

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093612.D
 Acq On : 13 Mar 2017 17:29
 Operator : SJ/MA
 Sample : I2174-22
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-71

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-BF030717.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	2.412	44	46	57	rVB	63485	156843	3.22%	0.376%
2	3.121	105	108	114	rBV	69756	188884	3.88%	0.453%
3	4.184	196	201	217	rBV2	158789	547563	11.23%	1.314%
4	4.401	217	220	223	rBV	39937	78175	1.60%	0.188%
5	4.870	258	261	277	rBV	807539	1673684	34.34%	4.016%
6	5.316	298	300	323	rBV	3131682	4874333	100.00%	11.695%
7	5.716	333	335	342	rVB	44618	70597	1.45%	0.169%
8	6.367	390	392	400	rBV	3431598	4437922	91.05%	10.648%
9	6.481	400	402	405	rVB	4583925	4457090	91.44%	10.694%
10	6.710	420	422	430	rVB	936687	980154	20.11%	2.352%
11	6.859	433	435	438	rBV	3472578	3501058	71.83%	8.400%
12	7.282	470	472	487	rBV	2859537	3233167	66.33%	7.757%
13	8.002	532	535	548	rVB	1190230	1328340	27.25%	3.187%
14	9.076	627	629	632	rBV	3825839	4771670	97.89%	11.449%
15	9.762	686	689	691	rBV	1051104	1399590	28.71%	3.358%
16	10.550	756	758	761	rBV	2249968	2608557	53.52%	6.259%
17	11.248	817	819	824	rBV	1491732	1406603	28.86%	3.375%
18	12.836	955	958	961	rBV	4182425	4282836	87.87%	10.276%
19	13.899	1049	1051	1059	rVB	753853	1002775	20.57%	2.406%
20	15.305	1171	1174	1182	rBV	418127	678588	13.92%	1.628%

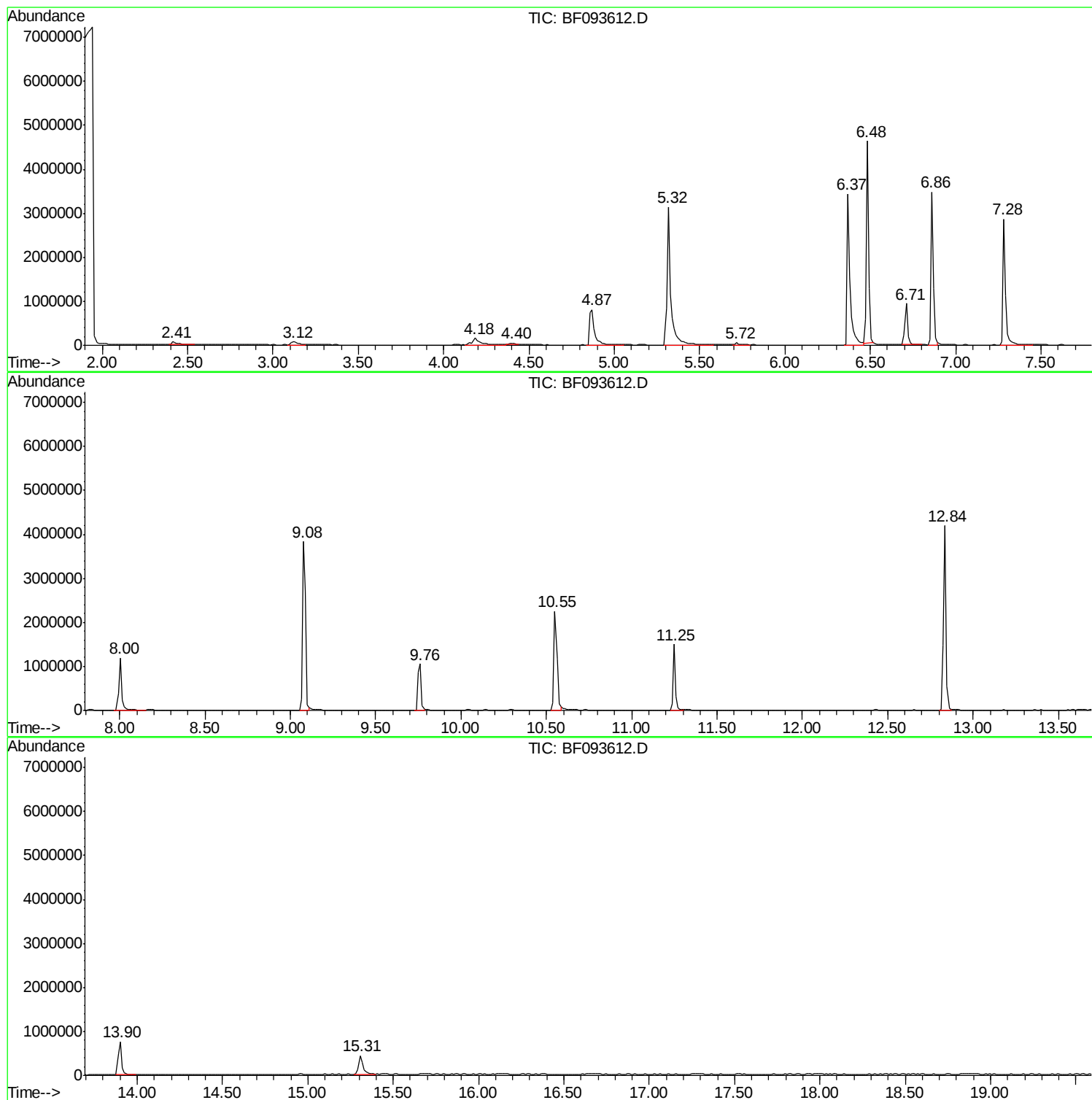
