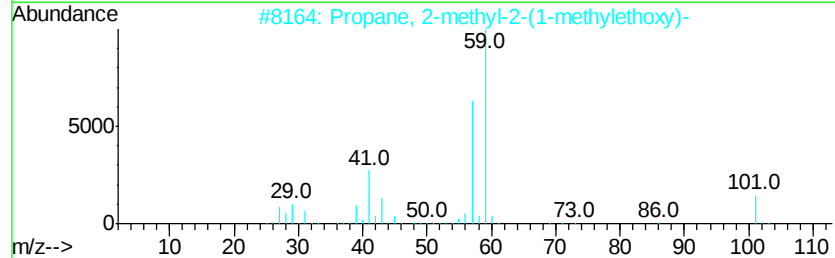
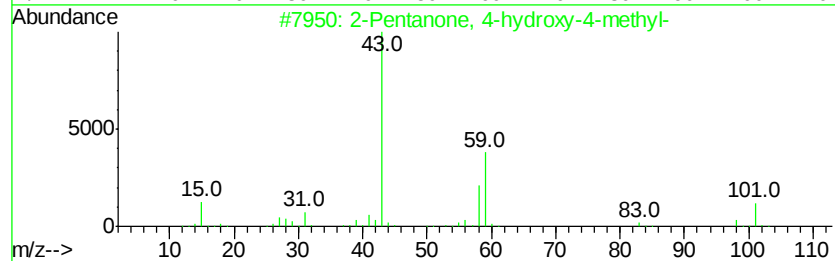
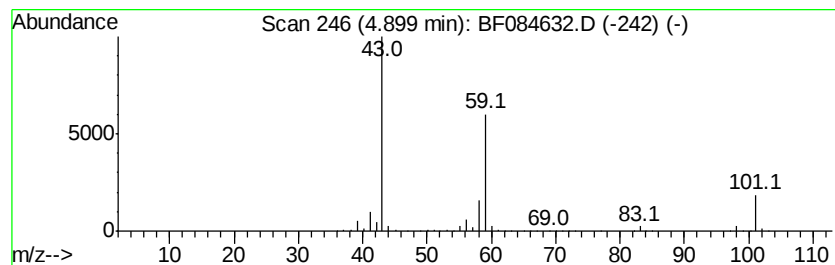
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	108.47 ng	5608520	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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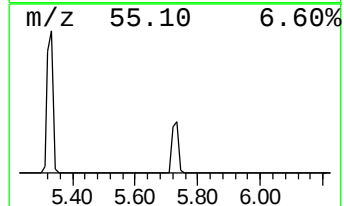
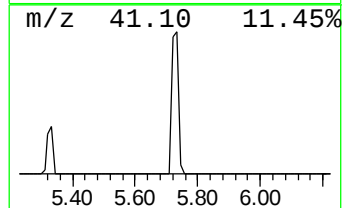
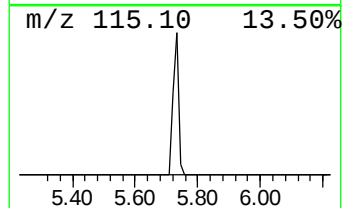
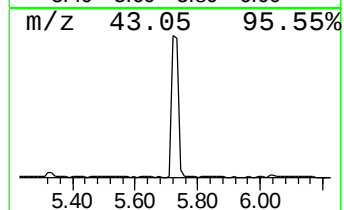
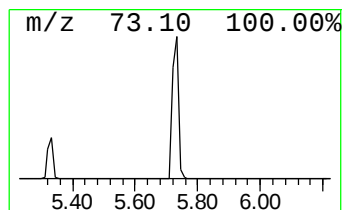
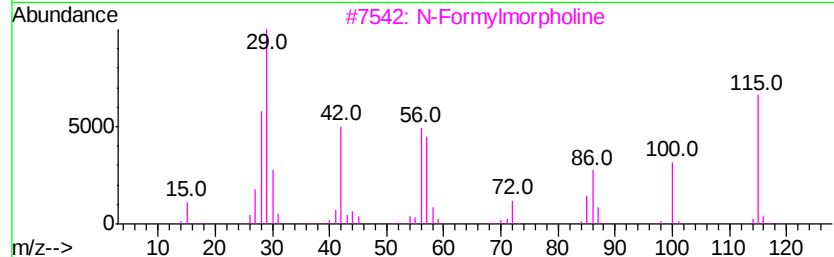
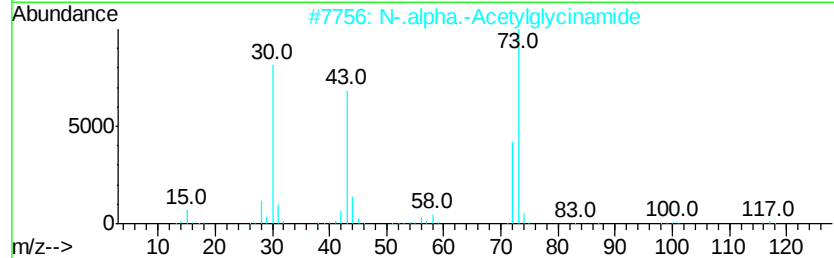
