

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022317\
 Data File : BF093139.D
 Acq On : 24 Feb 2017 9:16
 Operator : SJ/MA
 Sample : I1955-08
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1-4

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-BF013017.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	2.453	22	32	42	rVV2	21066	109615	2.62%	0.321%
2	2.613	44	46	53	rVB	149213	211839	5.06%	0.621%
3	4.350	195	198	200	rBV	37529	50918	1.22%	0.149%
4	5.024	254	257	265	rBV	1041932	1814192	43.29%	5.317%
5	5.447	291	294	296	rBV	3645680	3952018	94.31%	11.583%
6	6.487	382	385	387	rBV	3222764	3832798	91.47%	11.233%
7	6.613	393	396	398	rBV	3974993	4006403	95.61%	11.742%
8	6.842	414	416	418	rBV	993367	869428	20.75%	2.548%
9	7.002	427	430	432	rBV	2636007	3064660	73.14%	8.982%
10	7.413	463	466	468	rBV	2537834	2736867	65.31%	8.021%
11	8.122	526	528	531	rBV	1077583	1066722	25.46%	3.126%
12	9.208	620	623	625	rBV	3582129	4190385	100.00%	12.281%
13	9.882	679	682	684	rBV	848899	977803	23.33%	2.866%
14	10.671	748	751	753	rBV	1559027	1808884	43.17%	5.302%
15	10.785	759	761	765	rVB	52765	73902	1.76%	0.217%
16	11.356	809	811	814	rBV	743920	771120	18.40%	2.260%
17	12.694	927	928	932	rBV	82500	125377	2.99%	0.367%
18	12.762	932	934	936	rVB	53543	52151	1.24%	0.153%
19	12.945	947	950	953	rBV	2942703	2797979	66.77%	8.200%
20	13.117	963	965	967	rBV	35021	43590	1.04%	0.128%
21	13.471	993	996	997	rBV2	36817	50006	1.19%	0.147%
22	13.997	1039	1042	1045	rVB	834137	770272	18.38%	2.258%
23	15.425	1164	1167	1172	rVB	563980	699532	16.69%	2.050%
