

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071717\
 Data File : BM010860.D
 Acq On : 18 Jul 2017 06:32
 Operator : SJ/JU
 Sample : I4199-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3568-SPP3

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	4.640	293	298	305	rVB	192299	273153	1.12%	0.234%
2	5.081	367	373	386	rBV	3083397	4176634	17.12%	3.572%
3	6.634	630	637	646	rVB	1844680	2746536	11.26%	2.349%
4	6.981	689	696	706	rBV	5654032	8743687	35.83%	7.478%
5	7.440	767	774	783	rVB	1361557	2089981	8.56%	1.787%
6	7.757	820	828	836	rVB	5447125	8404816	34.44%	7.188%
7	8.593	961	970	979	rBV	4781110	7648368	31.34%	6.541%
8	10.204	1236	1244	1253	rBV	1778853	2950692	12.09%	2.524%
9	10.845	1344	1353	1362	rBV	1978519	3368831	13.81%	2.881%
10	12.704	1657	1669	1676	rBV	11946527	17669583	72.41%	15.112%
11	14.092	1898	1905	1915	rBV2	2620342	3924360	16.08%	3.356%
12	15.310	2106	2112	2120	rBV2	254998	385194	1.58%	0.329%
13	15.592	2154	2160	2169	rBV	10057138	14133403	57.92%	12.088%
14	16.845	2367	2373	2384	rVB2	3195435	4619213	18.93%	3.951%
15	18.080	2578	2583	2591	rBV2	366266	604183	2.48%	0.517%
16	19.068	2747	2751	2757	rBV2	240161	275889	1.13%	0.236%
17	19.510	2820	2826	2831	rBV	20200291	24402750	100.00%	20.871%
18	21.004	3076	3080	3085	rBV	1244206	1407334	5.77%	1.204%
19	21.062	3085	3090	3098	rVV	3959746	4711434	19.31%	4.030%
20	21.909	3231	3234	3239	rVB4	227565	297936	1.22%	0.255%
21	23.192	3446	3452	3460	rVB2	2350426	4088545	16.75%	3.497%

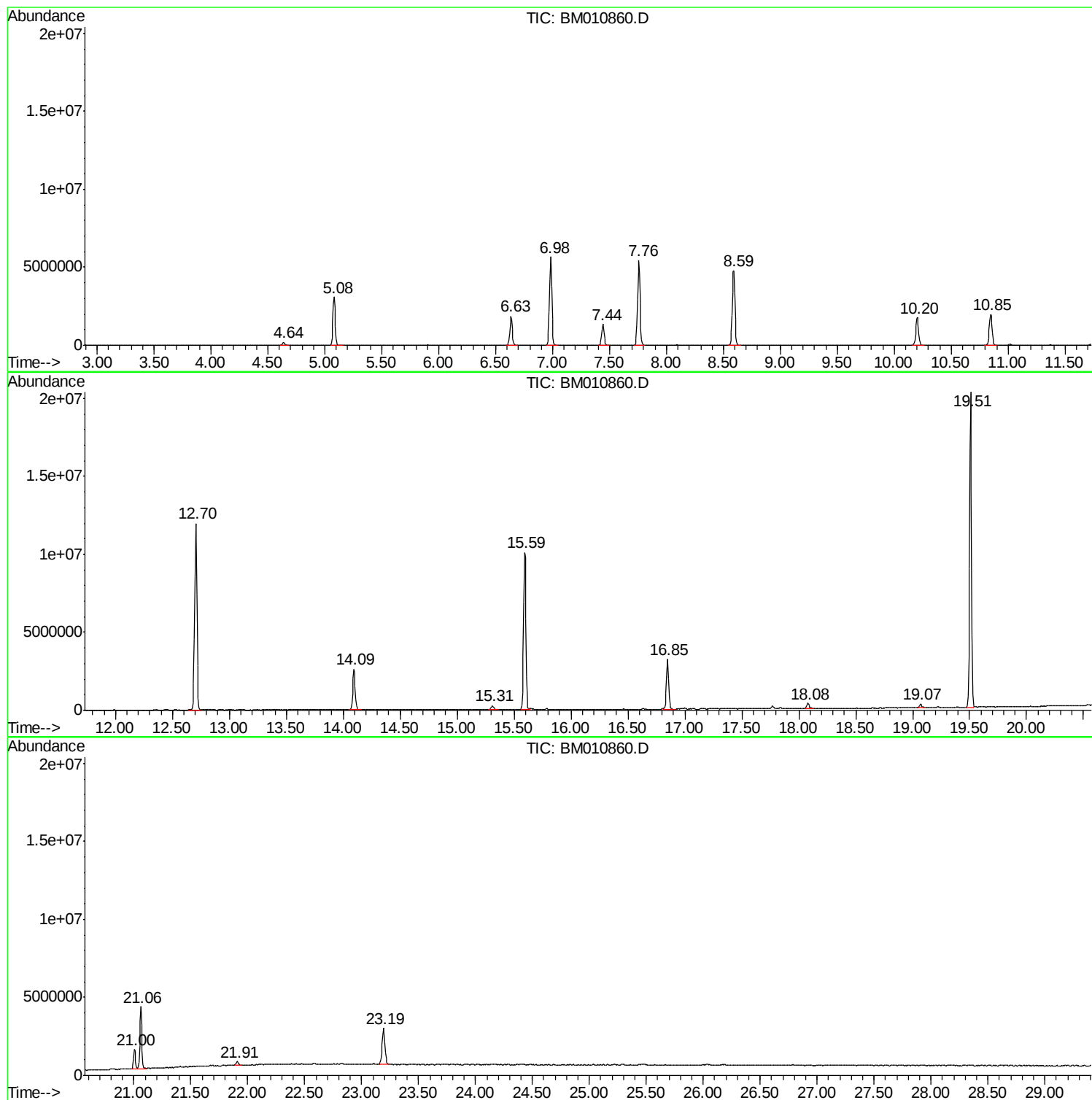
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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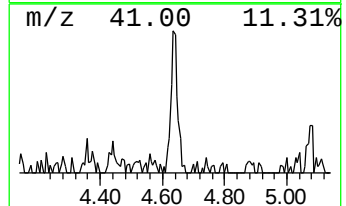
