

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050316\
 Data File : BF086662.D
 Acq On : 4 May 2016 00:54
 Operator : UM/SJ
 Sample : H2716-14
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26WARD-4-CS-3(16-23FTBGS)

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-BF042716.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	2.487	33	35	41	rVB	88219	131430	1.50%	0.311%
2	3.218	96	99	108	rBV	167499	320148	3.65%	0.758%
3	4.270	186	191	193	rBV	4734379	8780798	100.00%	20.789%
4	4.921	246	248	257	rBV	428576	628131	7.15%	1.487%
5	5.356	283	286	288	rBV	2709443	3684400	41.96%	8.723%
6	6.396	374	377	379	rBV	3335566	3686141	41.98%	8.727%
7	6.521	385	388	390	rBV	4008184	3925038	44.70%	9.293%
8	6.750	406	408	415	rBV	1240962	1206849	13.74%	2.857%
9	6.910	419	422	424	rBV	3021533	3036679	34.58%	7.190%
10	7.322	455	458	460	rBV	2241130	2550830	29.05%	6.039%
11	8.042	518	521	523	rBV	1133254	1463973	16.67%	3.466%
12	9.116	612	615	617	rBV	4361445	3843037	43.77%	9.099%
13	9.790	671	674	676	rBV	1450864	1347944	15.35%	3.191%
14	10.579	740	743	745	rBV	1483159	1945987	22.16%	4.607%
15	11.265	801	803	806	rBV	968575	1010006	11.50%	2.391%
16	12.854	939	942	954	rBV	3196503	3075932	35.03%	7.282%
17	13.894	1031	1033	1042	rBV	787623	939148	10.70%	2.223%
18	15.288	1152	1155	1158	rBV	522303	660933	7.53%	1.565%

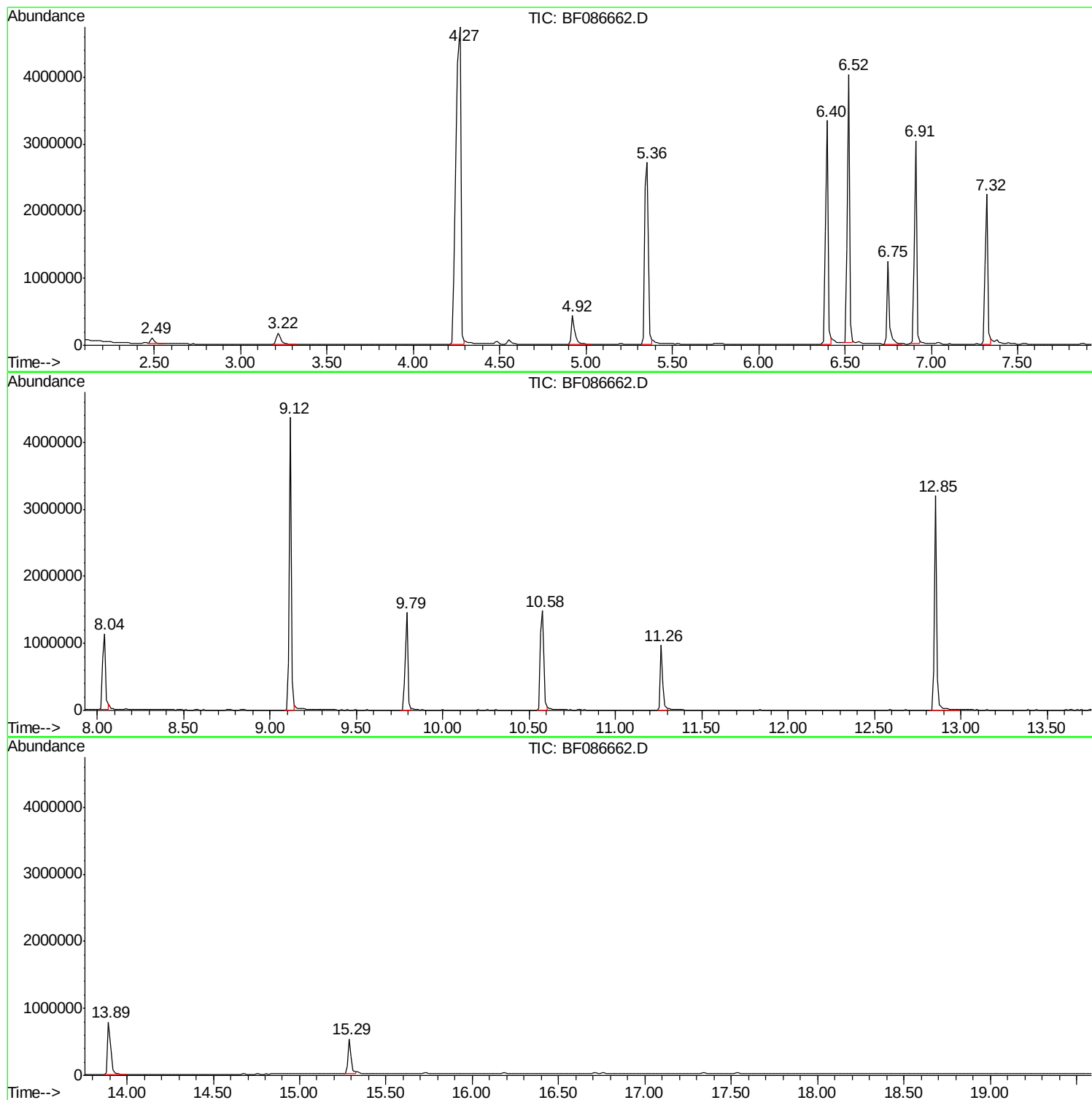
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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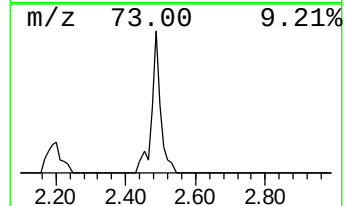