24	15.848	1201	1204	1209	rVB	22508	43440	1.04%	0.127%

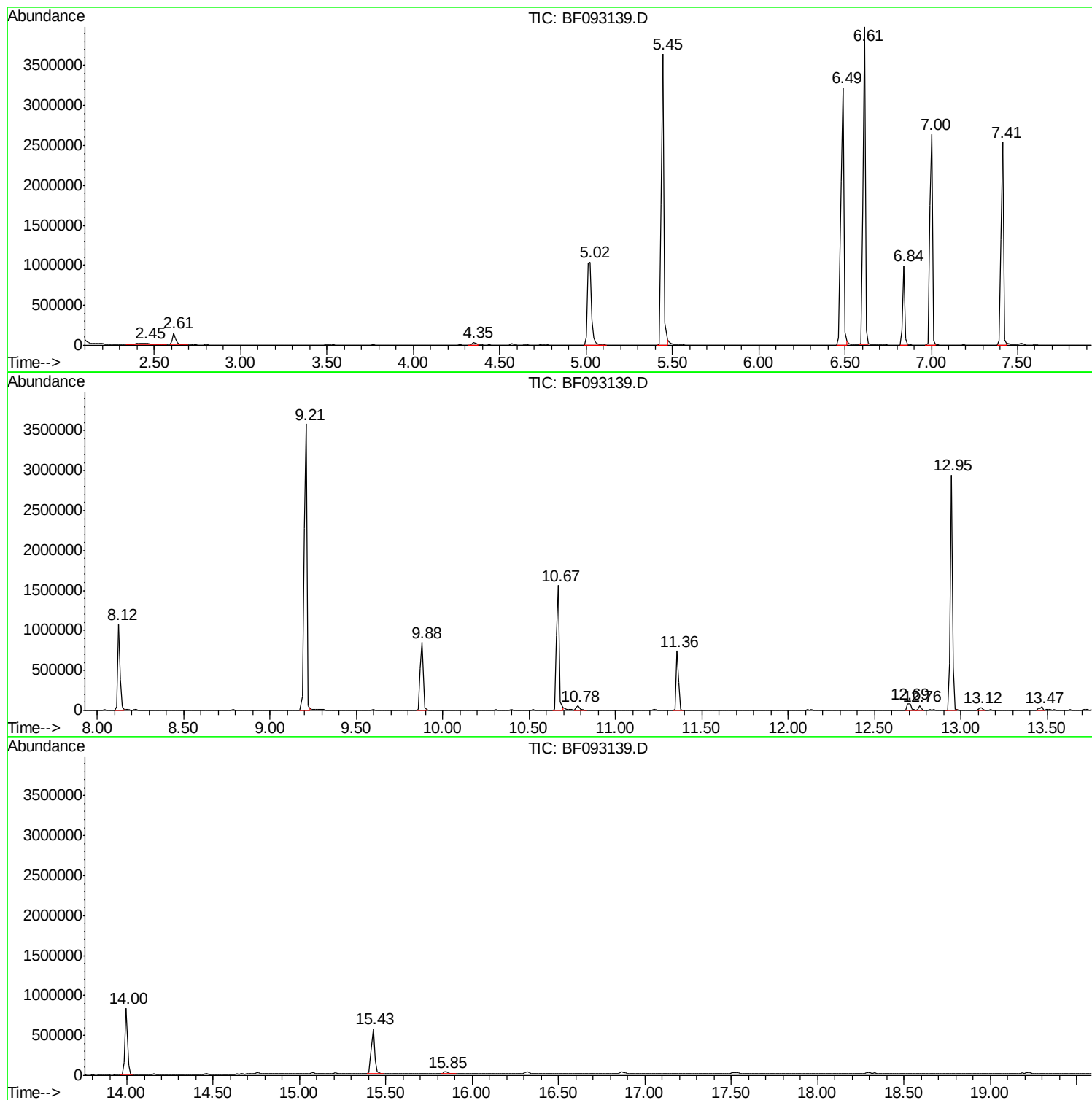
Sum of corrected areas: 34119901

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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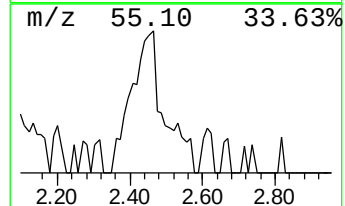
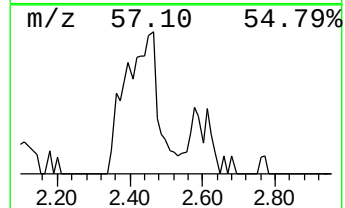
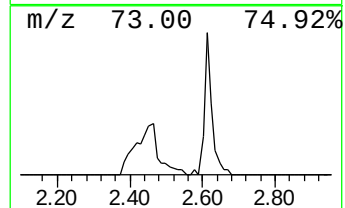
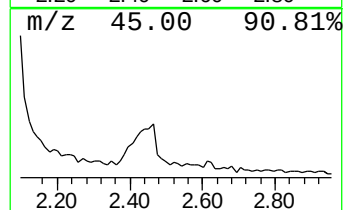
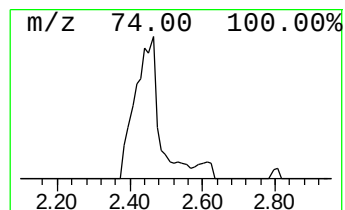
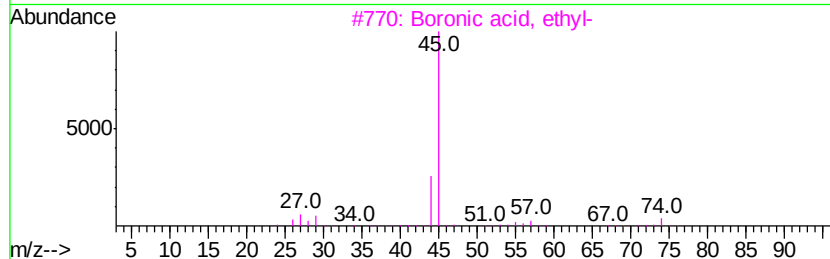
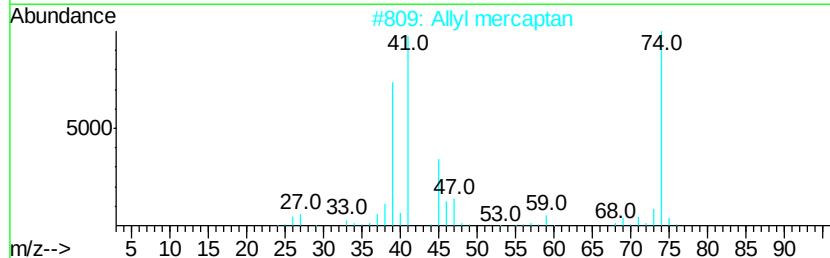
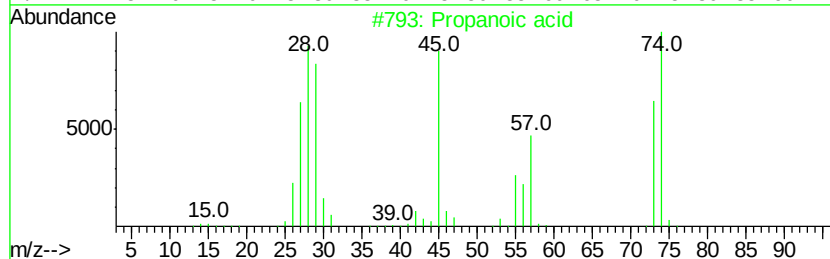
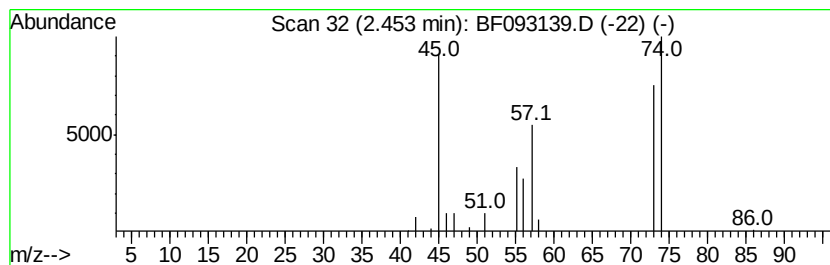
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.45	2.52 ng	109615	1,4-Dichlorobenzene-d4	6.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid	74	C3H6O2	000079-09-4	90
