

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083117\
 Data File : BF098209.D
 Acq On : 31 Aug 2017 22:03
 Operator : SJ/JU
 Sample : I4963-13
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3832-PA3-DUP

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-BF081517.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	4.904	475	479	489	rVB	169770	200111	5.16%	0.772%
2	5.328	546	551	554	rBV	1724651	1551110	39.98%	5.982%
3	6.357	722	726	729	rBV	1195983	1017955	26.24%	3.926%
4	6.487	744	748	752	rBV	2649817	2722554	70.18%	10.500%
5	6.716	783	787	791	rBV	954863	775905	20.00%	2.992%
6	6.875	809	814	817	rBV	2897813	2651563	68.35%	10.226%
7	7.287	879	884	887	rBV	2251462	2299936	59.29%	8.870%
8	7.998	1001	1005	1009	rBV	1109126	1041045	26.84%	4.015%
9	8.281	1049	1053	1059	rBV	280488	261833	6.75%	1.010%
10	9.081	1183	1189	1192	rBV	3861517	3879319	100.00%	14.961%
11	9.198	1203	1209	1213	rVB2	36231	47576	1.23%	0.183%
12	9.751	1299	1303	1310	rVB2	1250469	1164255	30.01%	4.490%
13	10.545	1432	1438	1441	rBV	2127826	2184042	56.30%	8.423%
14	10.651	1453	1456	1461	rBV	93175	90670	2.34%	0.350%
15	11.233	1551	1555	1559	rBV	1347466	1175148	30.29%	4.532%
16	11.963	1675	1679	1685	rBV	101383	116534	3.00%	0.449%
17	12.827	1820	1826	1829	rBV	3117657	3359443	86.60%	12.956%
18	13.869	1999	2003	2007	rBV	868088	785521	20.25%	3.029%
19	15.286	2240	2244	2248	rBV	527728	605559	15.61%	2.335%

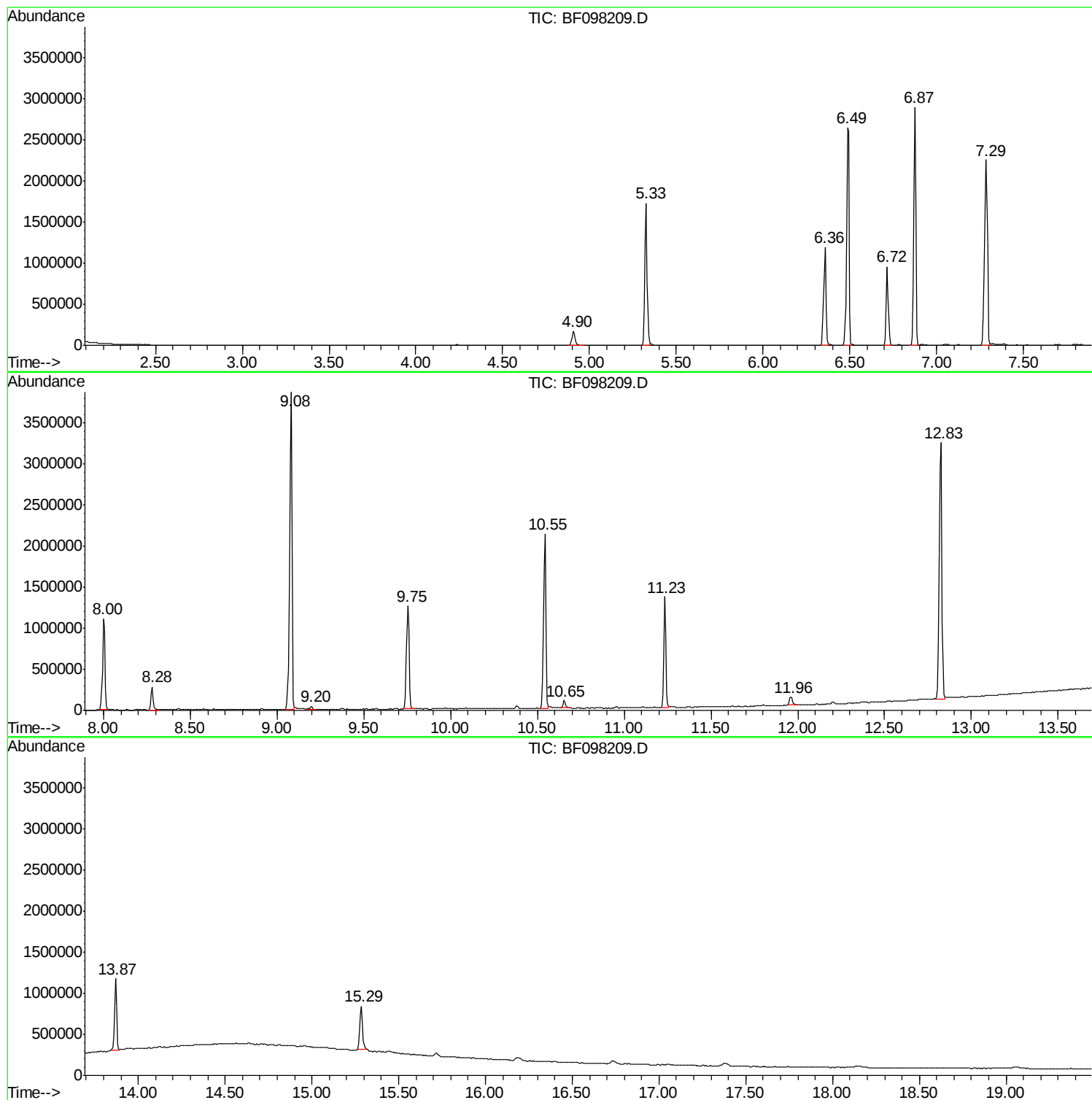