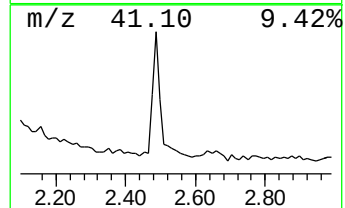
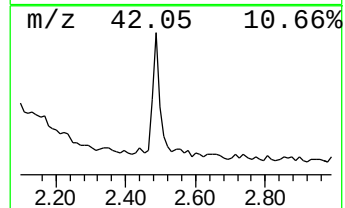
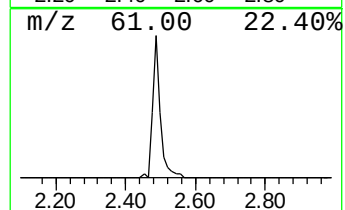
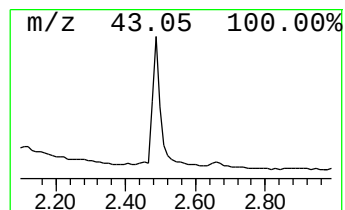
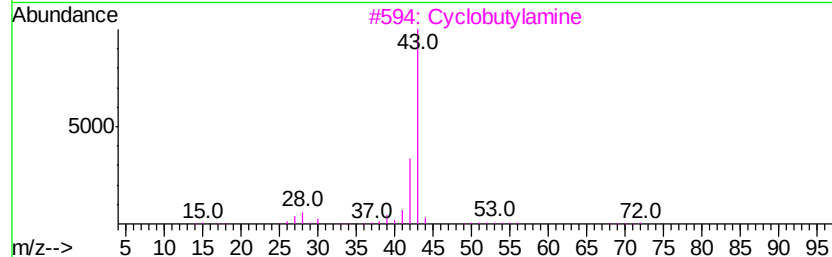
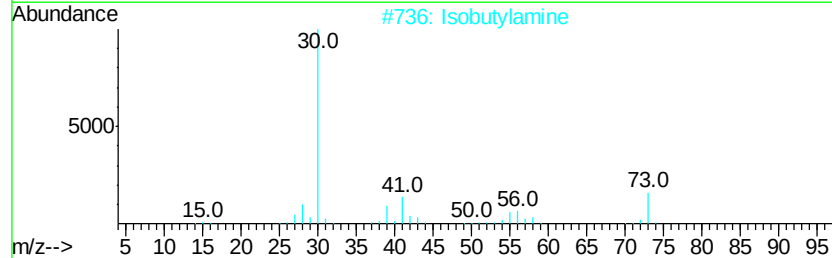
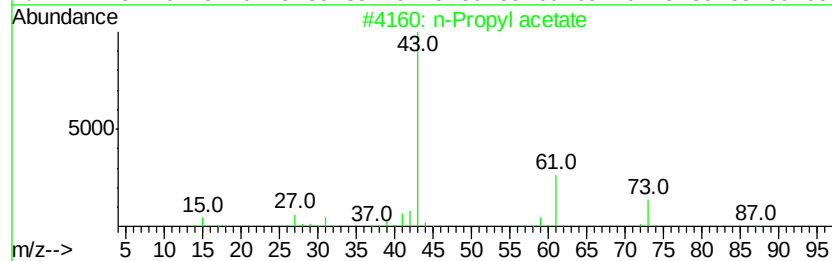
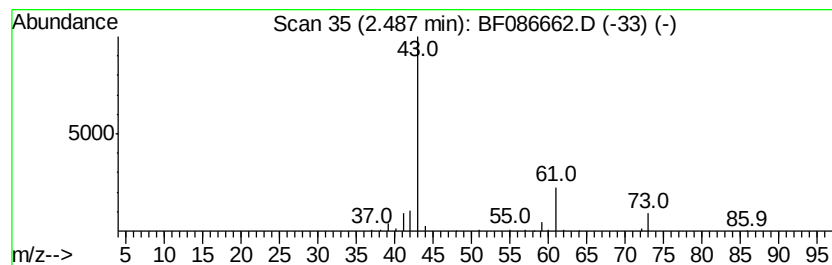
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF042716.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.49	2.18 ng	131430	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isobutylamine	73	C4H11N	000078-81-9	9
3		Cyclobutylamine	71	C4H9N	002516-34-9	9
4		1-Butanamine	73	C4H11N	000109-73-9	5
