

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050617\
 Data File : BM009939.D
 Acq On : 06 May 2017 13:38
 Operator : SJ/MA
 Sample : I2893-14
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3073-PA4

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-BM050517.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	4.910	305	310	317	rBV	182283	269305	2.34%	0.578%
2	5.369	381	388	398	rBV	1251396	1923222	16.73%	4.126%
3	6.963	653	659	670	rBV	796174	1293630	11.25%	2.775%
4	7.316	711	719	728	rBV	2373385	3870195	33.66%	8.303%
5	7.775	790	797	803	rBV2	472210	738939	6.43%	1.585%
6	8.092	844	851	859	rBV	2078743	3270217	28.44%	7.016%
7	8.951	988	997	1008	rBV	2066326	3439969	29.92%	7.380%
8	10.569	1265	1272	1280	rBV	579418	1014381	8.82%	2.176%
9	11.239	1377	1386	1392	rBV2	68611	131574	1.14%	0.282%
10	13.045	1684	1693	1701	rBV	4602677	6505831	56.59%	13.957%
11	14.433	1922	1929	1935	rBV2	850511	1328862	11.56%	2.851%
12	15.933	2177	2184	2193	rBV	4146534	5688859	49.48%	12.204%
13	16.157	2218	2222	2231	rVB3	97534	168478	1.47%	0.361%
14	17.186	2391	2397	2409	rBV2	1174648	1726346	15.02%	3.704%
15	18.068	2543	2547	2552	rBV6	99154	151469	1.32%	0.325%
16	19.350	2762	2765	2772	rVB7	73885	116107	1.01%	0.249%
17	19.815	2838	2844	2849	rBV	9534714	11496935	100.00%	24.665%
18	21.374	3105	3109	3114	rBV	1600969	2008328	17.47%	4.309%
19	23.680	3496	3501	3509	rVB2	800769	1470314	12.79%	3.154%

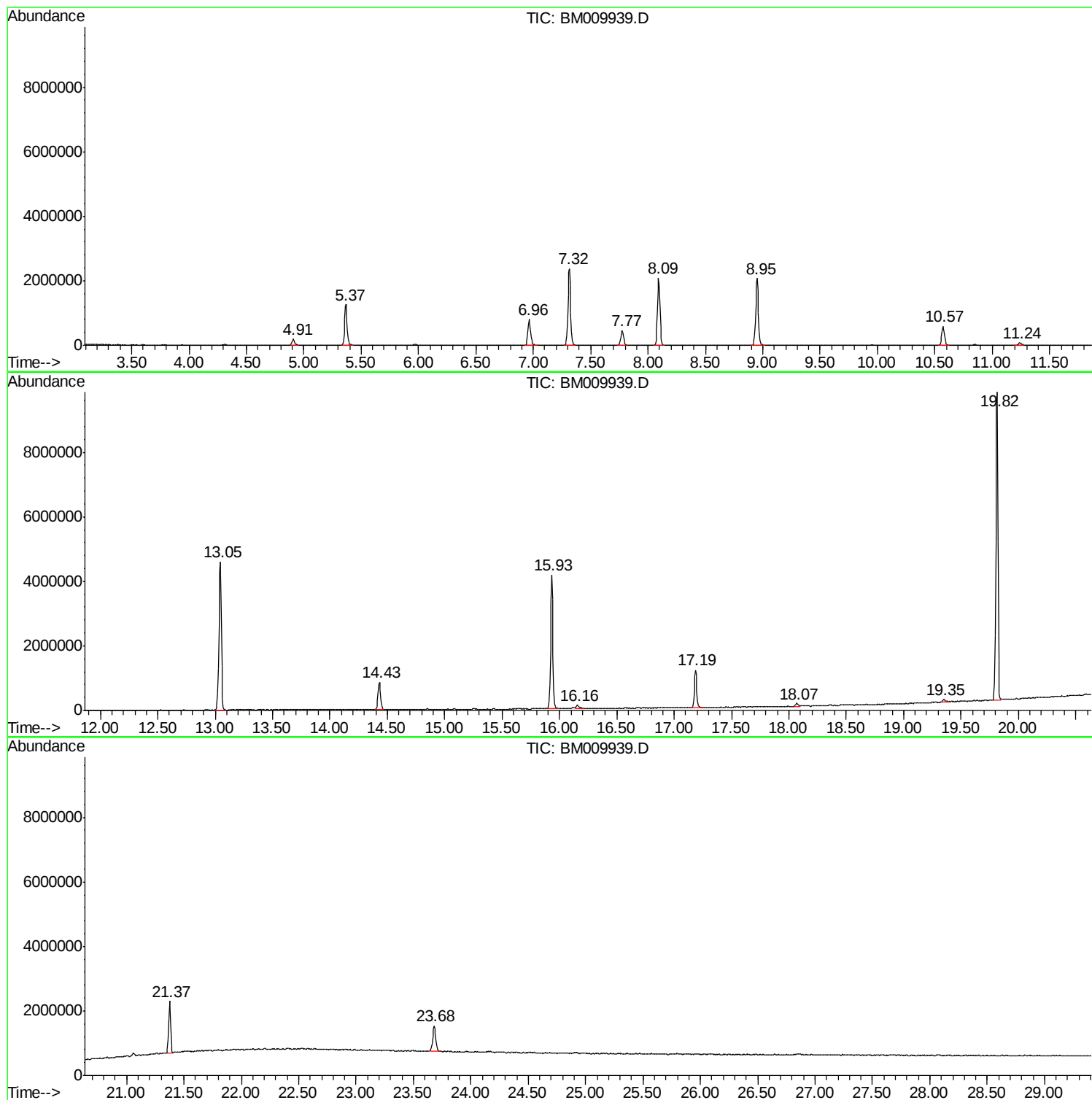
Sum of corrected areas: 46612961

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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