

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
 Data File : BM011386.D
 Acq On : 31 Aug 2017 23:45
 Operator : SJ/JU
 Sample : I4963-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3825-SPP2

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_M\METHODS\8270-BM083117.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	3.058	40	46	56	rBV	1170927	2102980	5.60%	1.182%
2	3.134	56	59	69	rVB	507799	645880	1.72%	0.363%
3	5.081	382	390	398	rBV	398459	613630	1.64%	0.345%
4	5.546	461	469	481	rBV	5225721	7507899	20.01%	4.219%
5	7.134	727	739	747	rBV	2985492	4707046	12.54%	2.645%
6	7.516	796	804	818	rBV	9252207	14895789	39.70%	8.371%
7	7.987	875	884	891	rBV	1945378	3191672	8.51%	1.794%
8	8.316	932	940	954	rVB	8280935	13567083	36.16%	7.624%
9	9.151	1074	1082	1092	rBV	6715021	11252387	29.99%	6.323%
10	10.798	1351	1362	1373	rBV	2916132	4814007	12.83%	2.705%
11	11.445	1466	1472	1483	rVB	397239	738928	1.97%	0.415%
12	13.245	1769	1778	1786	rBV	17747673	26266544	70.00%	14.761%
13	14.621	2005	2012	2020	rBV2	4016639	6263973	16.69%	3.520%
14	16.104	2257	2264	2288	rBV	13740891	19412252	51.73%	10.909%
15	17.357	2471	2477	2488	rBV2	5124936	7434977	19.81%	4.178%
16	19.968	2915	2921	2927	rBV	29635731	37523244	100.00%	21.086%
17	21.521	3180	3185	3191	rBV	7591314	8997432	23.98%	5.056%
18	23.903	3583	3590	3603	rVB	4027330	8014484	21.36%	4.504%

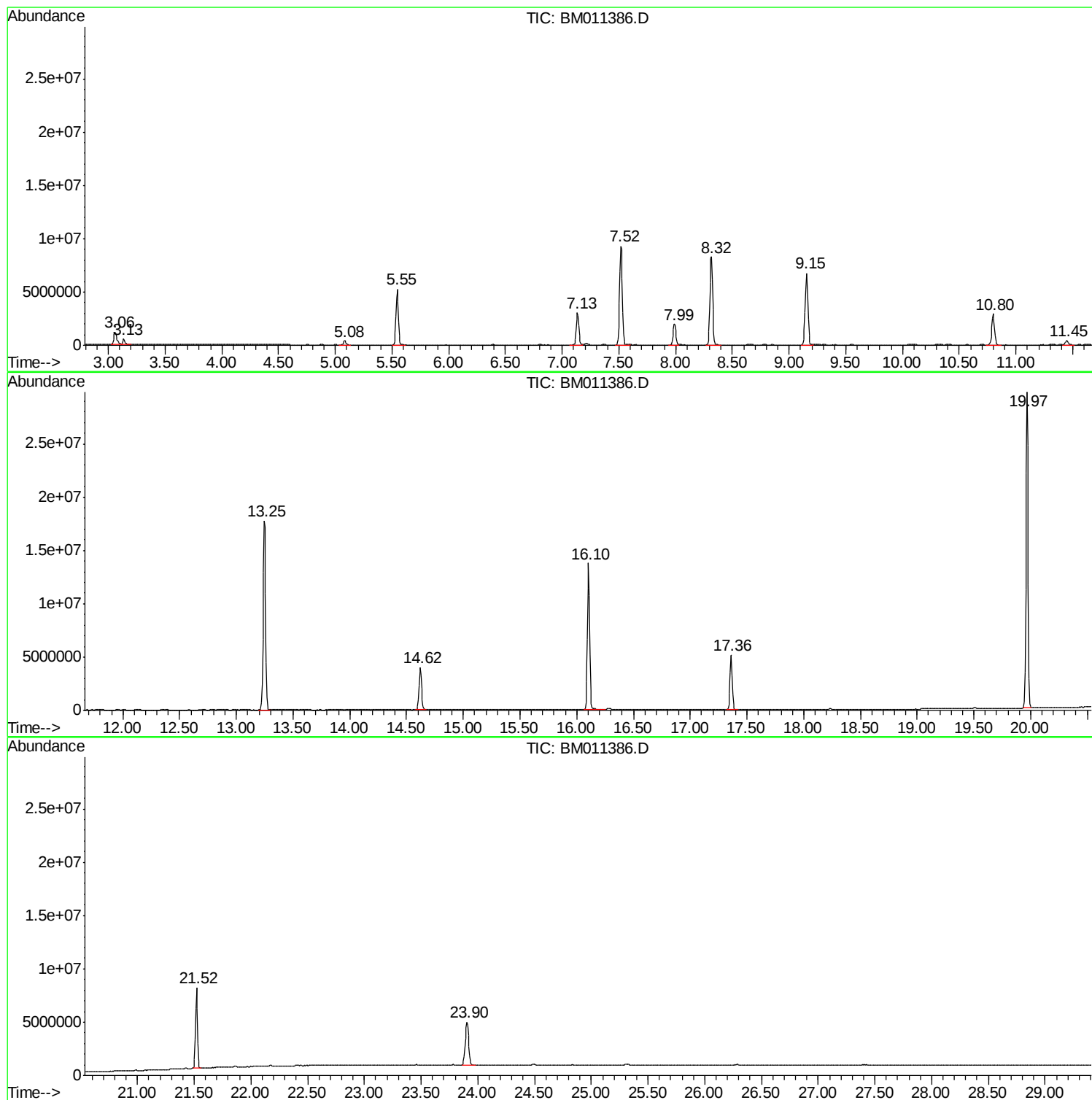
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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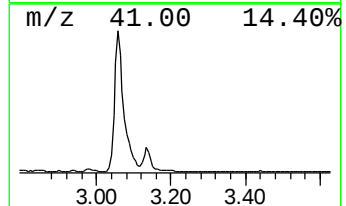
