

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071717\
 Data File : BM010858.D
 Acq On : 18 Jul 2017 05:20
 Operator : SJ/JU
 Sample : I4199-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3566-SPP1

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	5.081	366	373	382	rBV	3097159	4218388	16.39%	3.592%
2	6.634	631	637	646	rBV	1906245	2841307	11.04%	2.419%
3	6.981	689	696	708	rVB	5780219	8889699	34.55%	7.570%
4	7.440	768	774	783	rVB	1310081	2038500	7.92%	1.736%
5	7.757	821	828	837	rBV	5403216	8271428	32.14%	7.043%
6	8.592	962	970	978	rBV	4689689	7574272	29.43%	6.450%
7	10.204	1235	1244	1251	rBV	1763610	2871884	11.16%	2.445%
8	10.845	1345	1353	1363	rBV	1772090	3070259	11.93%	2.614%
9	12.704	1663	1669	1677	rVB	12432041	18060419	70.19%	15.379%
10	14.092	1898	1905	1915	rBV2	2527854	3842844	14.93%	3.272%
11	15.592	2153	2160	2169	rBV	10735101	15396138	59.83%	13.110%
12	15.786	2188	2193	2202	rVB	437703	652435	2.54%	0.556%
13	16.845	2367	2373	2381	rVB2	3094502	4436874	17.24%	3.778%
14	18.080	2578	2583	2592	rBV2	362365	563615	2.19%	0.480%
15	19.509	2820	2826	2831	rBV	21624887	25732572	100.00%	21.912%
16	21.062	3085	3090	3095	rVV	3894592	4662641	18.12%	3.970%
17	21.909	3231	3234	3239	rVB3	306059	342190	1.33%	0.291%
18	23.191	3446	3452	3460	rVB2	2224890	3972796	15.44%	3.383%

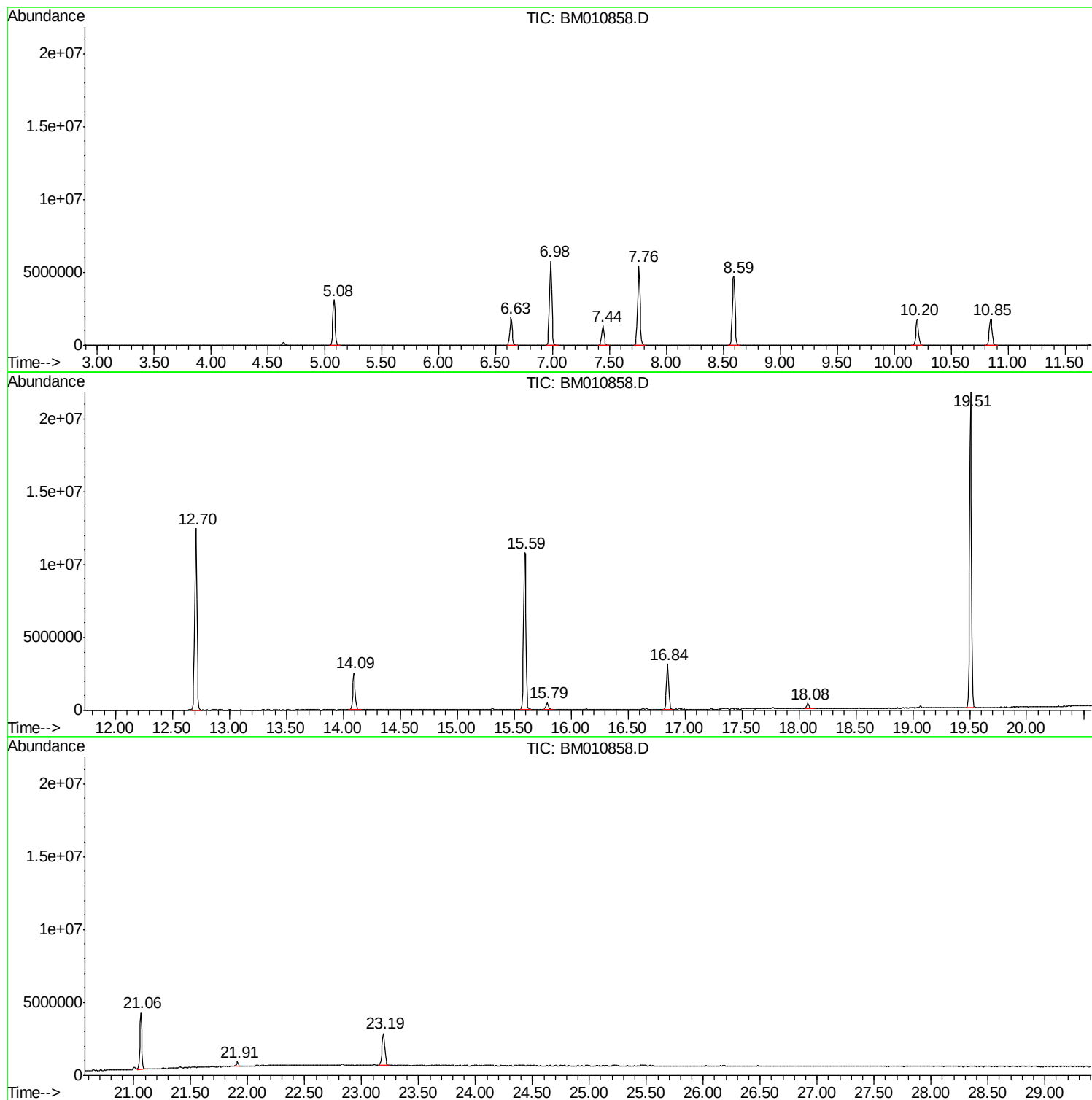
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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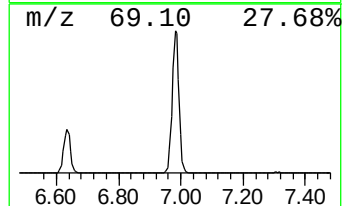
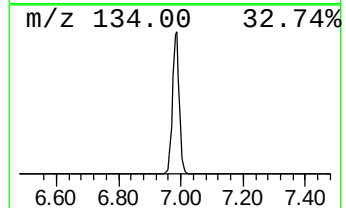
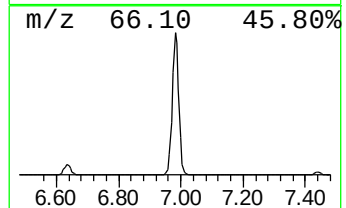
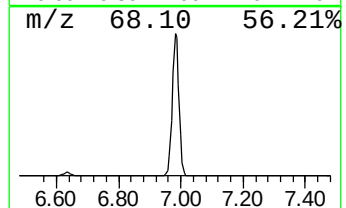