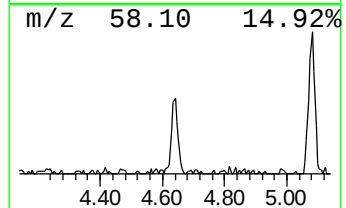
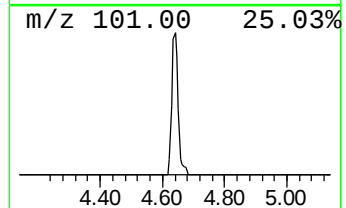
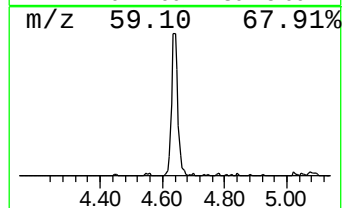
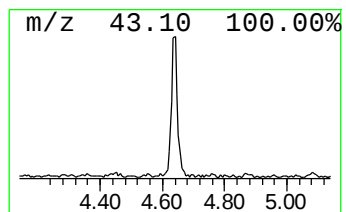
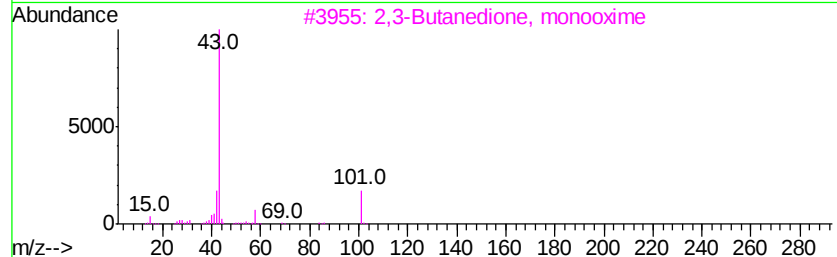
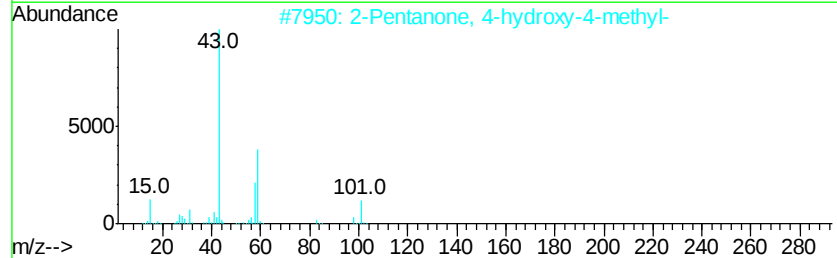
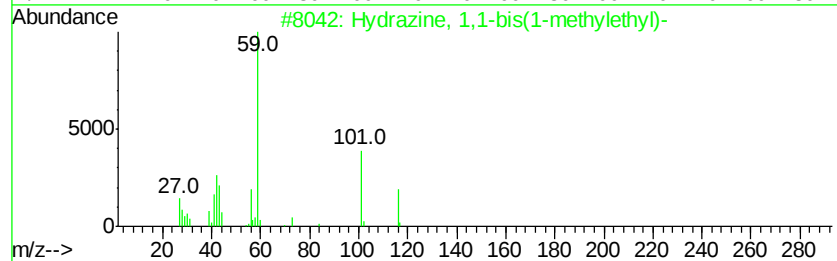
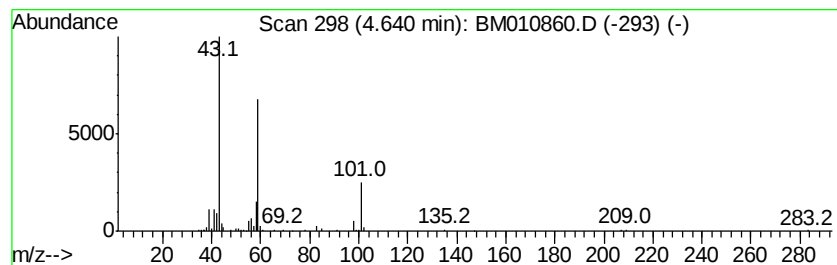
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hydrazine, 1,1-bis(1-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	2.61 ng	273153	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	32
5		Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	32



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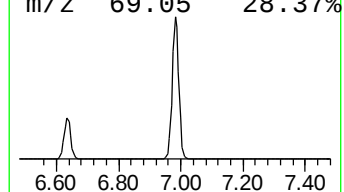
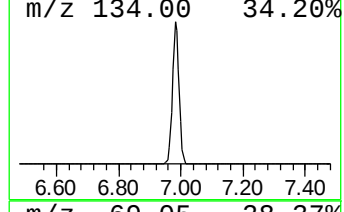
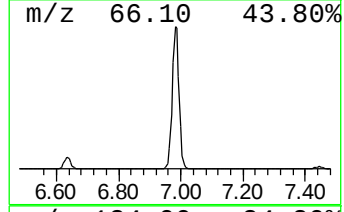