5		Pentane	72	C5H12	000109-66-0	4



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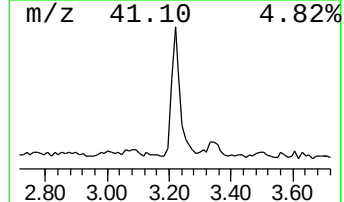
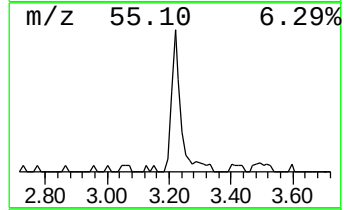
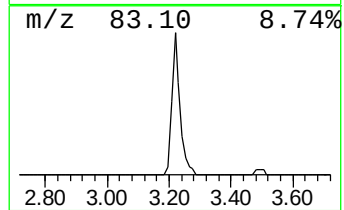
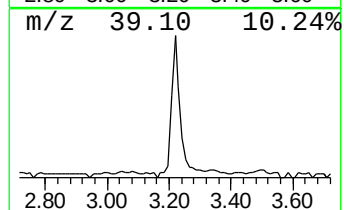
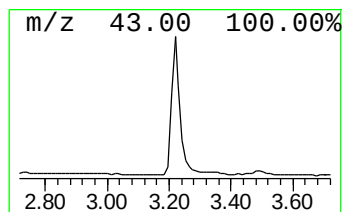
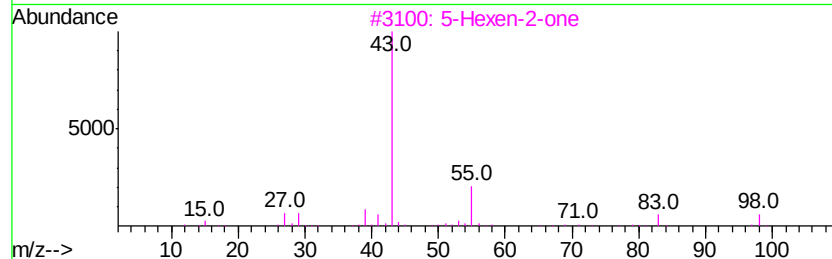
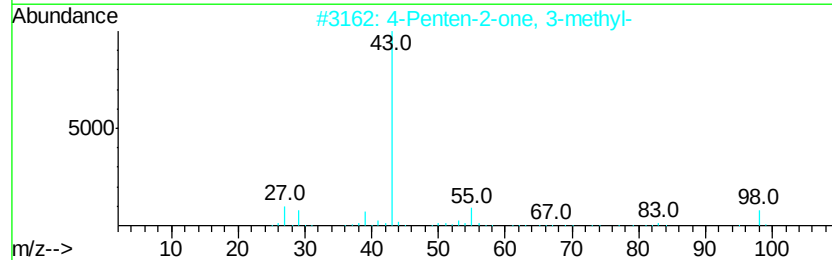
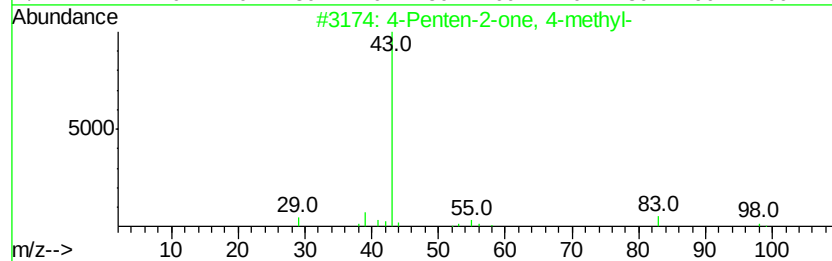
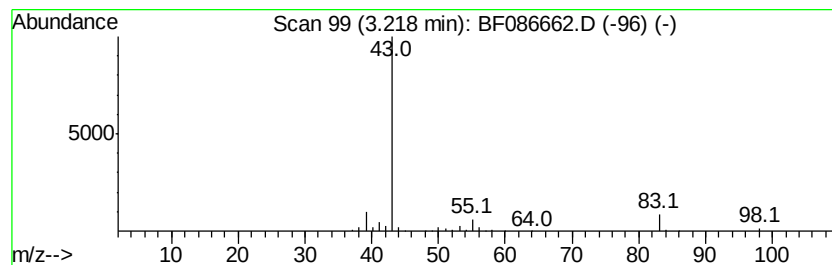
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Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	5.31 ng	320148	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	59
3		5-Hexen-2-one	98	C6H10O	000109-49-9	42
4		4-Hexen-2-one	98	C6H10O	025659-22-7	9