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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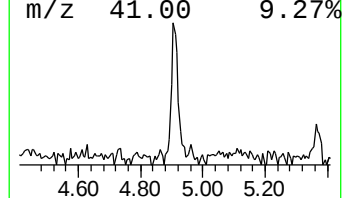
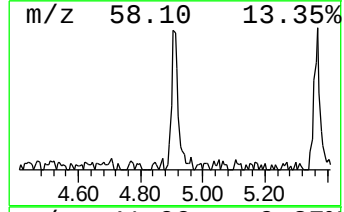
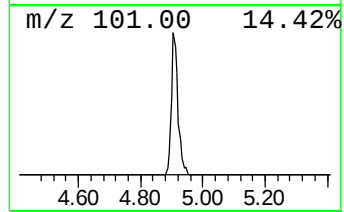
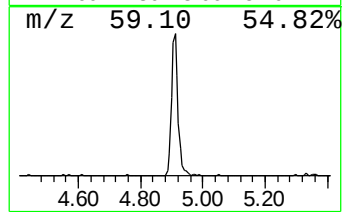
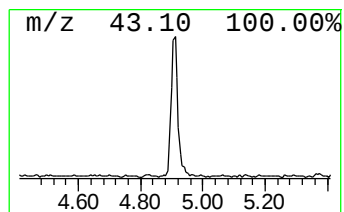
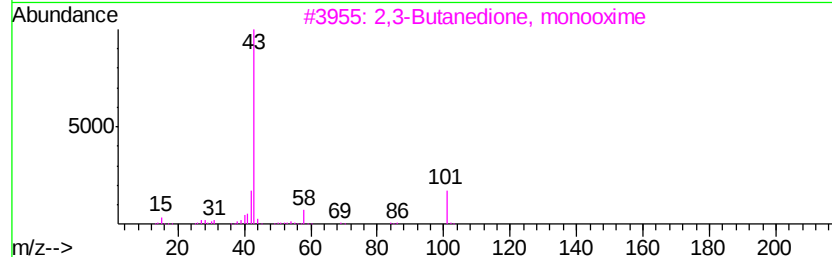
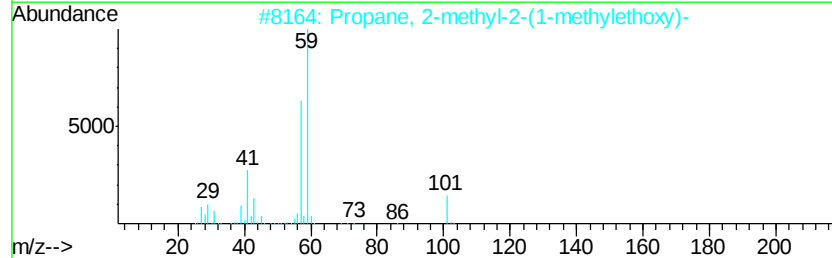
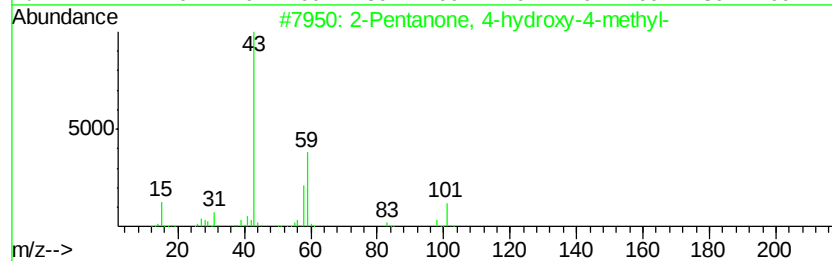
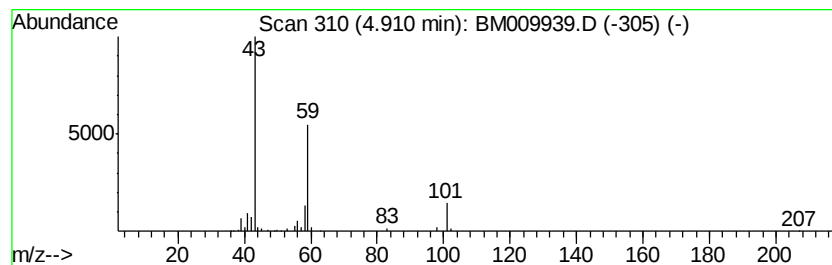
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	7.29 ng	269305	1,4-Dichlorobenzene-d4	7.77

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	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Propylamine	59	C3H9N	000107-10-8	9
5		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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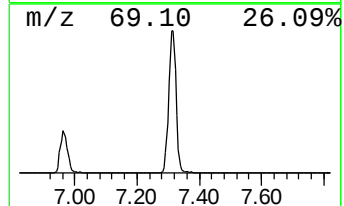