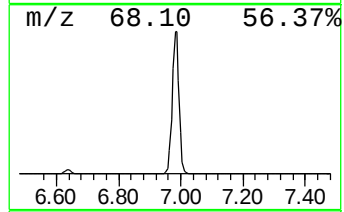
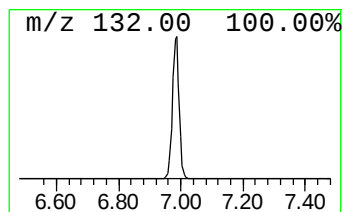
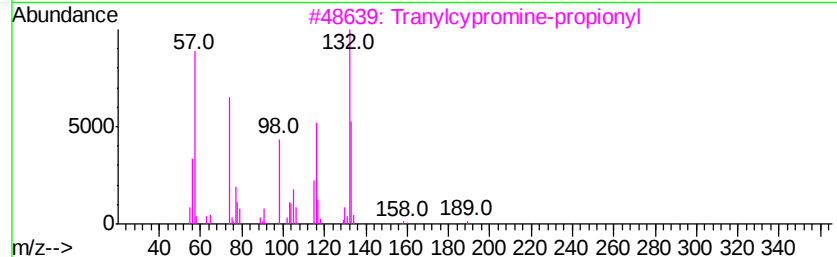
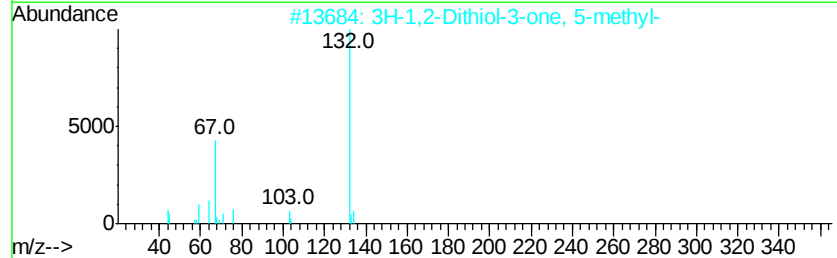
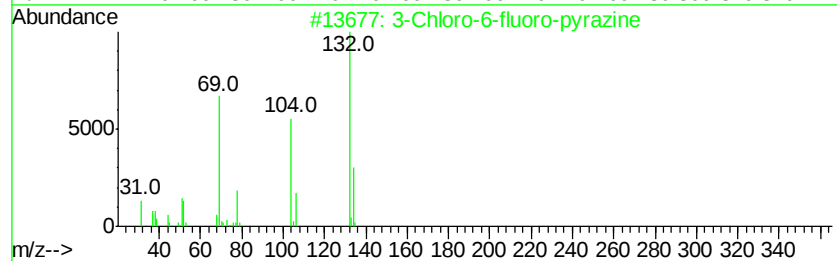
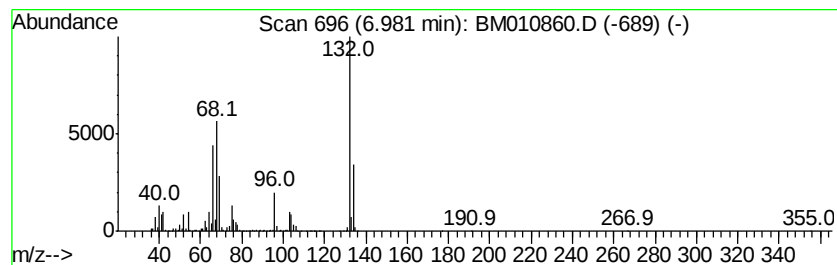
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	83.67 ng	8743690	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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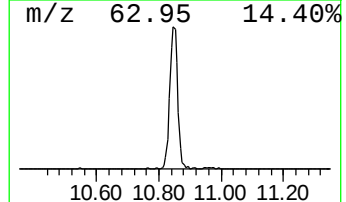
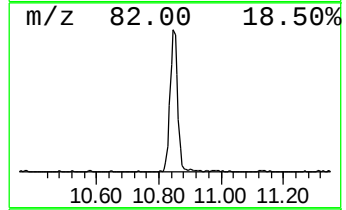
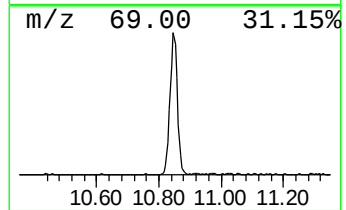
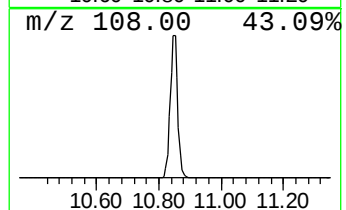
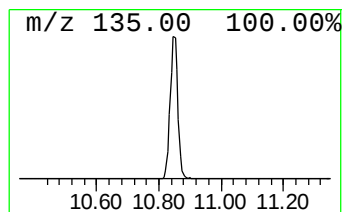
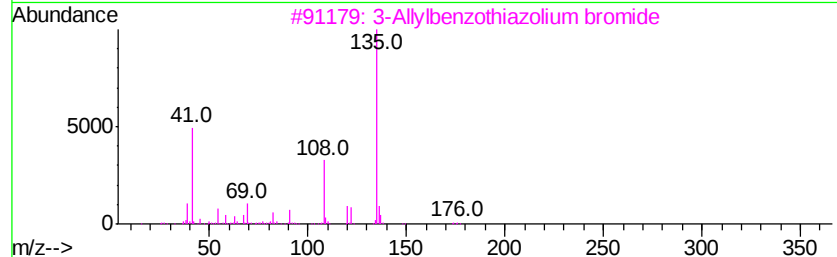
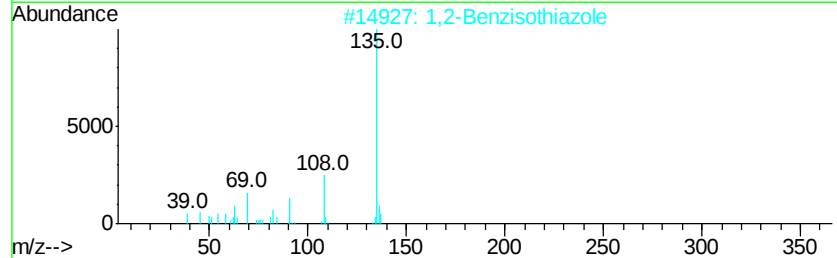
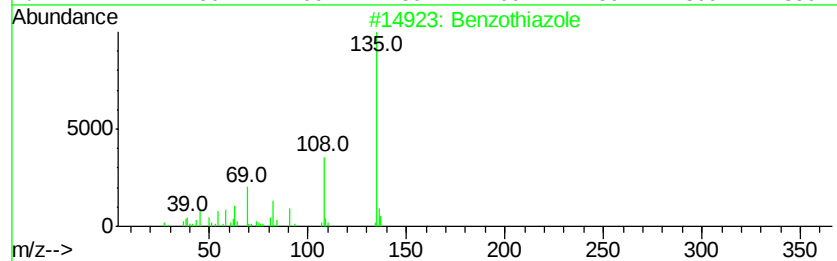
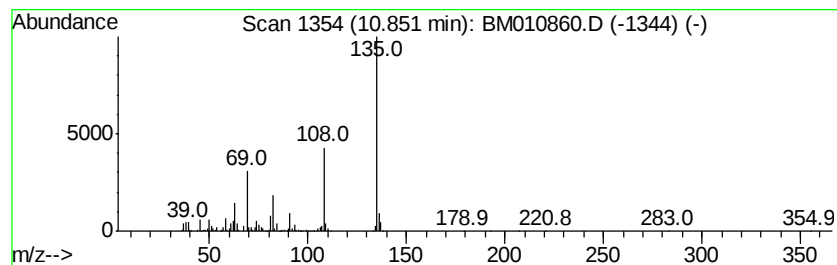
