

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071717\
 Data File : BM010853.D
 Acq On : 18 Jul 2017 02:21
 Operator : SJ/JU
 Sample : I4199-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3561-PP1

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-BM071217.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	4.634	292	297	304	rBV	162912	224806	1.10%	0.230%
2	5.081	366	373	383	rVB	2785430	3872494	19.01%	3.960%
3	6.634	630	637	647	rBV	1679994	2548971	12.51%	2.607%
4	6.981	689	696	704	rBV	5367305	8064715	39.60%	8.248%
5	7.440	767	774	783	rVB	1154764	1790506	8.79%	1.831%
6	7.757	818	828	839	rVB	5089142	7850018	38.54%	8.028%
7	8.587	960	969	979	rBV	4363444	7020525	34.47%	7.180%
8	10.204	1236	1244	1252	rVB	1450762	2420357	11.88%	2.475%
9	10.845	1346	1353	1361	rBV	371745	592078	2.91%	0.606%
10	12.704	1662	1669	1681	rBV	10751499	15800660	77.58%	16.159%
11	14.092	1898	1905	1914	rBV3	2062836	3141379	15.42%	3.213%
12	15.592	2153	2160	2171	rBV	8832217	11902996	58.44%	12.173%
13	16.845	2365	2373	2380	rBV2	2529729	3540770	17.38%	3.621%
14	17.768	2525	2530	2536	rBV2	192036	255060	1.25%	0.261%
15	19.068	2747	2751	2756	rBV	250663	331682	1.63%	0.339%
16	19.509	2820	2826	2835	rBV	16714623	20367968	100.00%	20.830%
17	21.003	3077	3080	3085	rVB	573074	638330	3.13%	0.653%
18	21.062	3085	3090	3095	rBV	3146310	3858207	18.94%	3.946%
19	23.192	3446	3452	3458	rVB	2034514	3558969	17.47%	3.640%

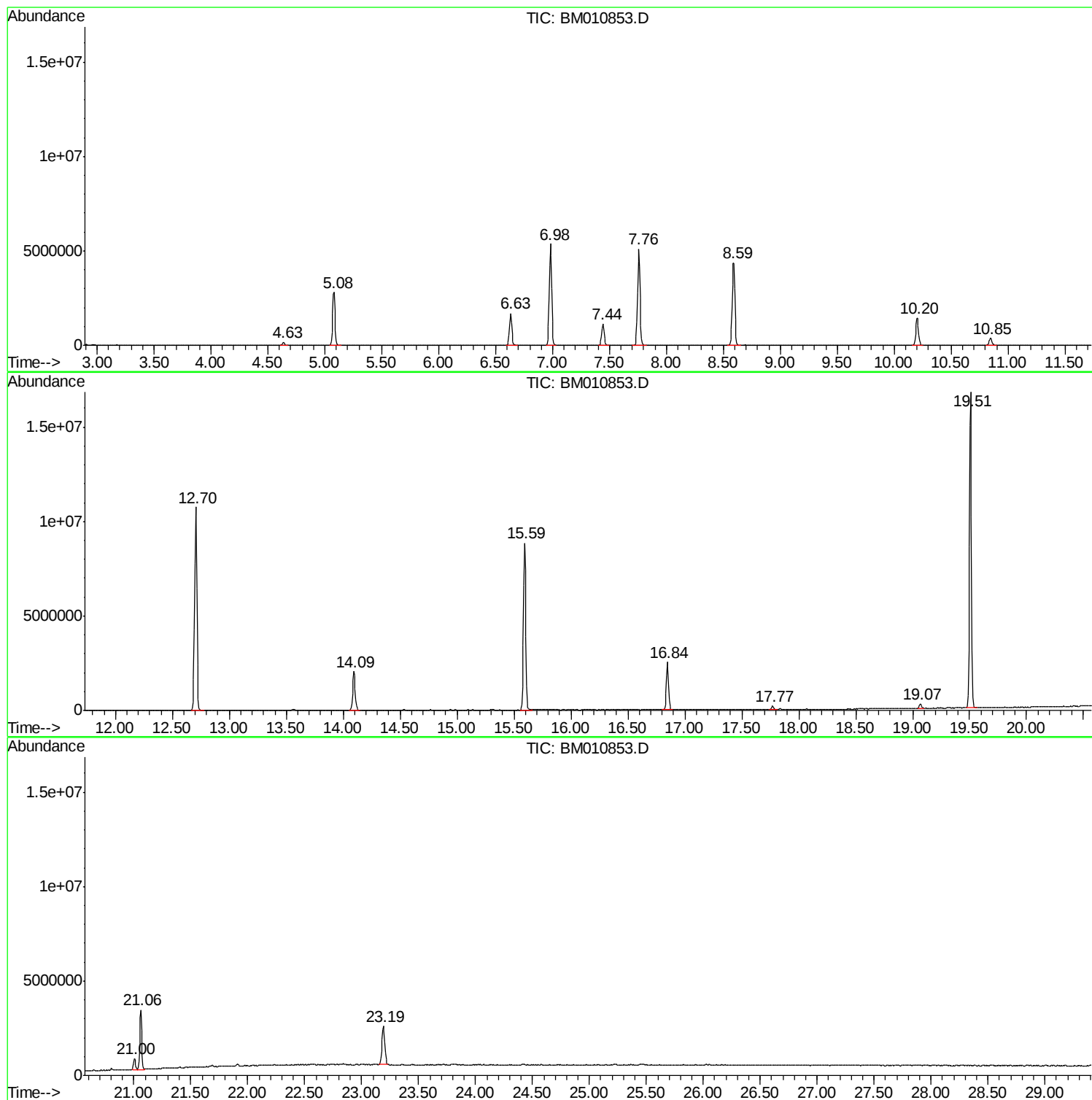
Sum of corrected areas: 97780491