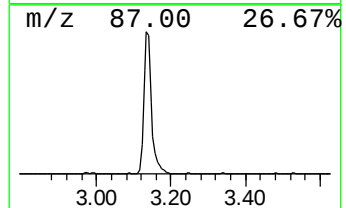
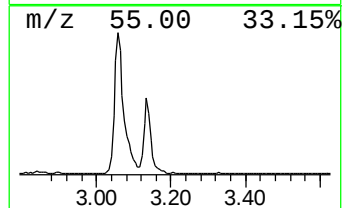
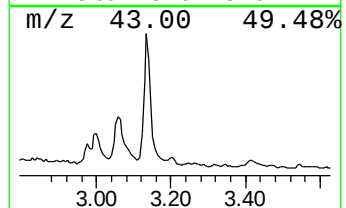
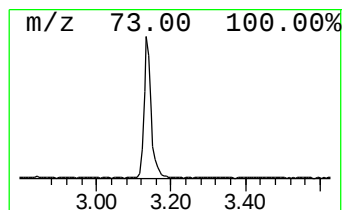
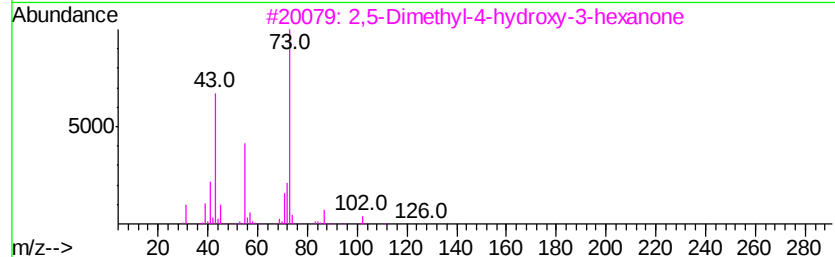
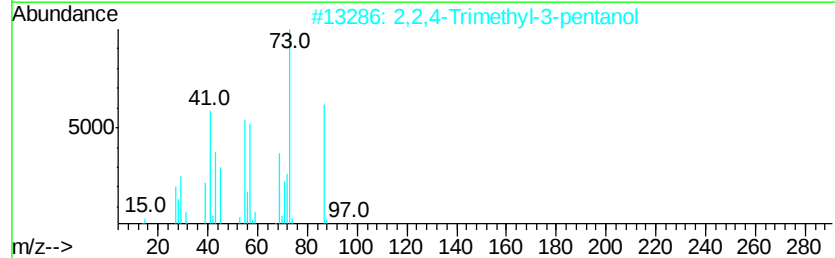
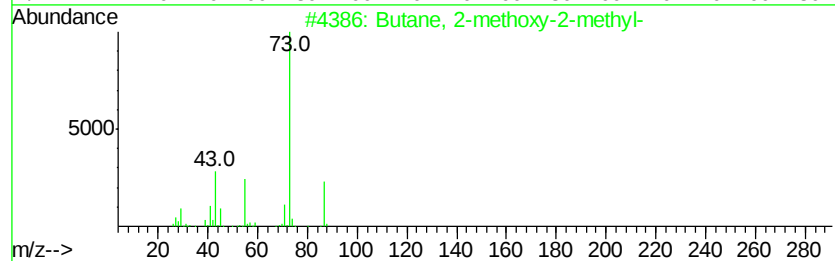
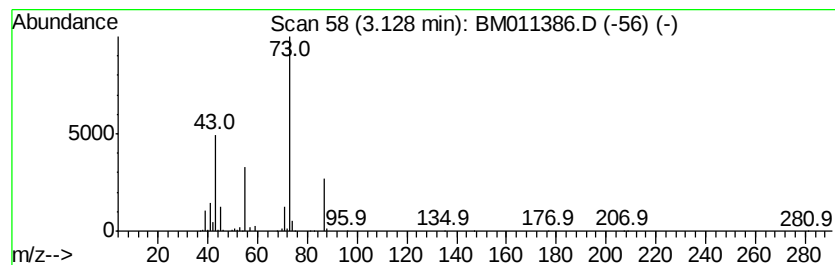
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	4.05 ng	645880	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	40
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32



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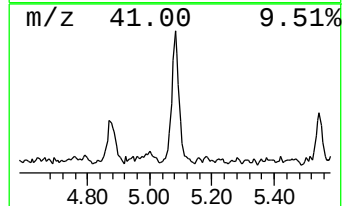
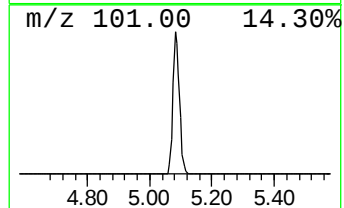
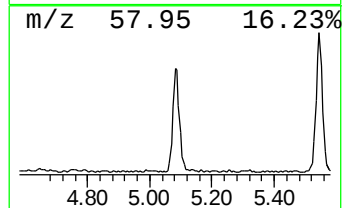