2	Allyl mercaptan	74	C3H6S	000870-23-5	9
3	Boronic acid, ethyl-	74	C2H7BO2	004433-63-0	9
4	Butane, 1-methoxy-2-methyl-	102	C6H14O	062016-48-2	9
5	Thiirane, methyl-	74	C3H6S	001072-43-1	7



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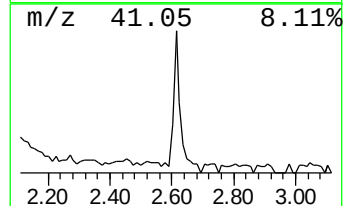
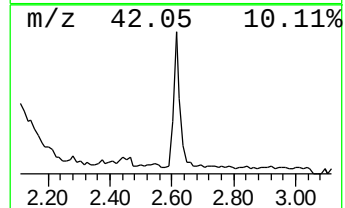
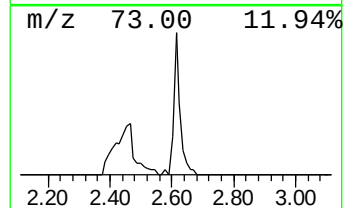
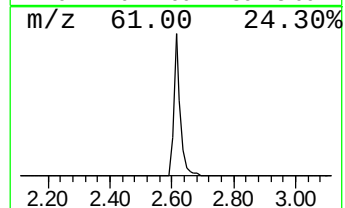
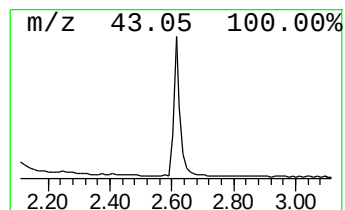
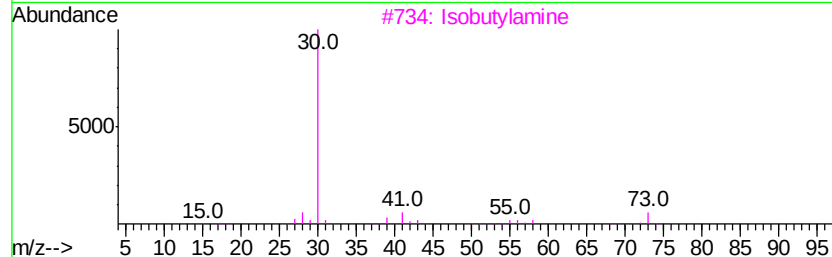
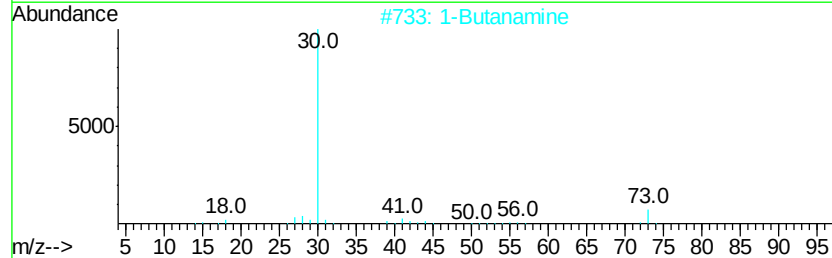
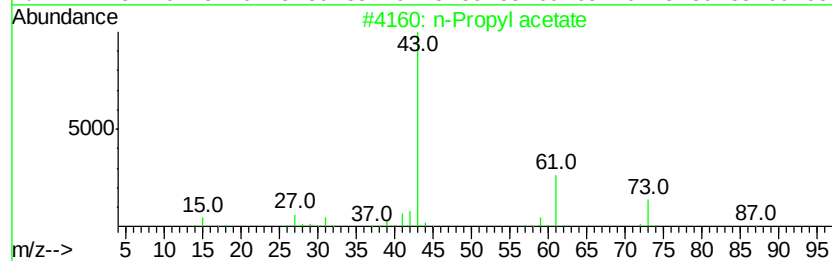
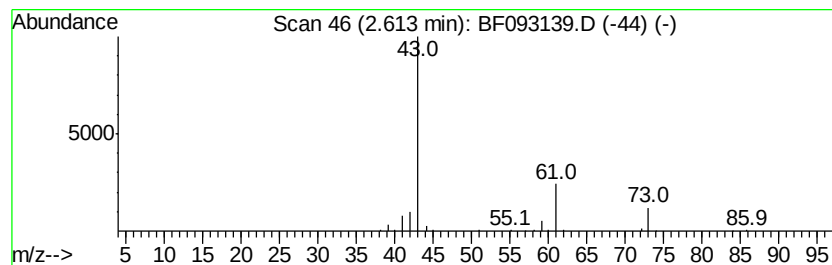
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Peak Number 2 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.61	4.87 ng	211839	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	7