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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.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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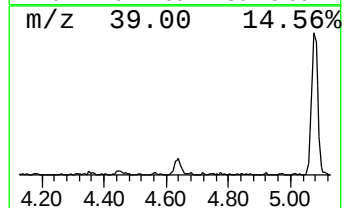
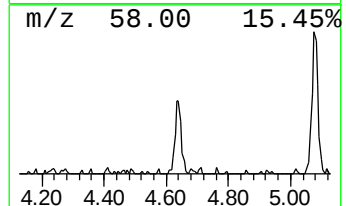
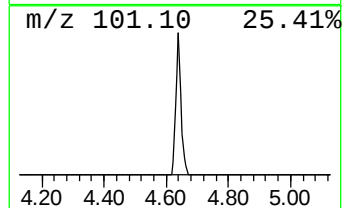
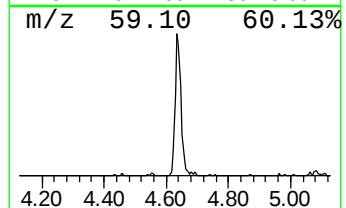
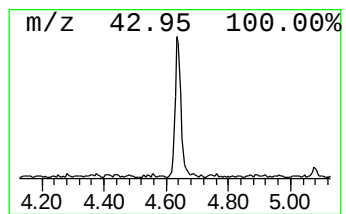
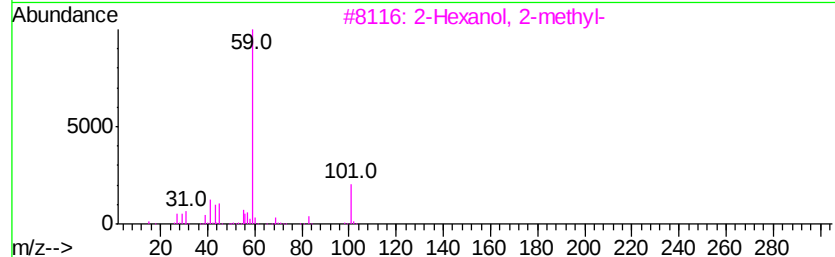
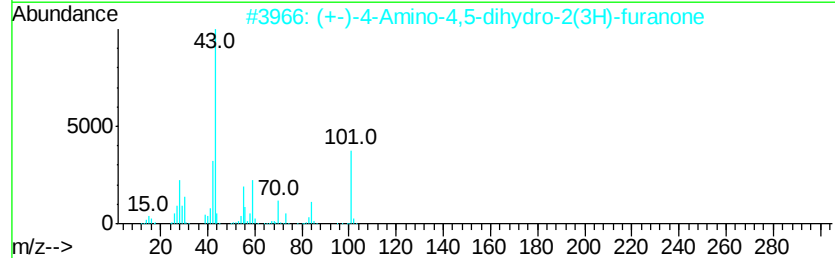
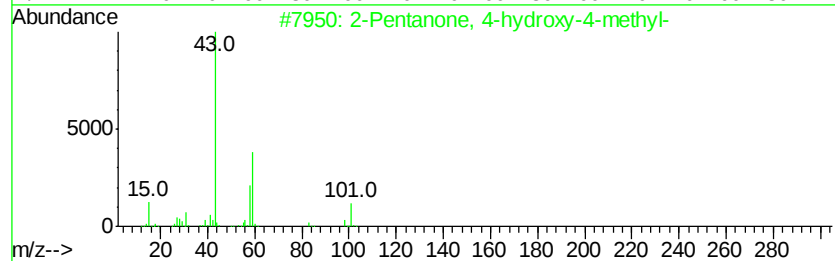
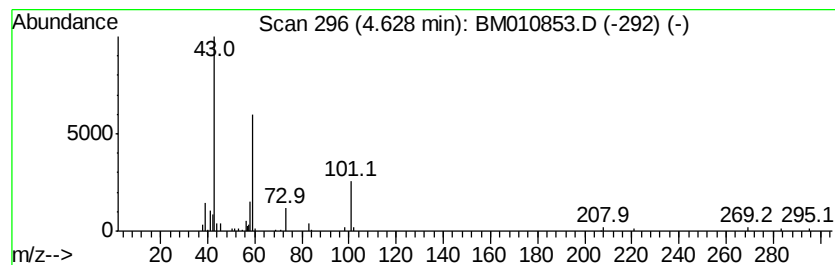
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	2.51 ng	224806	1,4-Dichlorobenzene-d4	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	28
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			1,3-Dioxolane-2-methanol, 2,4-dihydro-	132	C6H12O3	053951-43-2	25
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16