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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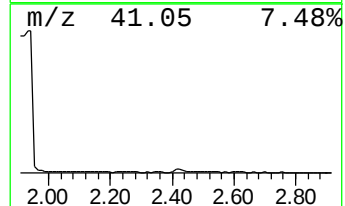
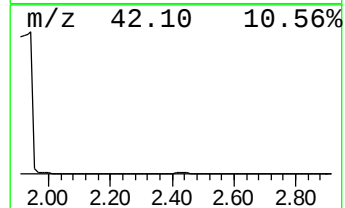
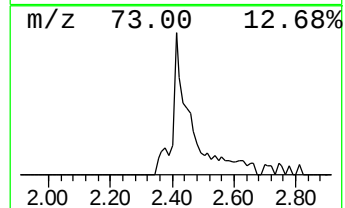
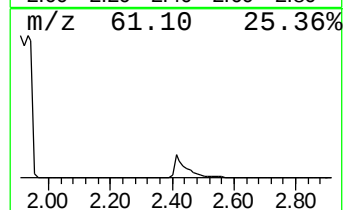
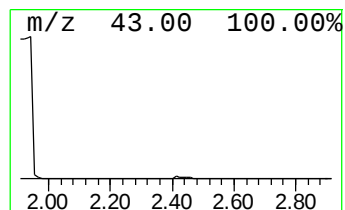
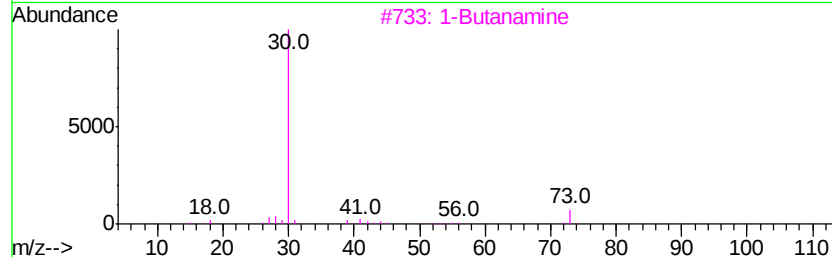
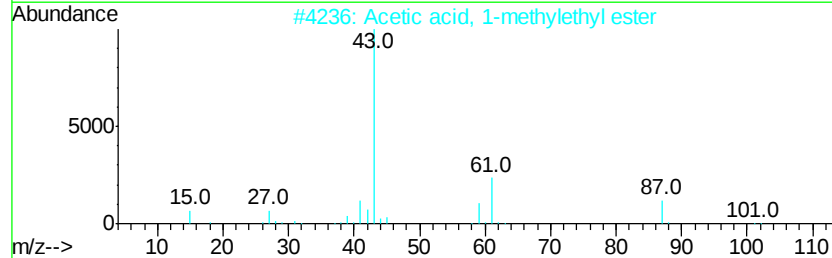
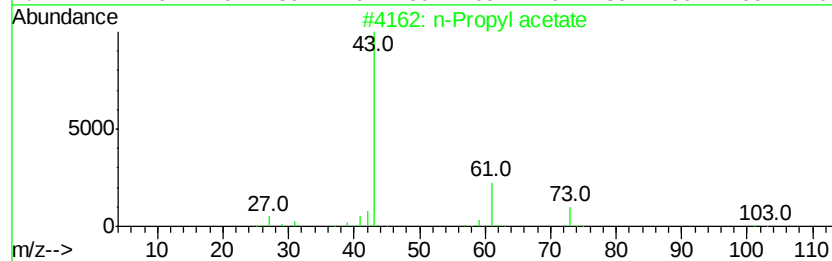
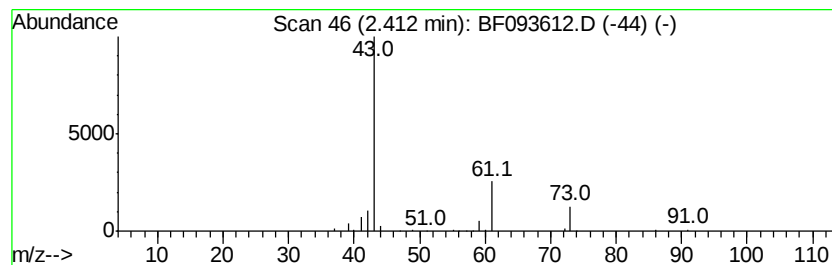
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	3.20 ng	156843	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78	
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	9	
3	1-Butanamine	73	C4H11N	000109-73-9	5	
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	5	