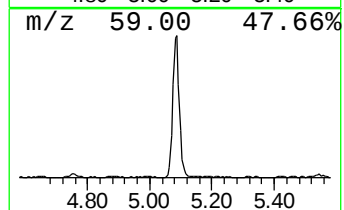
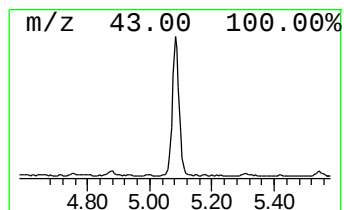
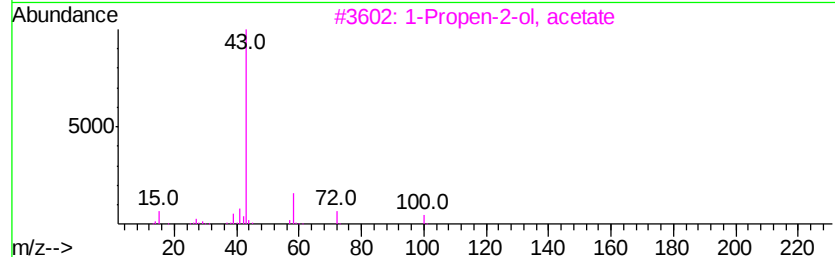
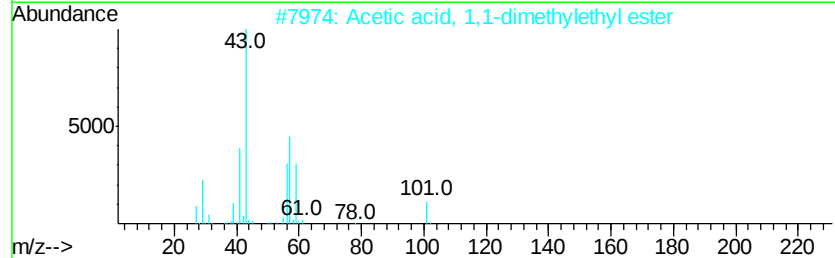
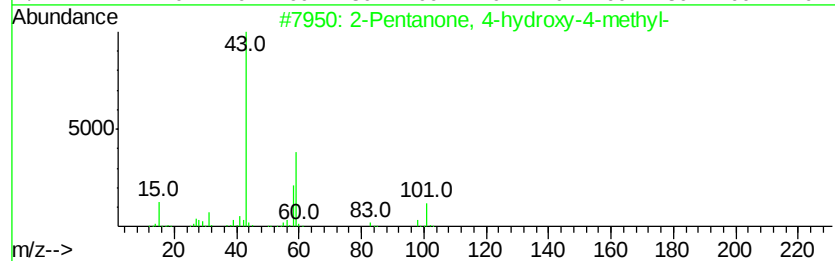
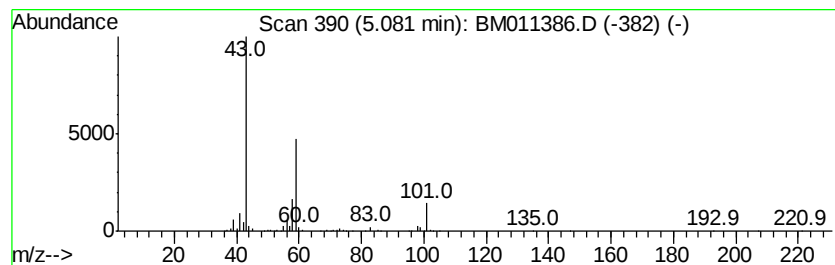
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	3.85 ng	613630	1,4-Dichlorobenzene-d4	7.99

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	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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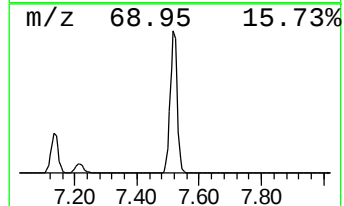
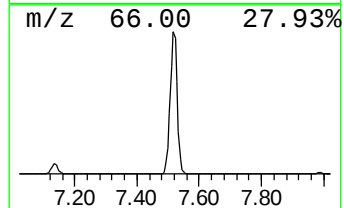
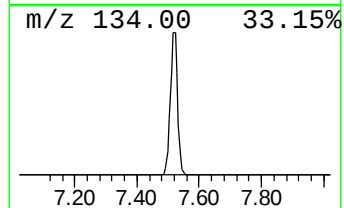
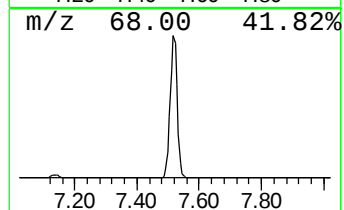
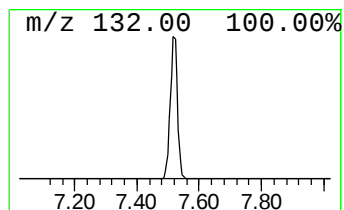
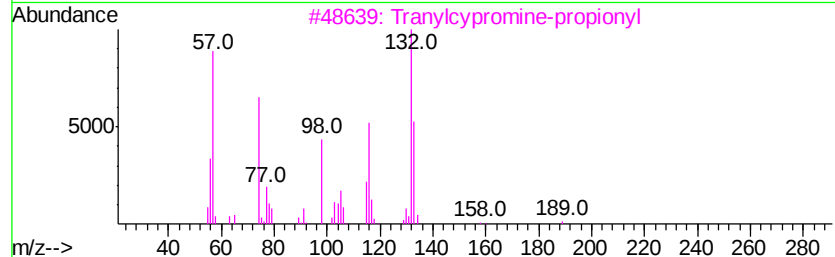