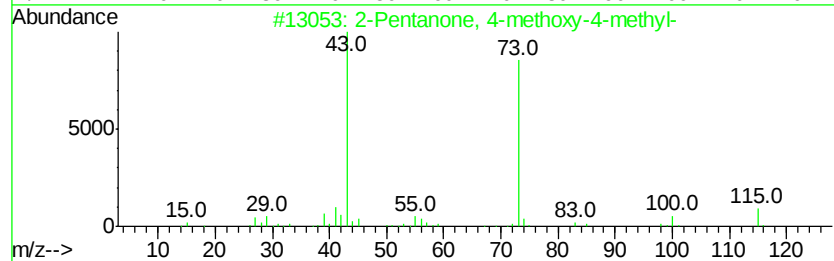
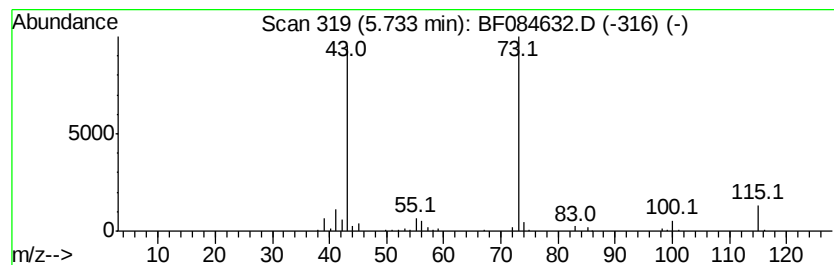
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	7.02 ng	363228	1,4-Dichlorobenzene-d4	6.73

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		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



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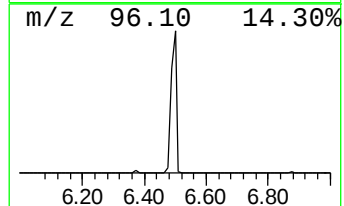
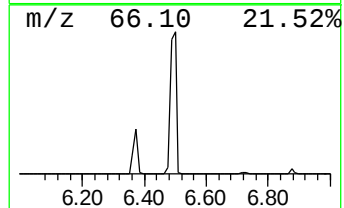
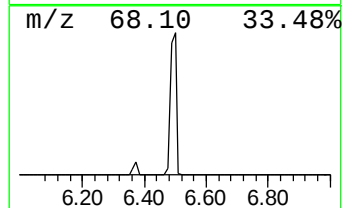
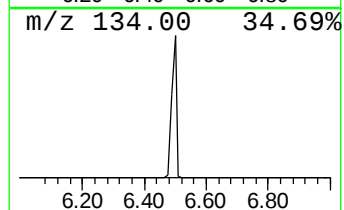
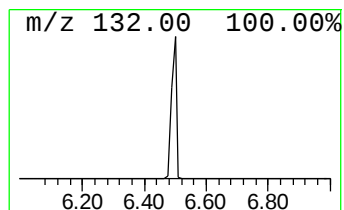