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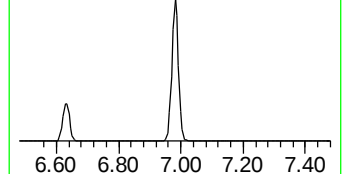
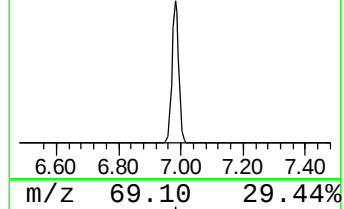
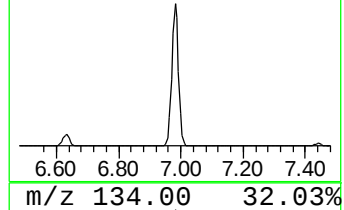
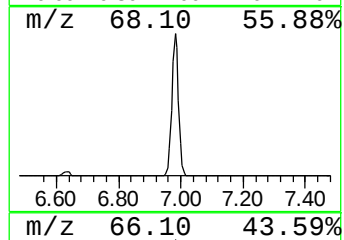
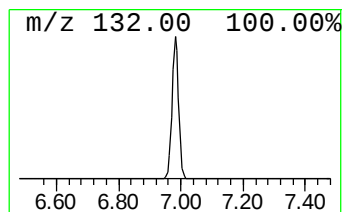
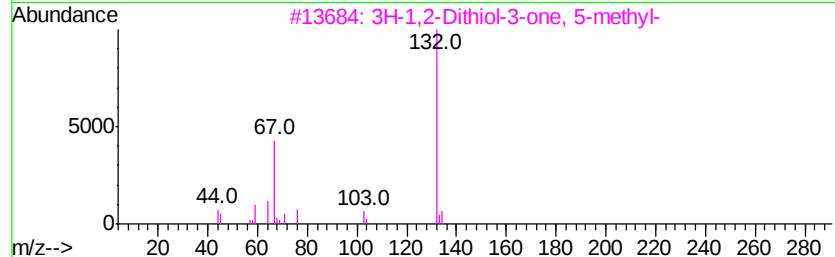
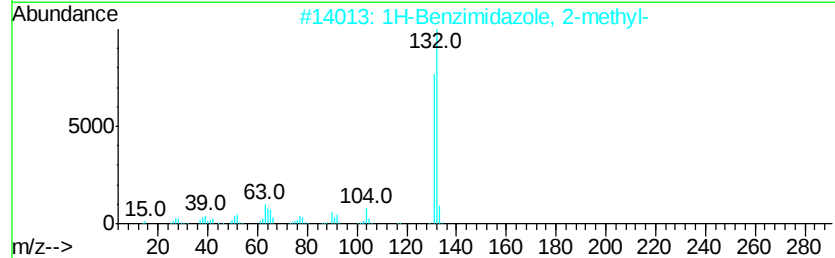
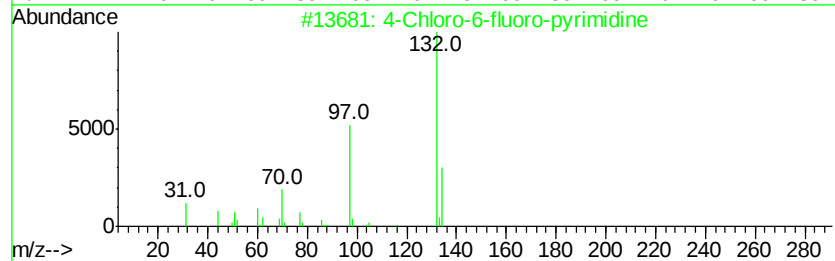
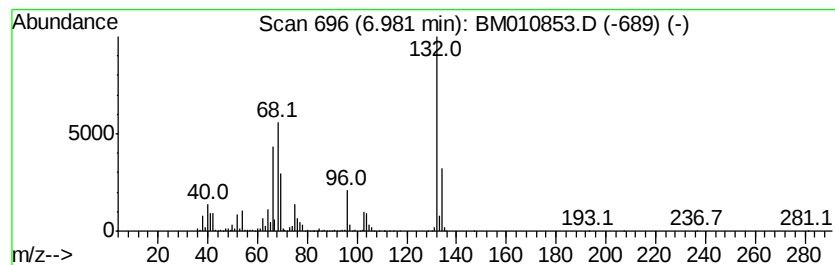
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	90.08 ng	8064720	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10



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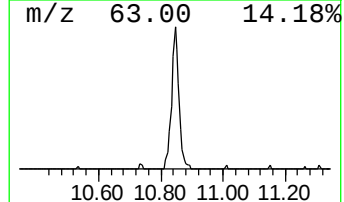
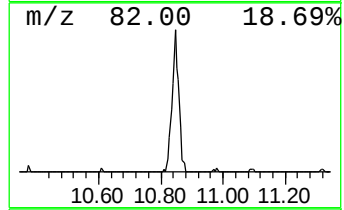
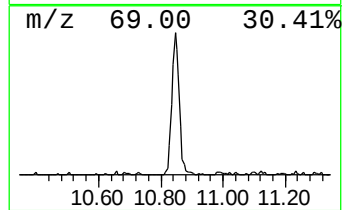
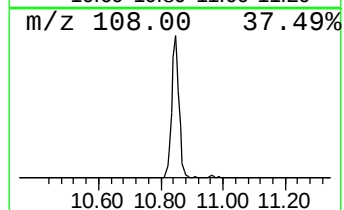