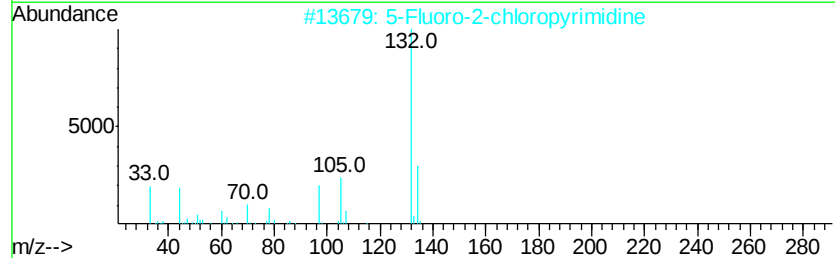
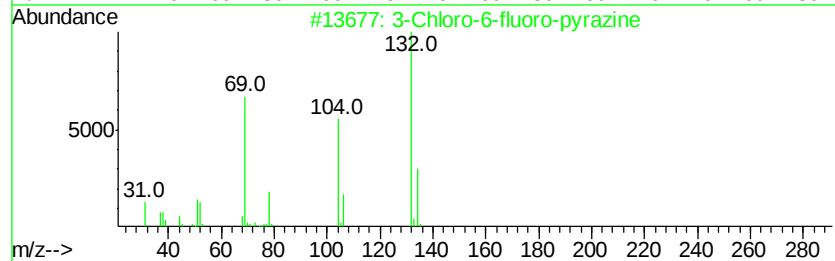
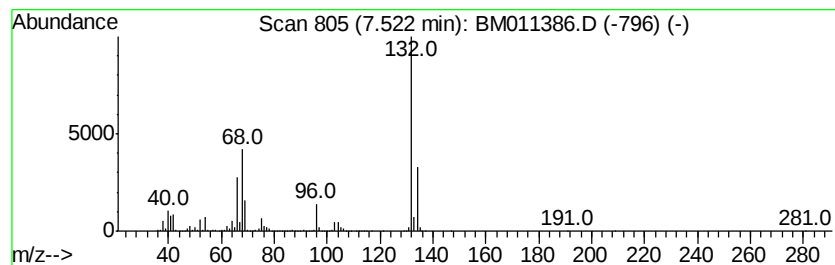
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Peak Number 4 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	93.34 ng	14895800	1,4-Dichlorobenzene-d4	7.99

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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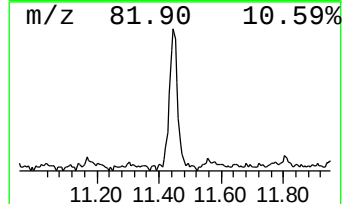
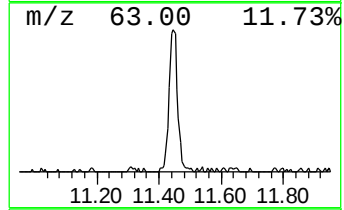
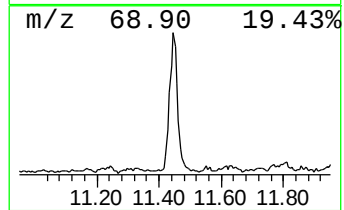
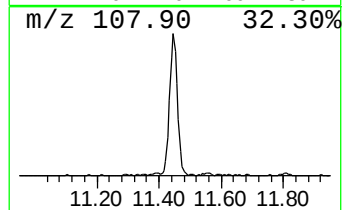
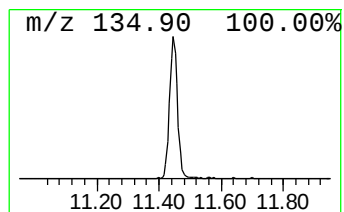
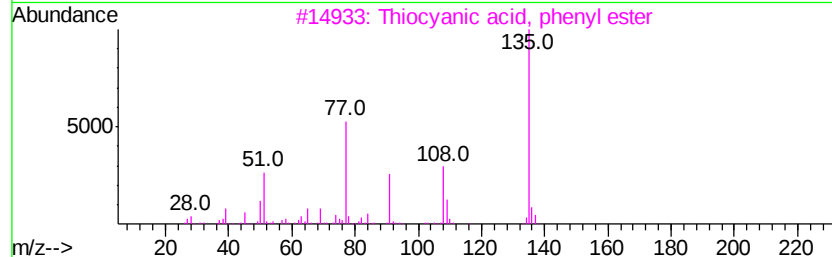
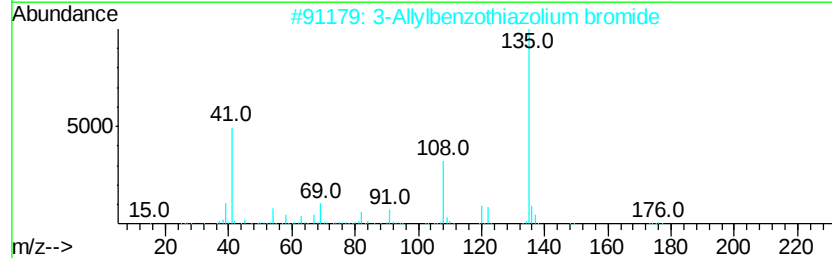
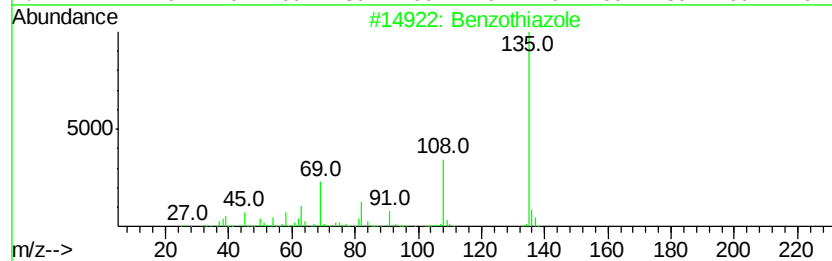