5		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9



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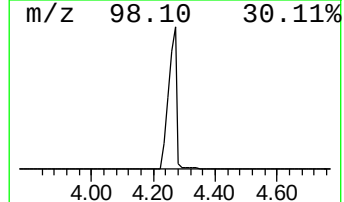
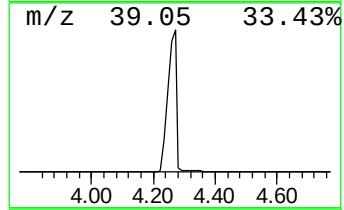
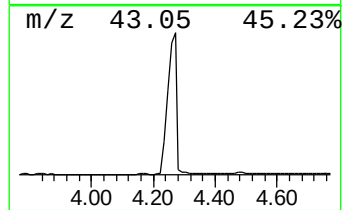
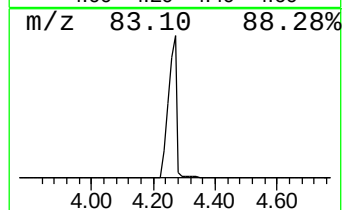
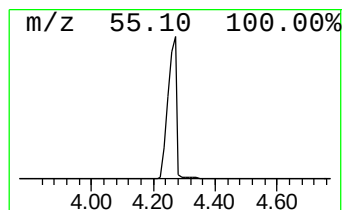
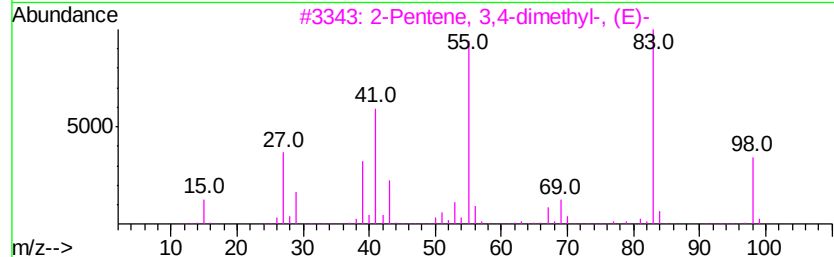
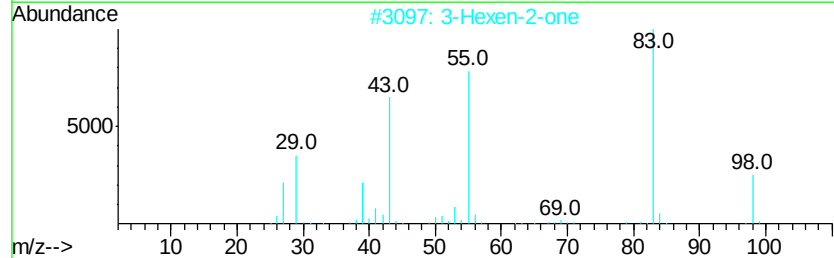
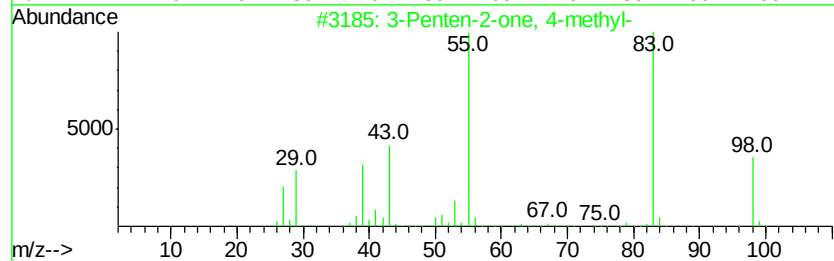
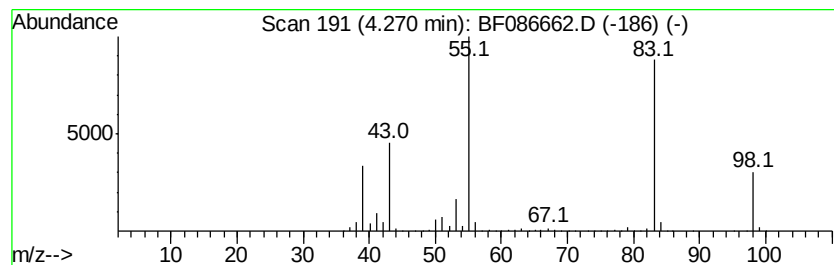
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	145.52 ng	8780800	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	86
4		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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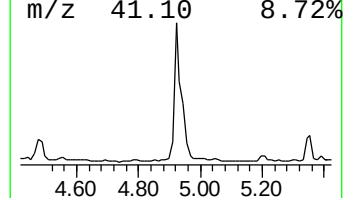