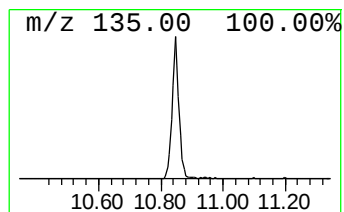
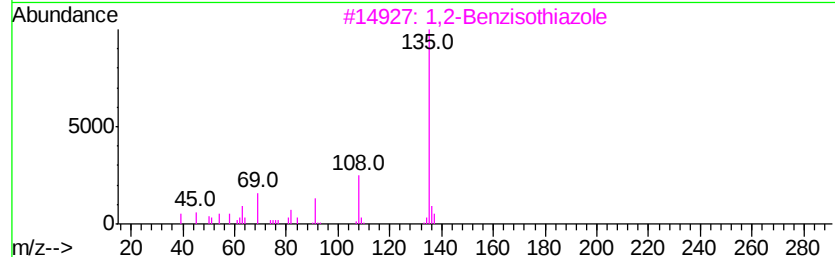
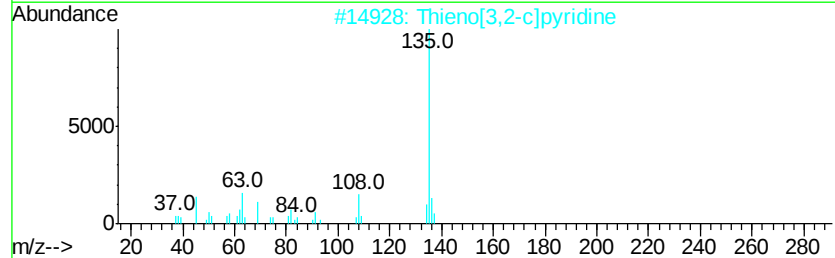
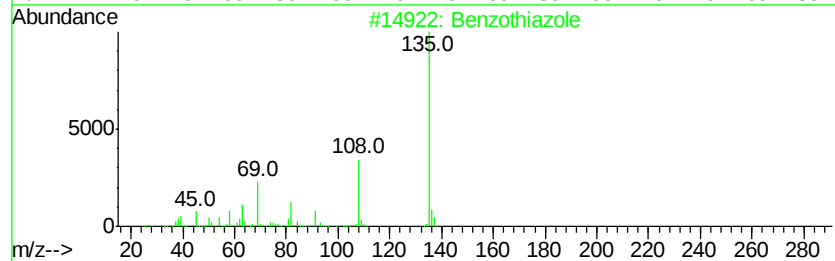
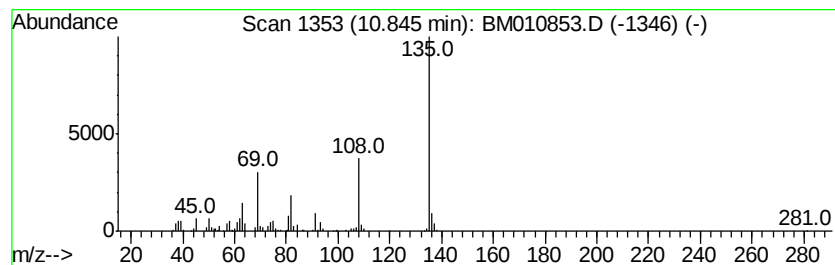
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Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	4.89 ng	592078	Naphthalene-d8	10.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	93
2		Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	87
3		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	72
4		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	53
5		Adenine	135	C5H5N5	000073-24-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	2.5	ng	224806	1	7.44	1790510	20.0
unknown6.98	6.98	90.1	ng	8064720	1	7.44	1790510	20.0
Benzothiazole	10.85	4.9	ng	592078	2	10.20	2420360	20.0