3		Isobutylamine	73	C4H11N	000078-81-9	5
4		Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4
5		Pentane	72	C5H12	000109-66-0	4



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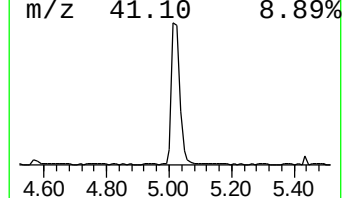
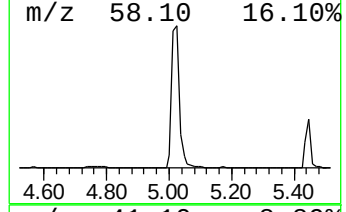
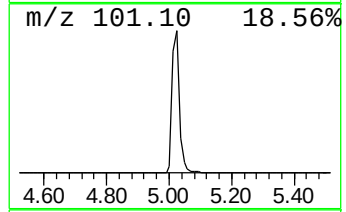
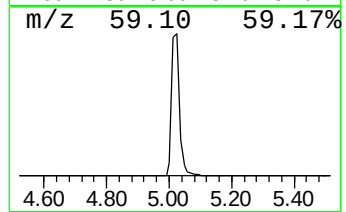
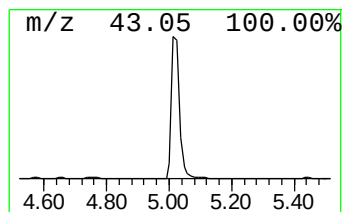
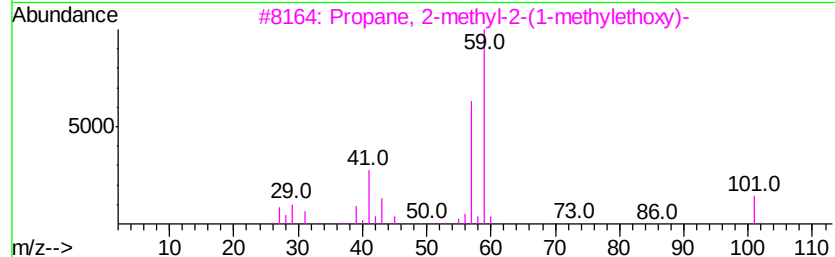
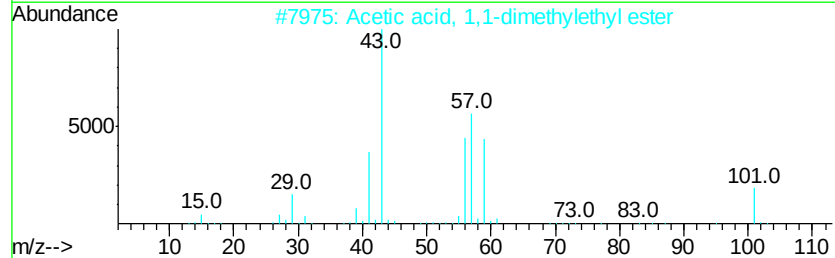
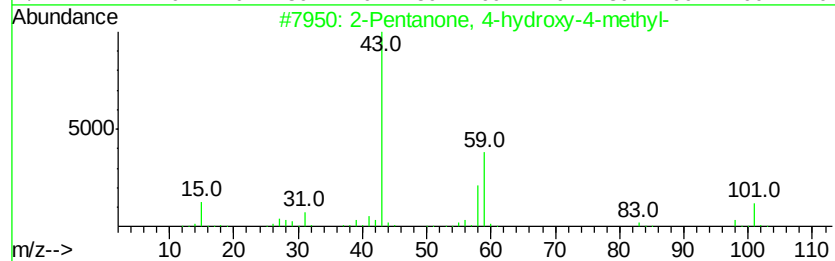
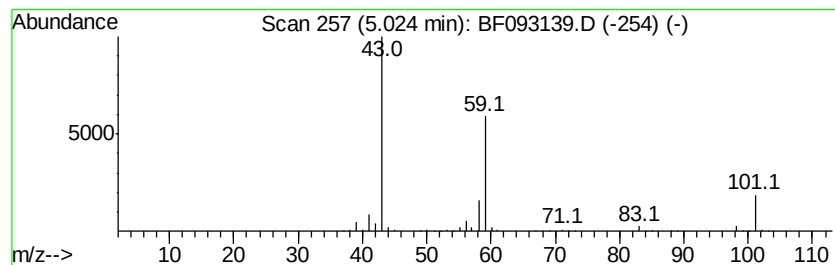
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	41.73 ng	1814190	1,4-Dichlorobenzene-d4	6.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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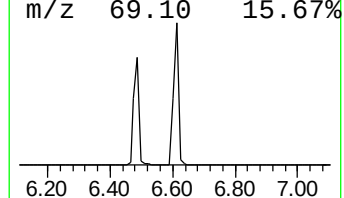