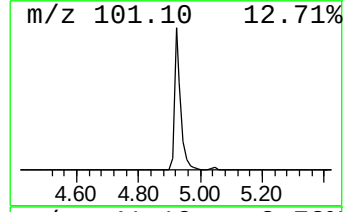
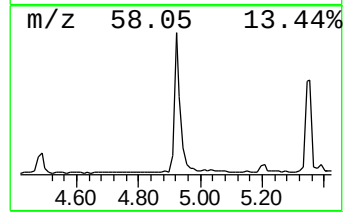
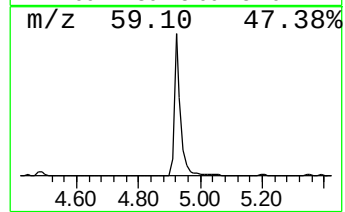
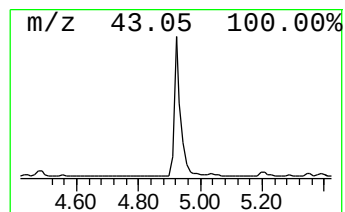
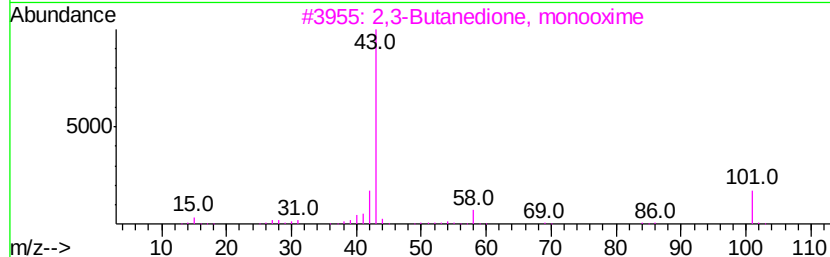
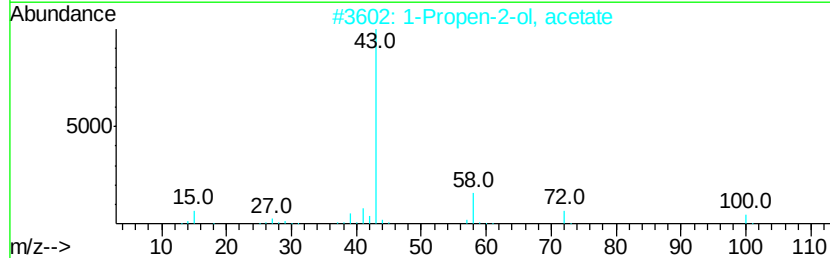
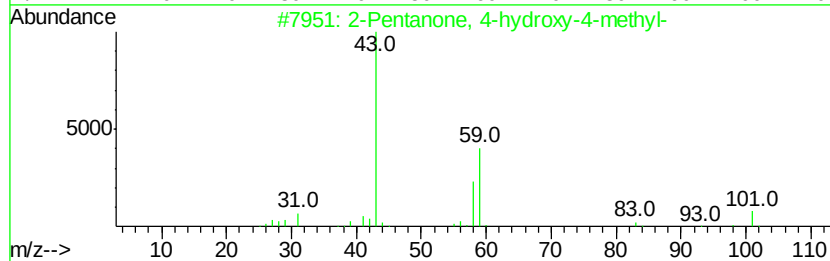
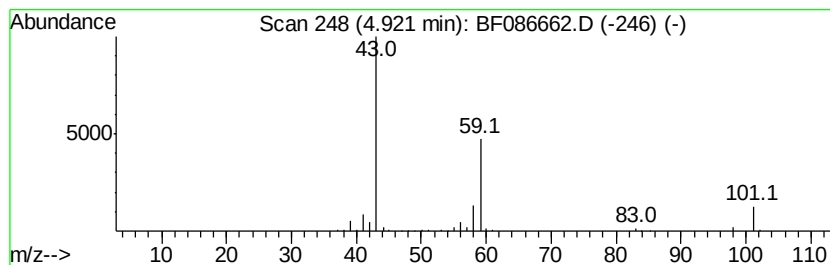
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	10.41 ng	628131	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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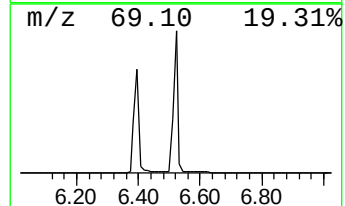
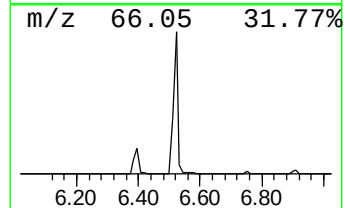
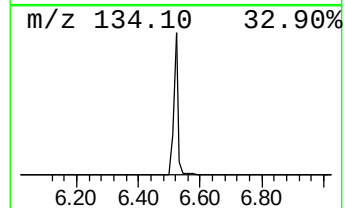
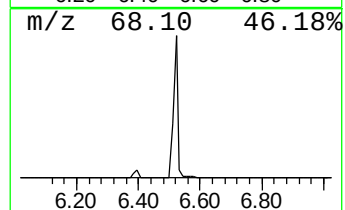