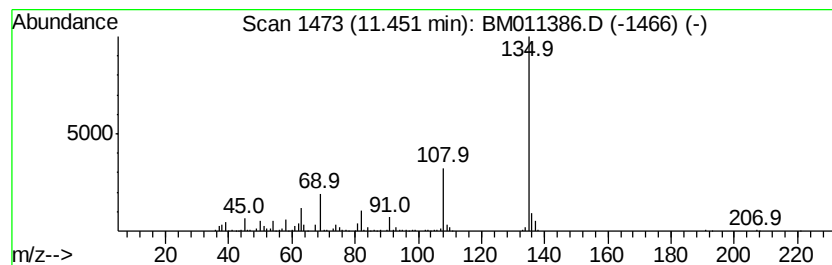
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Peak Number 6 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	3.07 ng	738928	Naphthalene-d8	10.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	97
2		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
3		Thiocyanic acid, phenyl ester	135	C7H5NS	005285-87-0	59
4		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59
5		4-Aminopyrazolo(3,4-d)pyrimidine	135	C5H5N5	020289-44-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	4.0	ng	645880	1	7.99	3191670	20.0
2-Pentanone, 4-hy...	5.08	3.9	ng	613630	1	7.99	3191670	20.0
unknown7.52	7.52	93.3	ng	14895800	1	7.99	3191670	20.0
Benzothiazole	11.45	3.1	ng	738928	2	10.80	4814010	20.0