5	Isobutylamine	73	C4H11N	000078-81-9	5	



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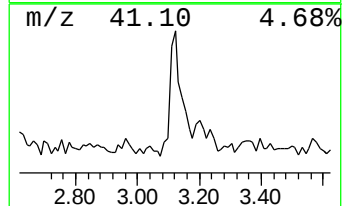
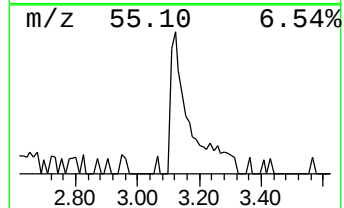
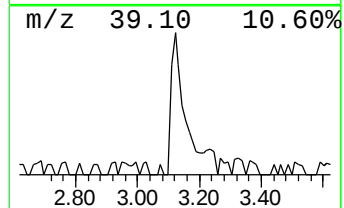
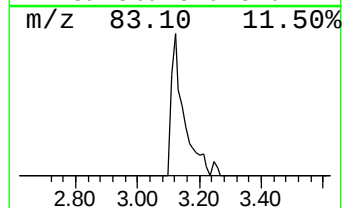
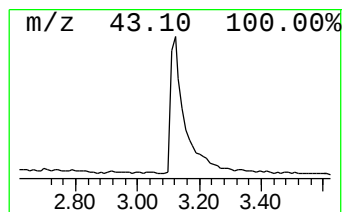
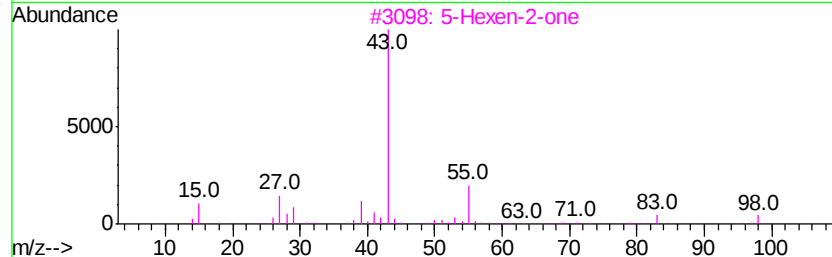
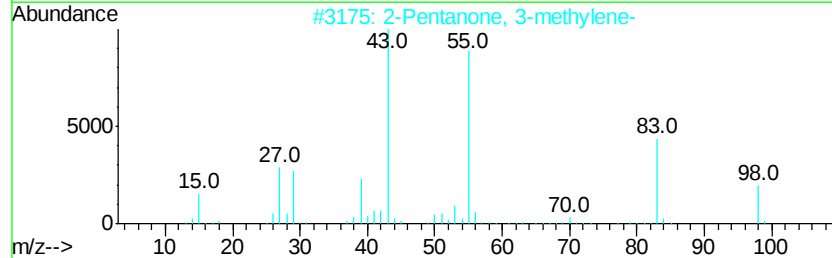
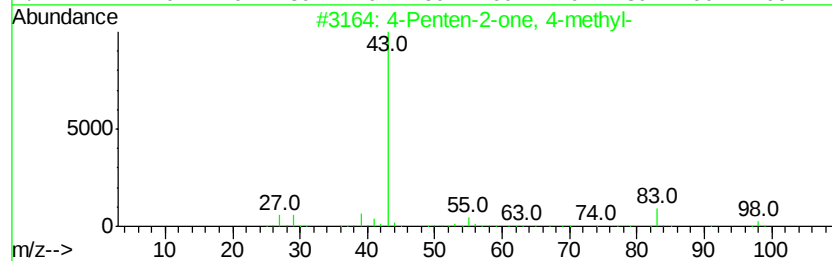
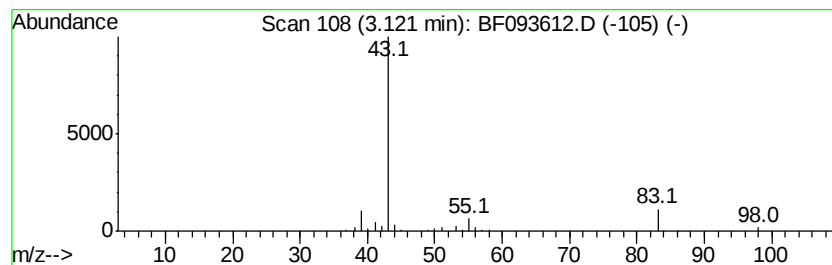
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Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	3.85 ng	188884	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	12
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