Sum of corrected areas: 25930079

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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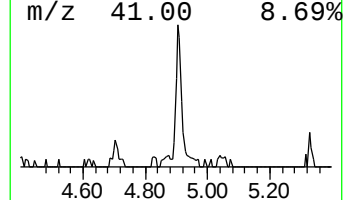
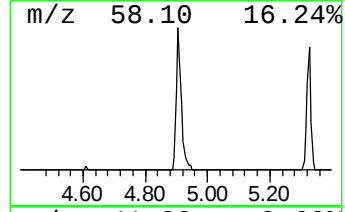
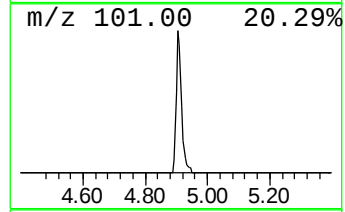
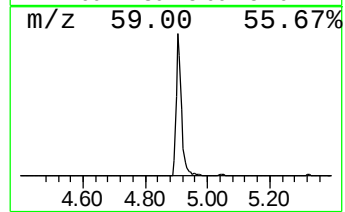
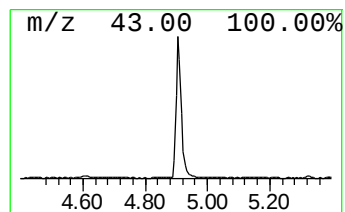
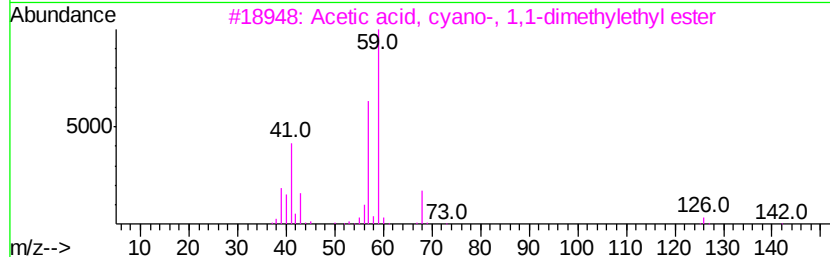
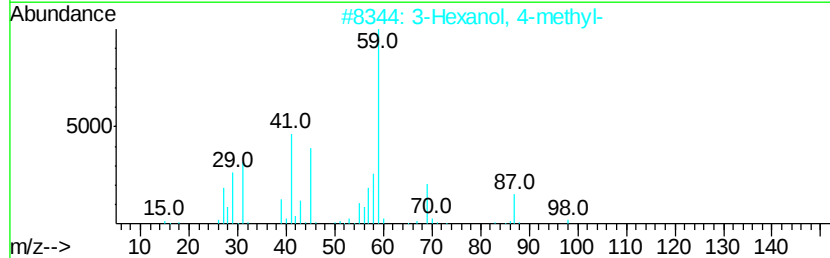
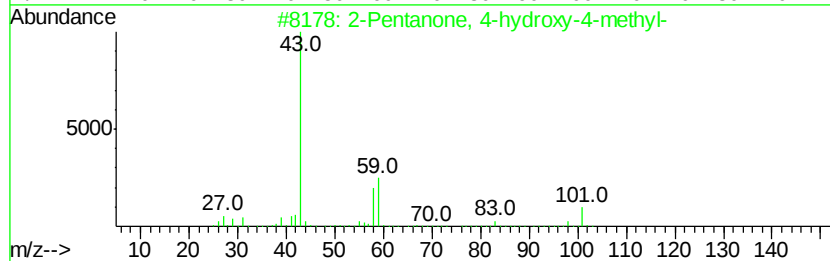
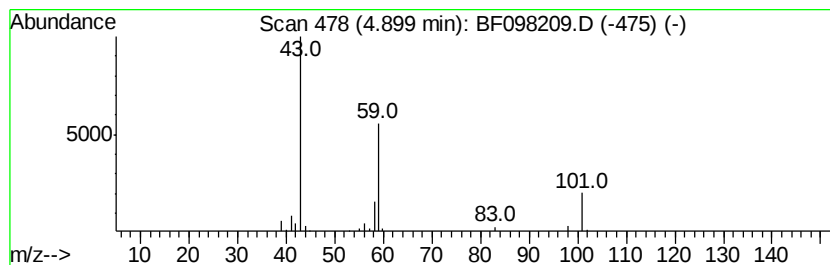
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.90	5.16 ng	200111	1,4-Dichlorobenzene-d4	6.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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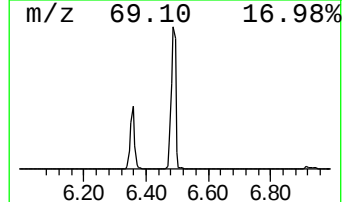