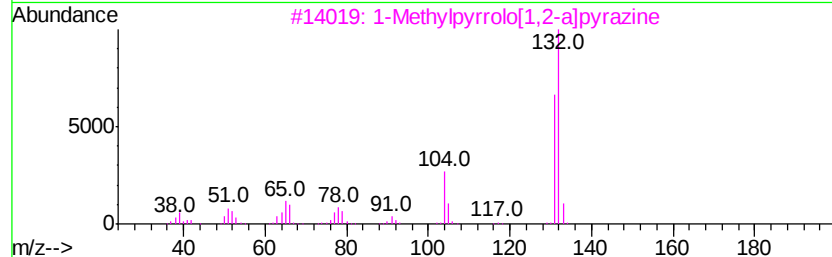
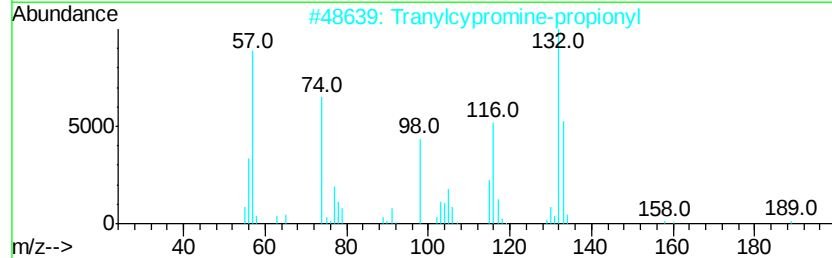
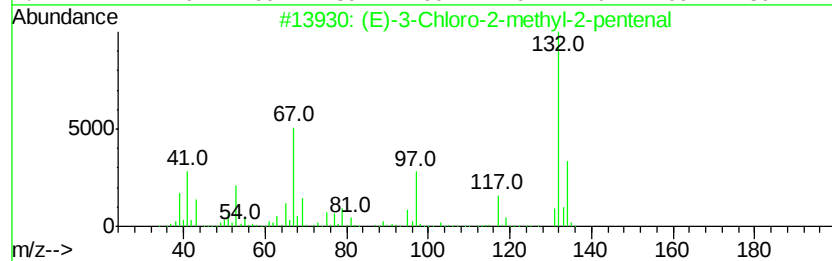
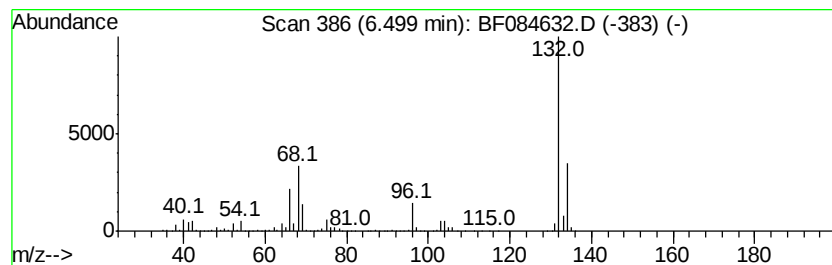
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Peak Number 4 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	92.91 ng	4804250	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.20	18.8	ng	974050	1	6.73	1034150	20.0
2-Pentanone, 4-hy...	4.90	108.5	ng	5608520	1	6.73	1034150	20.0
2-Pentanone, 4-me...	5.73	7.0	ng	363228	1	6.73	1034150	20.0
unknown6.50	6.50	92.9	ng	4804250	1	6.73	1034150	20.0