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Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	22.83 ng	3368830	Napthalene-d8	10.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzothiazole	135 C7H5NS	000095-16-9 97
2		1,2-Benzisothiazole	135 C7H5NS	000272-16-2 83
3		3-Allylbenzothiazolium bromide	255 C10H10BrNS	016407-55-9 78
4		Adenine	135 C5H5N5	000073-24-5 53
5		Thieno[2,3-c]pyridine	135 C7H5NS	000272-12-8 53



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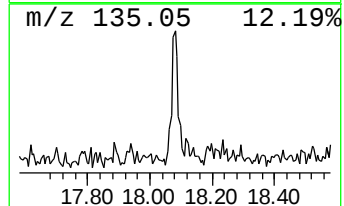
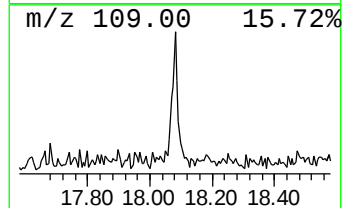
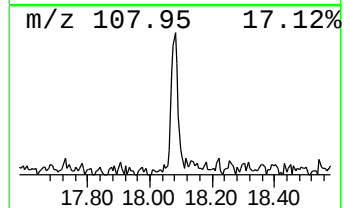
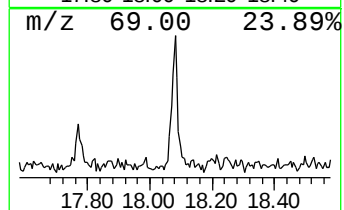
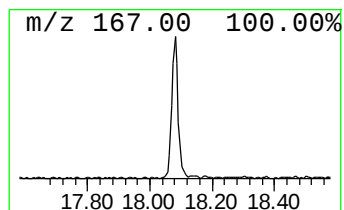
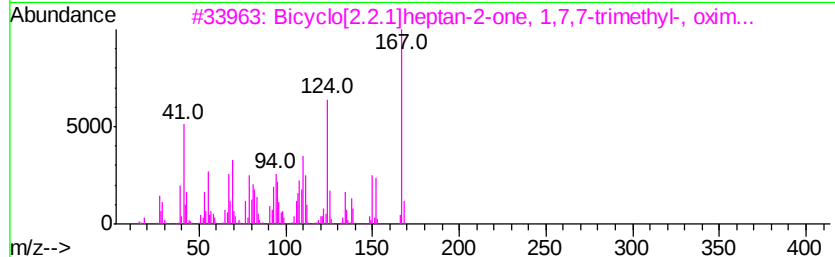
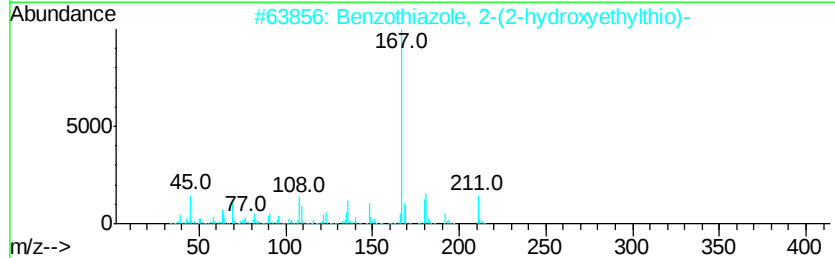
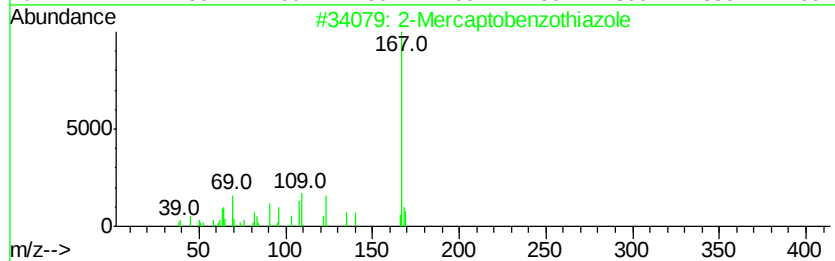