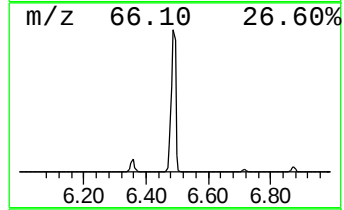
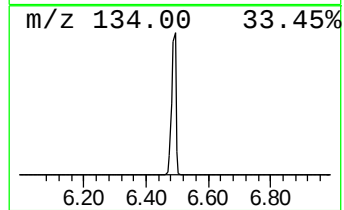
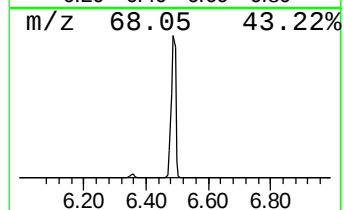
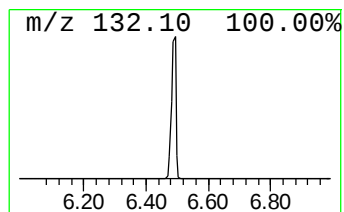
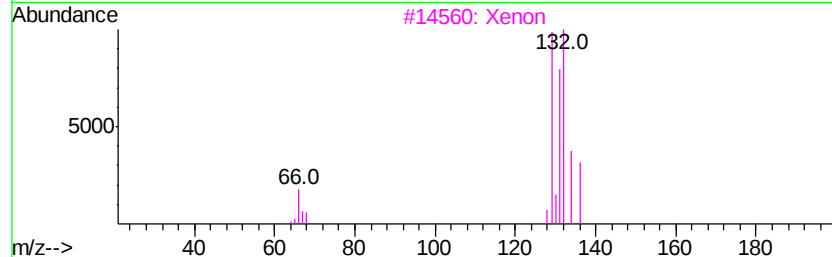
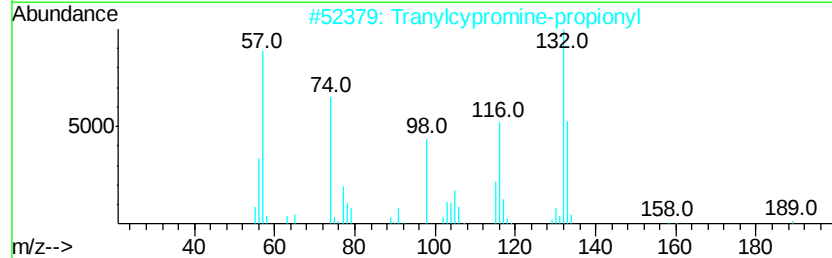
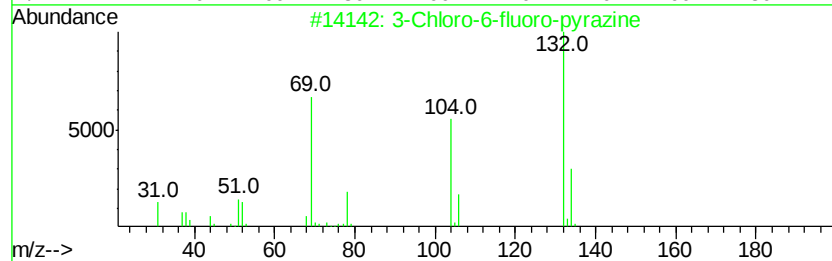
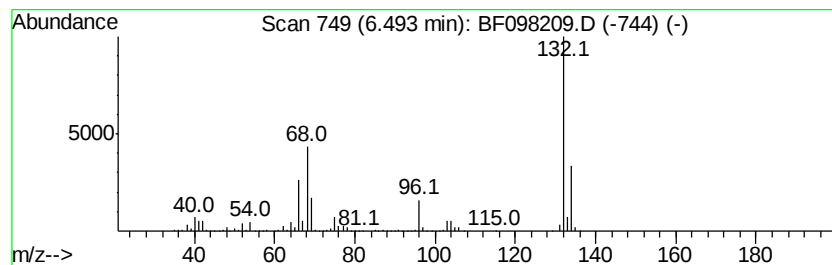
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	70.18 ng	2722550	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Xenon	132	Xe	007440-63-3	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



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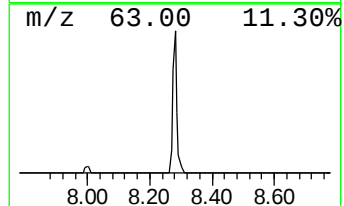
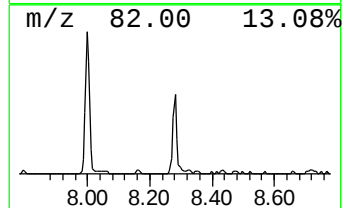
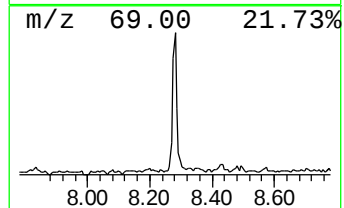