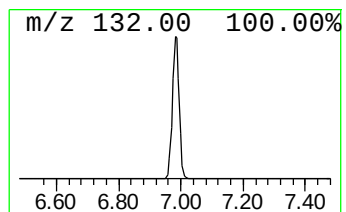
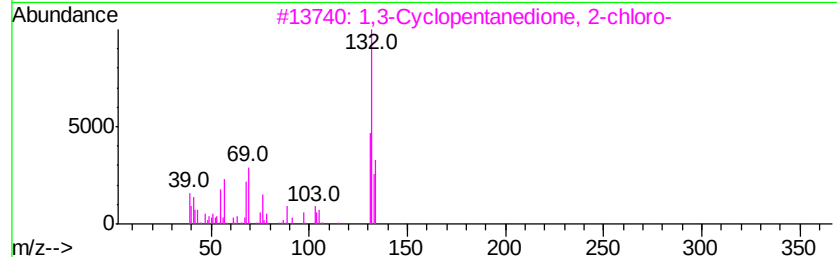
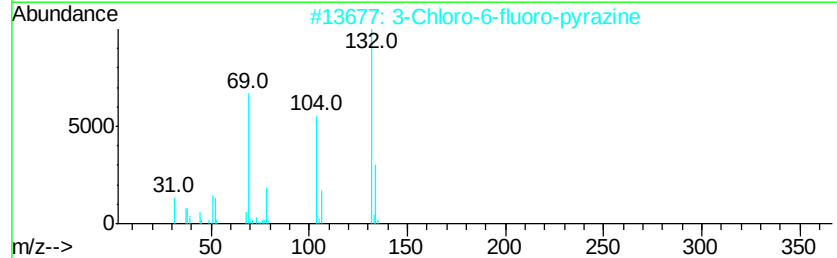
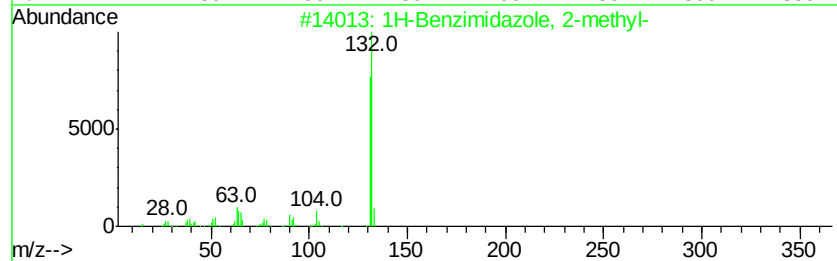
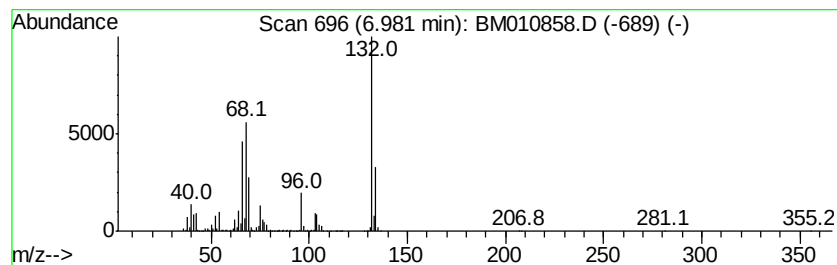
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	87.22 ng	8889700	1,4-Dichlorobenzene-d4	7.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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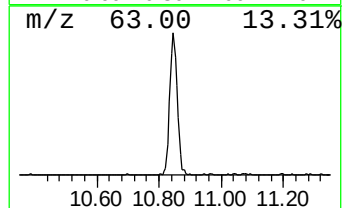
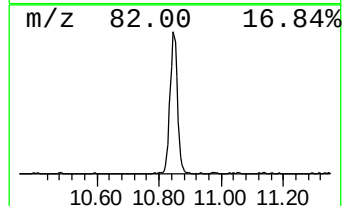
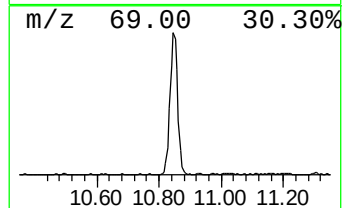
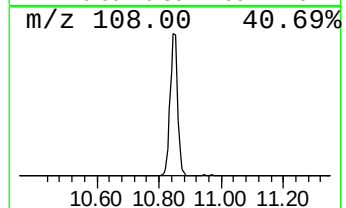
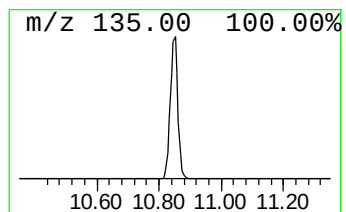
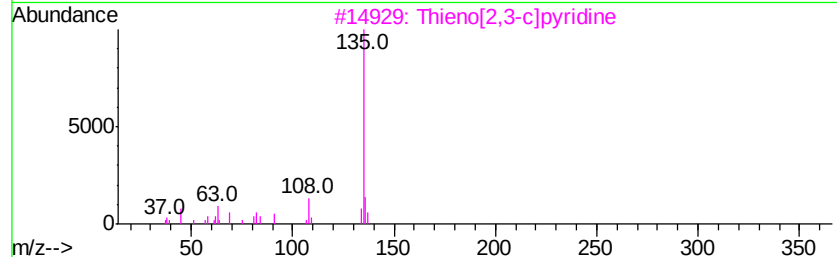
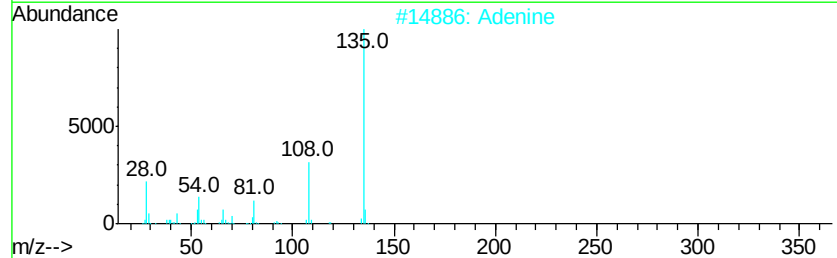
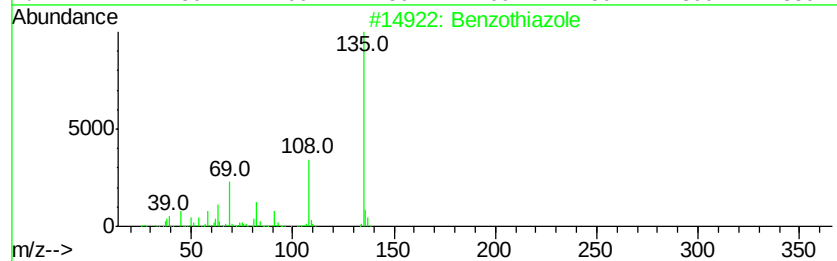
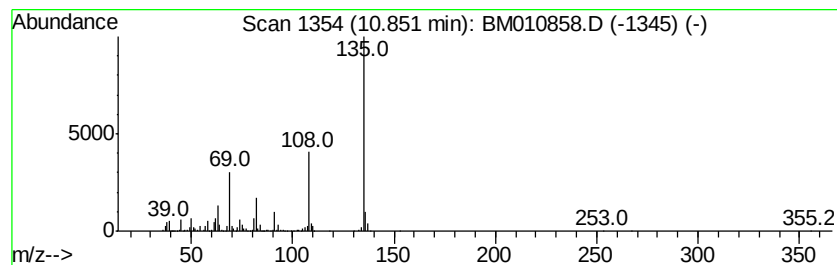