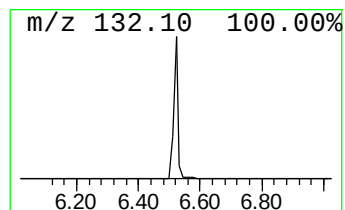
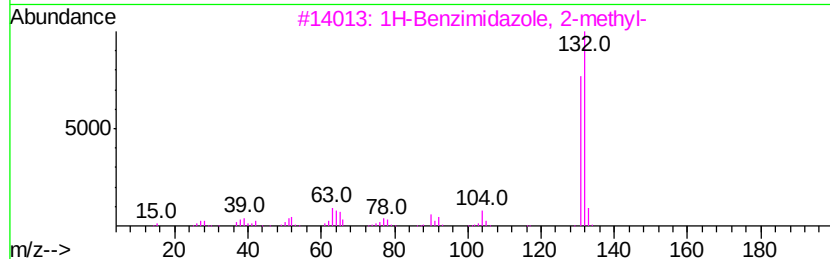
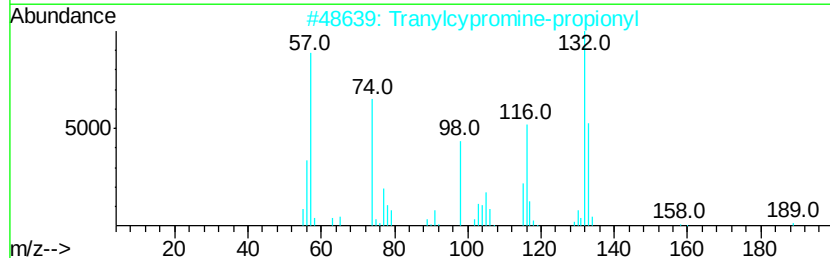
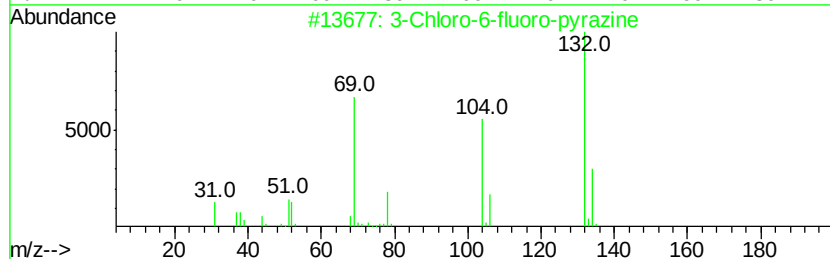
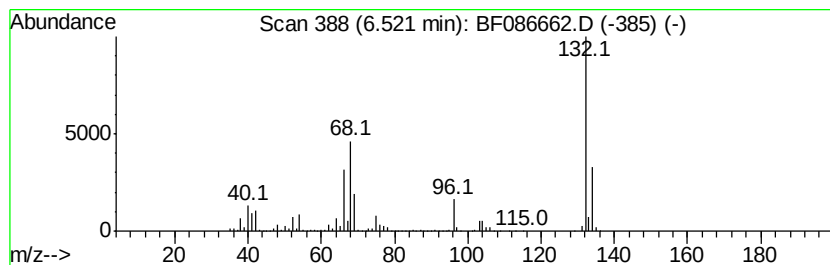
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Peak Number 5 unknown6.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	65.05 ng	3925040	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22	
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.49	2.2	ng	131430	1	6.75	1206850	20.0
4-Penten-2-one, 4...	3.22	5.3	ng	320148	1	6.75	1206850	20.0
3-Penten-2-one, 4...	4.27	145.5	ng	8780800	1	6.75	1206850	20.0
2-Pentanone, 4-hy...	4.92	10.4	ng	628131	1	6.75	1206850	20.0
unknown6.52	6.52	65.0	ng	3925040	1	6.75	1206850	20.0