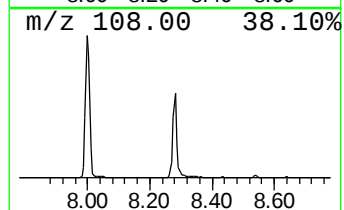
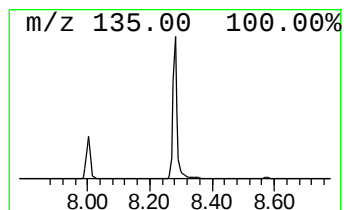
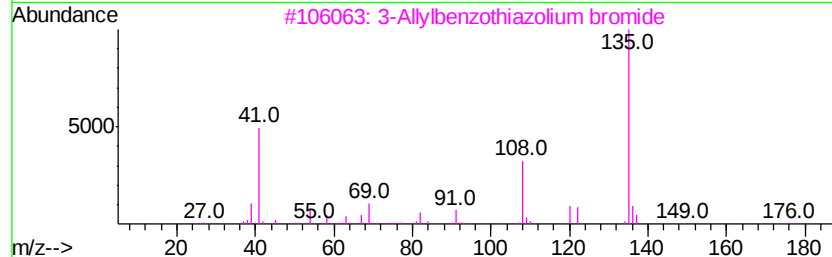
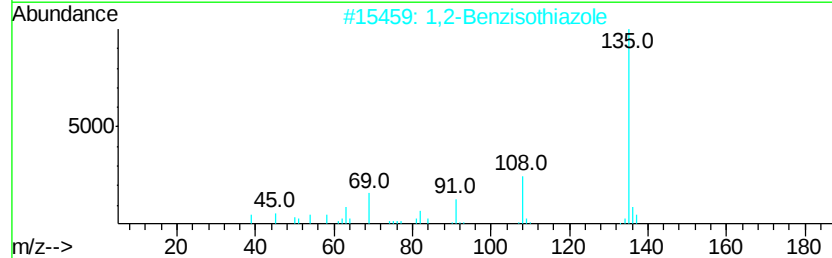
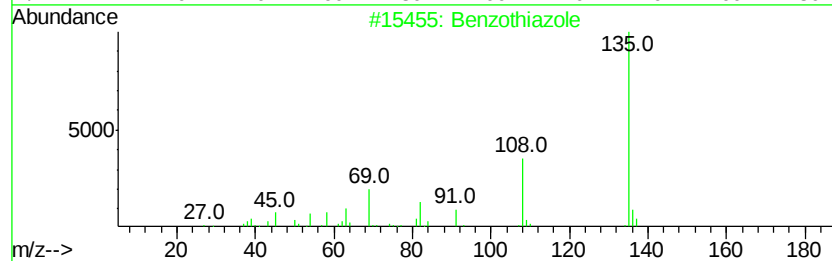
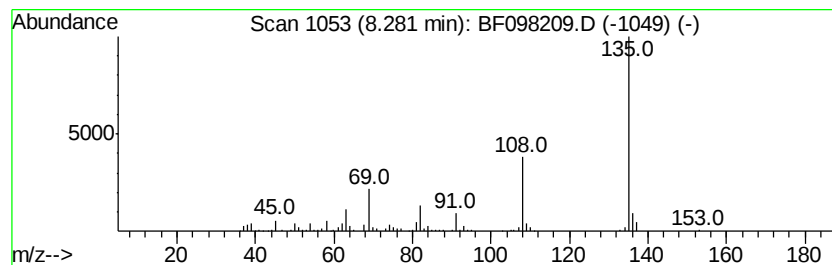
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Peak Number 4 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	5.03 ng	261833	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	97
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59
5		Adenine	135	C5H5N5	000073-24-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	5.2	ng	200111	1	6.72	775905	20.0
unknown6.49	6.49	70.2	ng	2722550	1	6.72	775905	20.0
Benzothiazole	8.28	5.0	ng	261833	2	8.00	1041050	20.0