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Peak Number 3 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	21.38 ng	3070260	Napthalene-d8	10.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzothiazole	135 C7H5NS	000095-16-9 96
2		Adenine	135 C5H5N5	000073-24-5 64
3		Thieno[2,3-c]pyridine	135 C7H5NS	000272-12-8 64
4		1,2-Benzisothiazole	135 C7H5NS	000272-16-2 64
5		3-Allylbenzothiazolium bromide	255 C10H10BrNS	016407-55-9 56



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Instrument :
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ClientSampled :
3566-SPP1

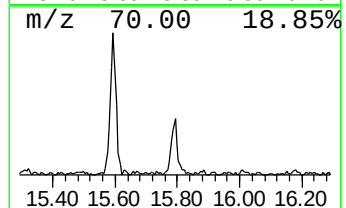
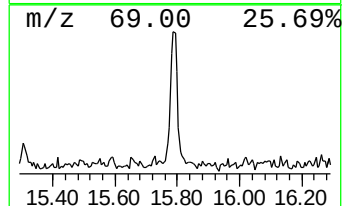
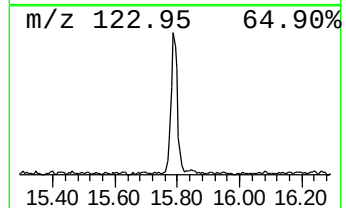
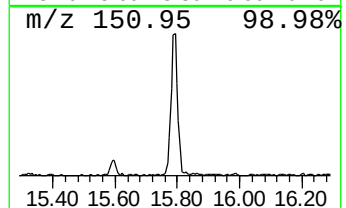
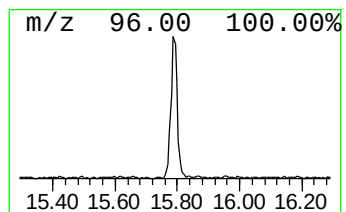
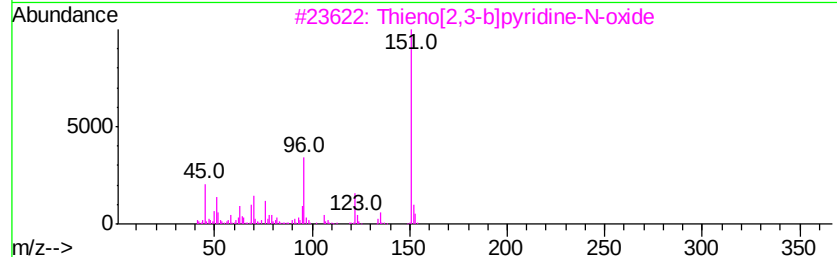
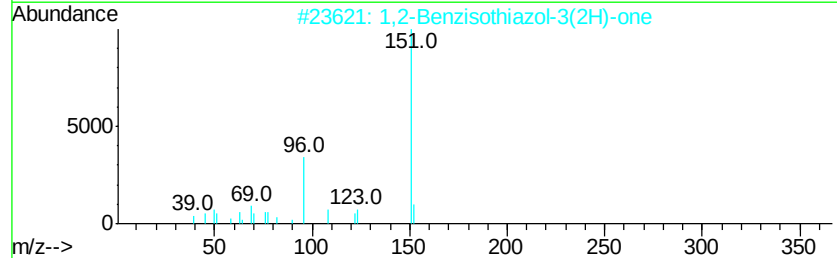