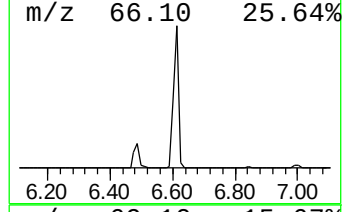
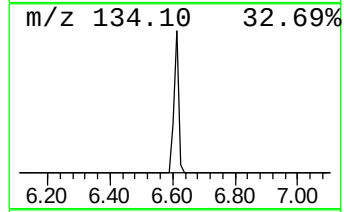
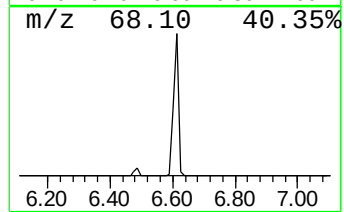
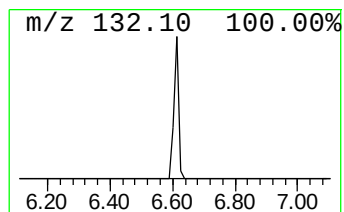
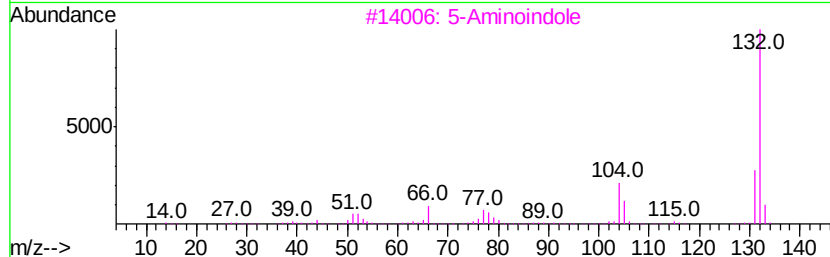
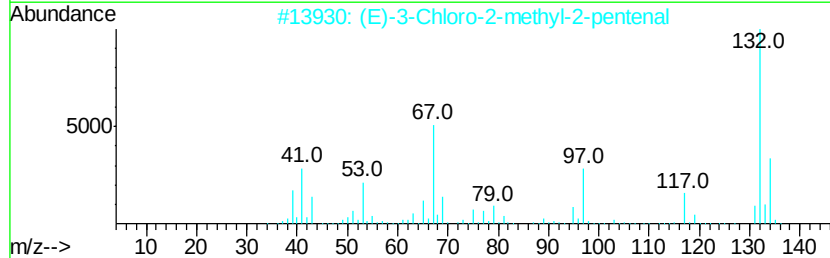
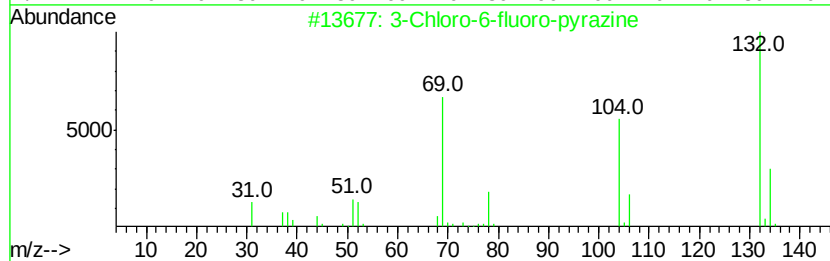
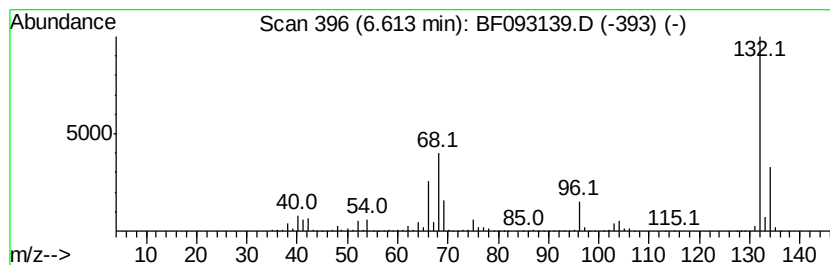
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Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	92.16 ng	4006400	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid	2.45	2.5	ng	109615	1	6.84	869428	20.0
n-Propyl acetate	2.61	4.9	ng	211839	1	6.84	869428	20.0
2-Pentanone, 4-hy...	5.02	41.7	ng	1814190	1	6.84	869428	20.0
unknown6.61	6.61	92.2	ng	4006400	1	6.84	869428	20.0