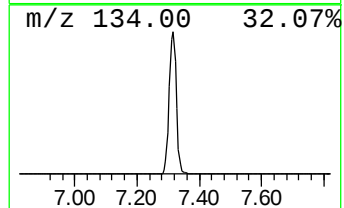
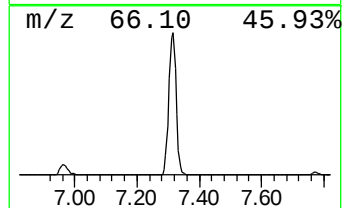
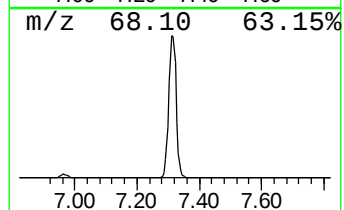
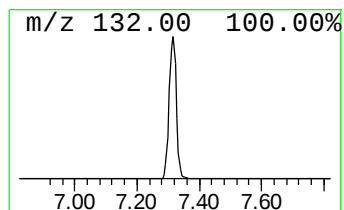
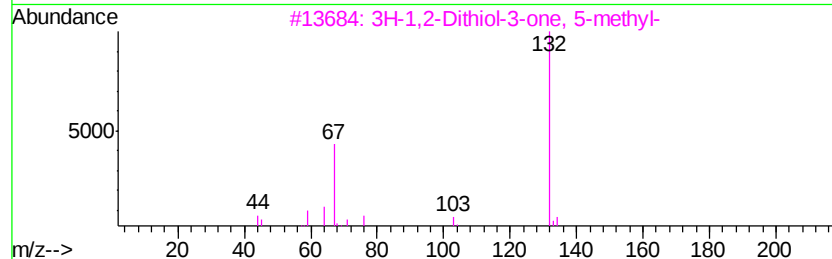
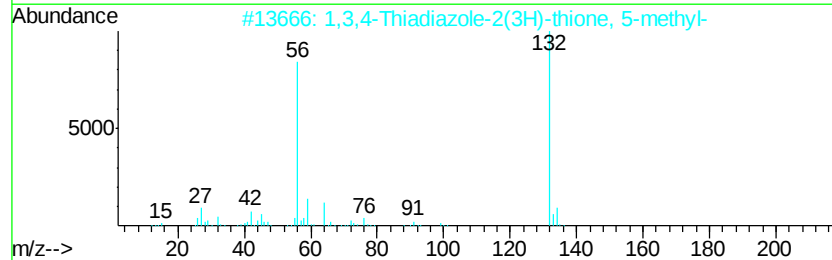
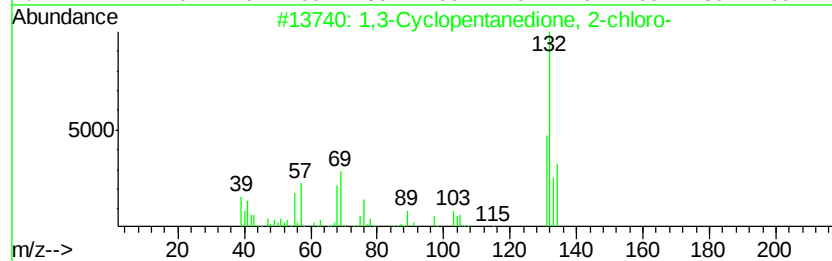
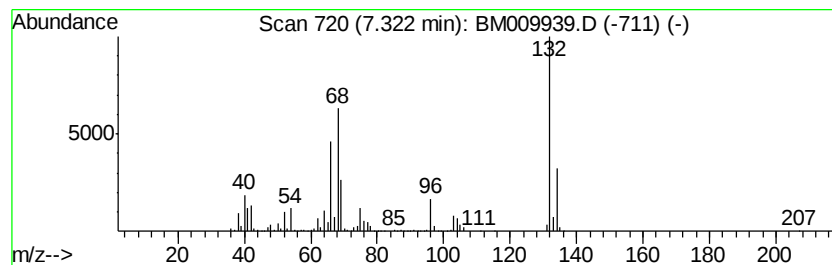
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Peak Number 2 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	104.75 ng	3870200	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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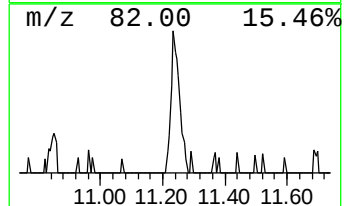
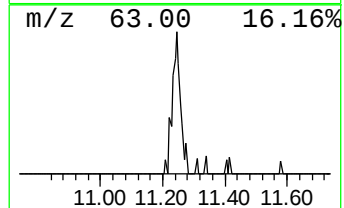
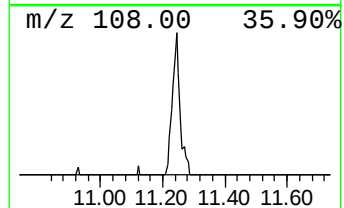
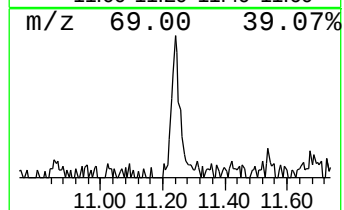