5			4-Hexen-2-one	98	C6H10O	025659-22-7	9



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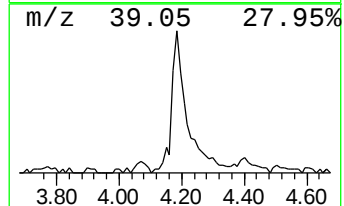
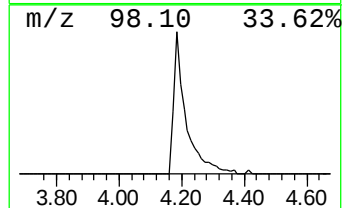
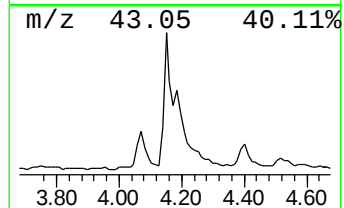
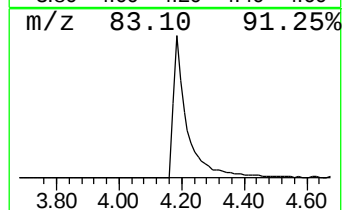
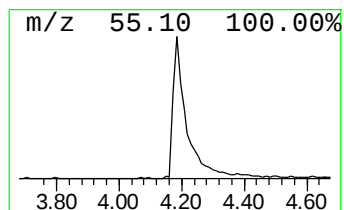
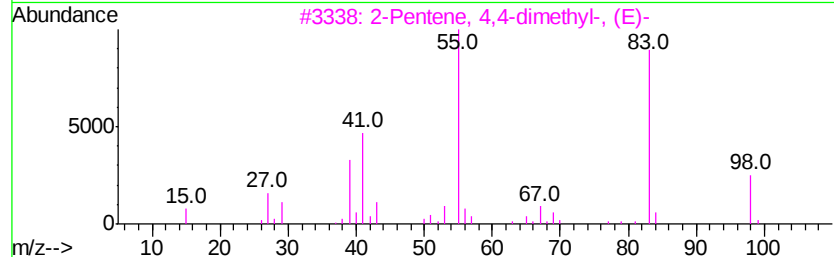
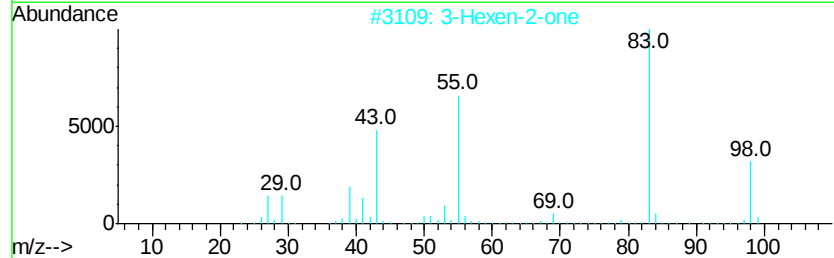
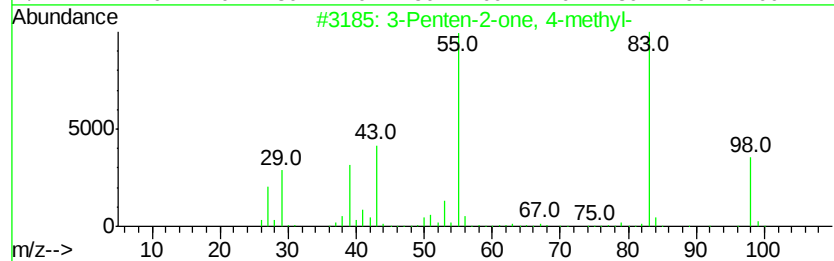
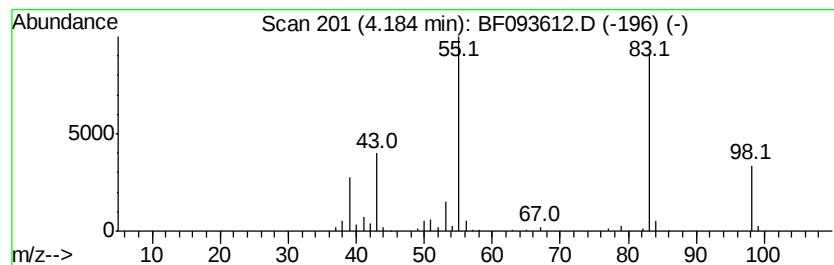
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	11.17 ng	547563	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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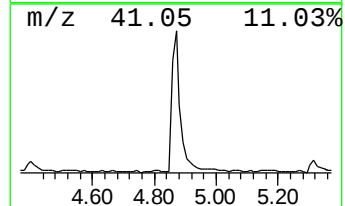
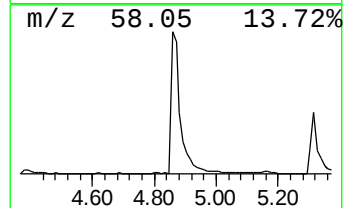