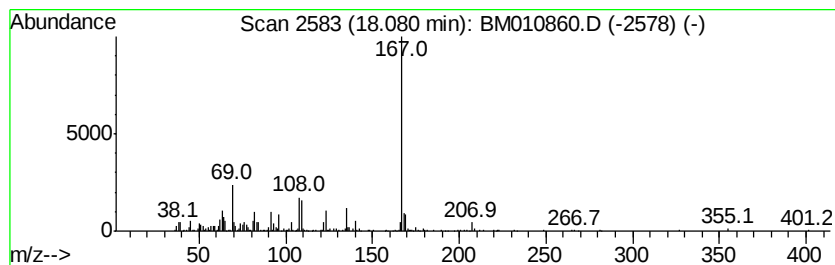
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Peak Number 5 2-Mercaptobenzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	2.62 ng	604183	Phenanthrene-d10	16.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	95
2		Benzo[thiazole, 2-(2-hydroxyethyl)...	211	C9H9NOS2	004665-63-8	64
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	167	C10H17NO	018674-50-5	59
4		Thioquanine	167	C5H5N5S	000154-42-7	53
5		1,3-Di(2-benzothiazolyl)-1,3-bis...	418	C17H14N4OS4	064216-20-2	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hydrazine, 1,1-bi...	4.64	2.6	ng	273153	1	7.44	2089980	20.0
unknown6.98	6.98	83.7	ng	8743690	1	7.44	2089980	20.0
Benzothiazole	10.85	22.8	ng	3368830	2	10.20	2950690	20.0
2-Mercaptobenzoth...	18.08	2.6	ng	604183	4	16.85	4619210	20.0