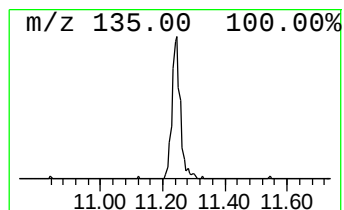
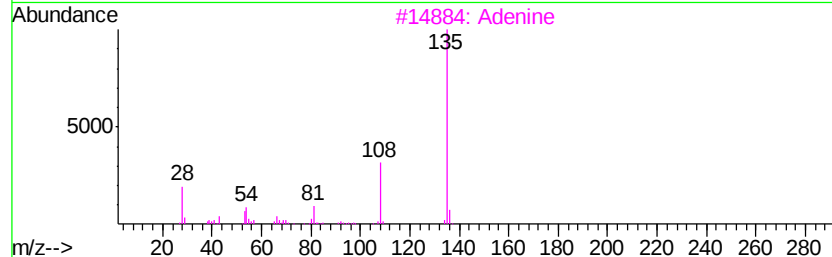
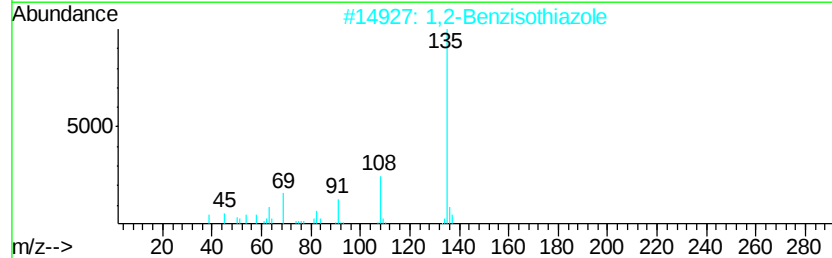
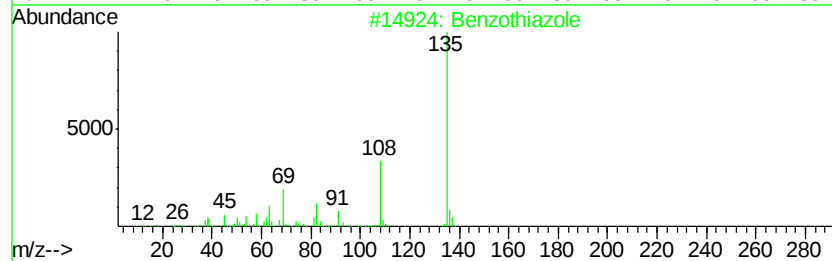
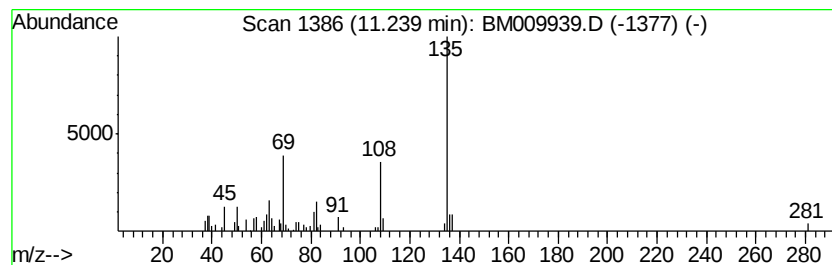
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Peak Number 4 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.59 ng	131574	Naphthalene-d8	10.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	90
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	83
3		Adenine	135	C5H5N5	000073-24-5	72
4		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64
5		5-Fluoro-2-methylbenzonitrile	135	C8H6FN	077532-79-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	7.3	ng	269305	1	7.77	738939	20.0
unknown7.32	7.32	104.8	ng	3870200	1	7.77	738939	20.0
Benzothiazole	11.24	2.6	ng	131574	2	10.57	1014380	20.0