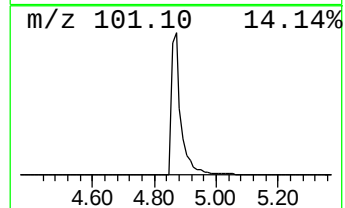
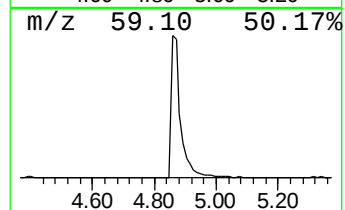
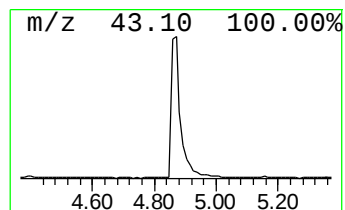
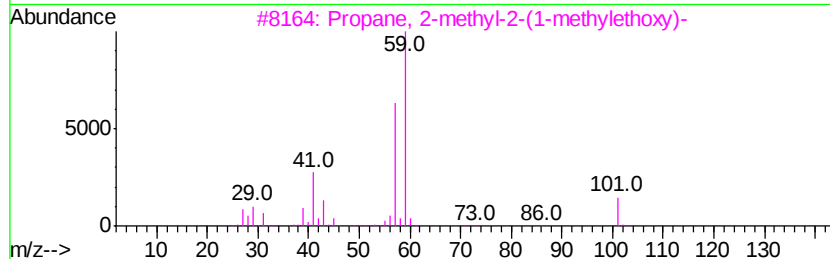
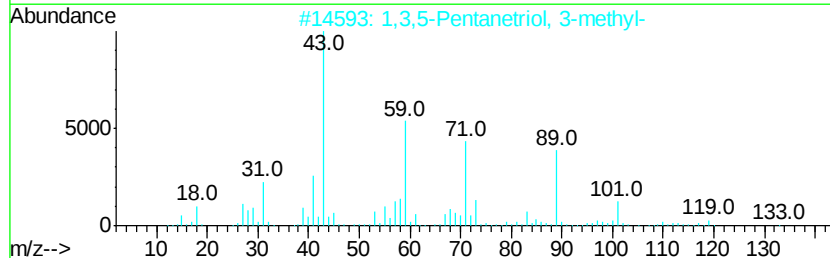
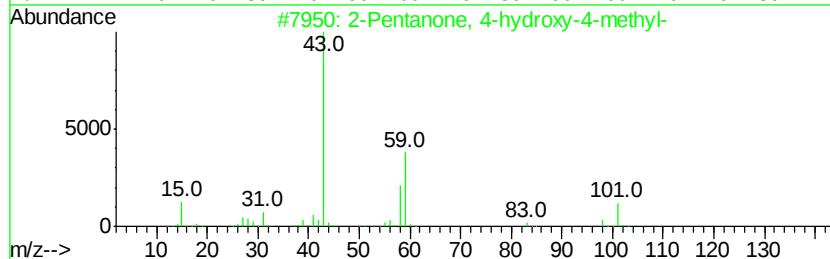
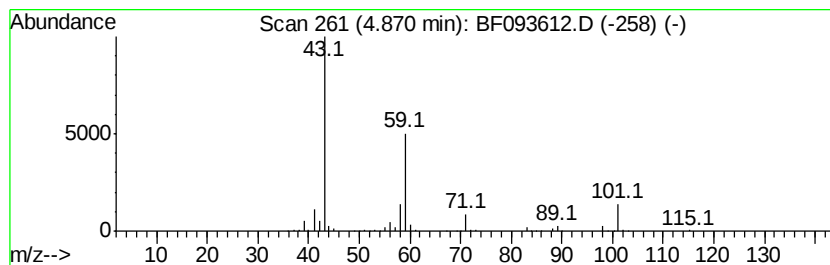
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	34.15 ng	1673680	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	39
3		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	33
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	32
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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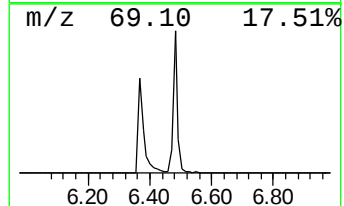
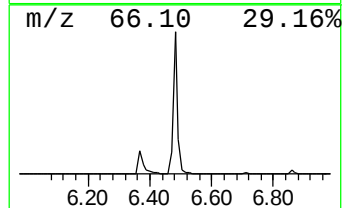
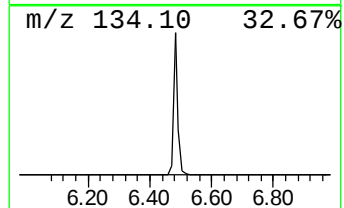
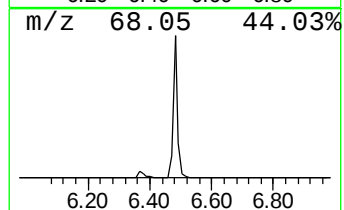
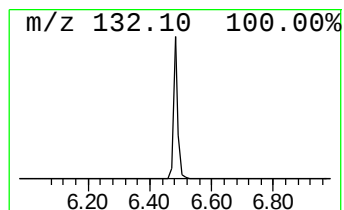
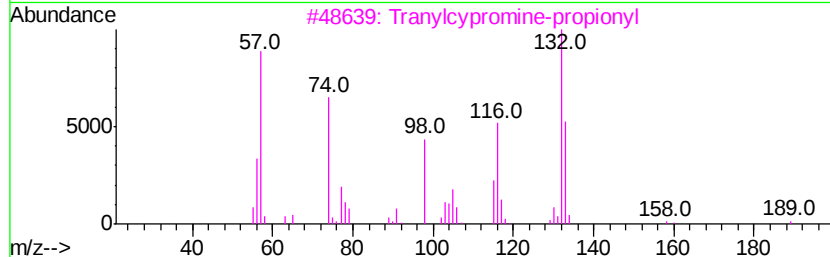
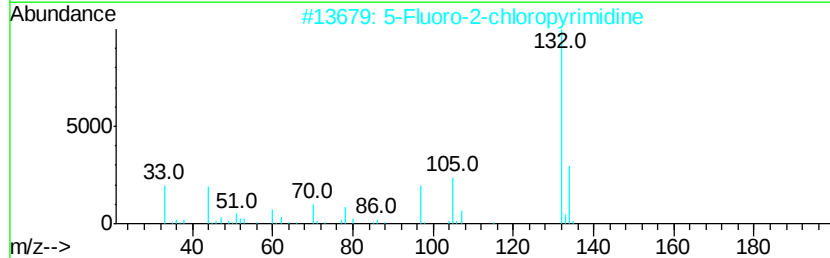
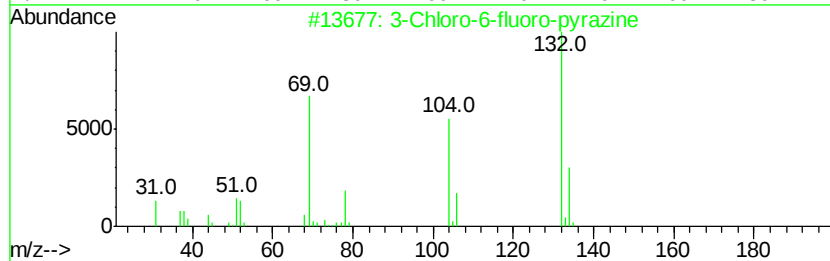
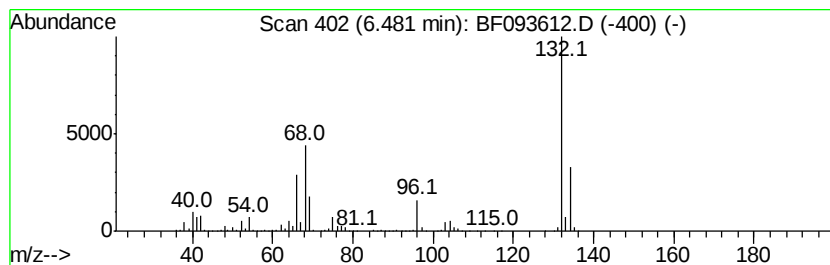
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.95 ng	4457090	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
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
n-Propyl acetate	2.41	3.2	ng	156843	1	6.71	980154	20.0
4-Penten-2-one, 4...	3.12	3.9	ng	188884	1	6.71	980154	20.0
3-Penten-2-one, 4...	4.18	11.2	ng	547563	1	6.71	980154	20.0
2-Pentanone, 4-hy...	4.87	34.1	ng	1673680	1	6.71	980154	20.0
unknown6.48	6.48	91.0	ng	4457090	1	6.71	980154	20.0