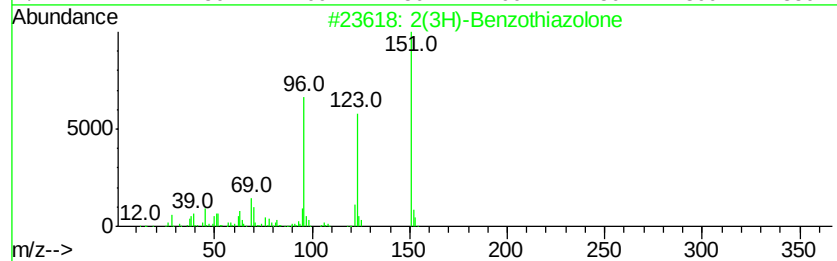
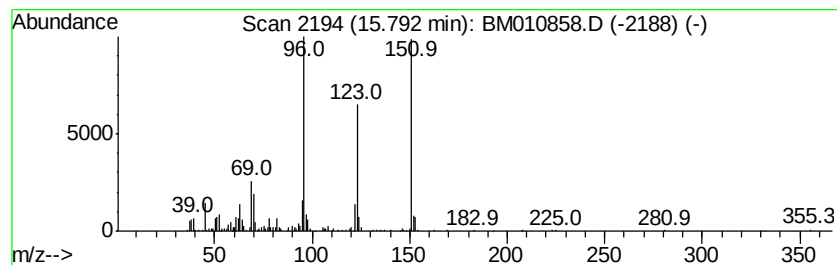
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Peak Number 4 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.94 ng	652435	Phenanthrene-d10	16.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	64
3		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	46
4		4-Methoxyformanilide	151	C8H9NO2	023896-88-0	35
5		5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	30



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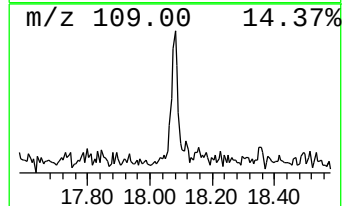
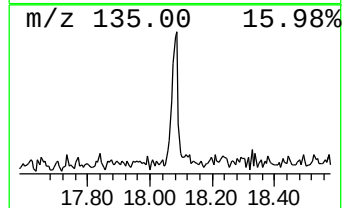
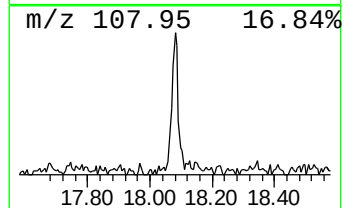
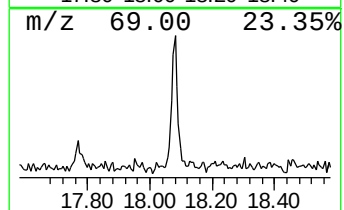
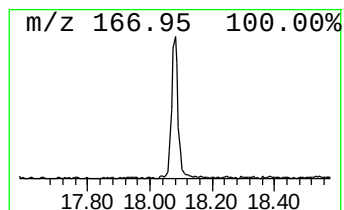
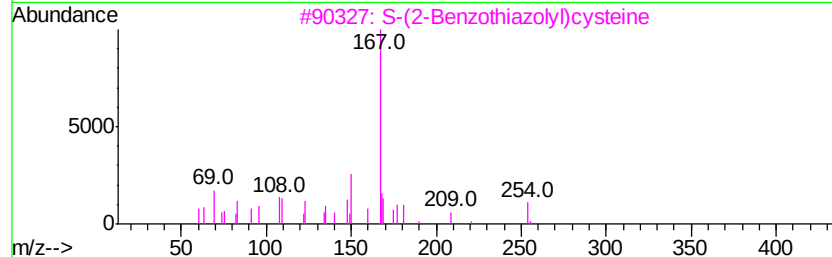
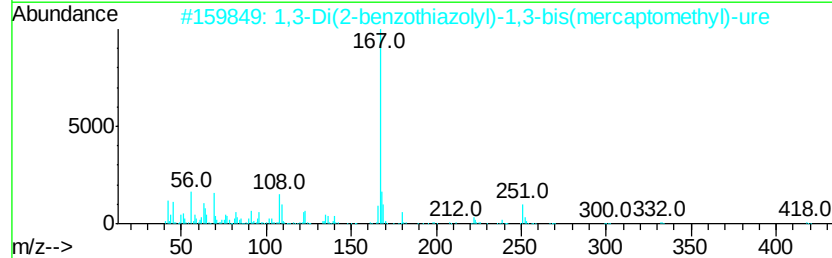
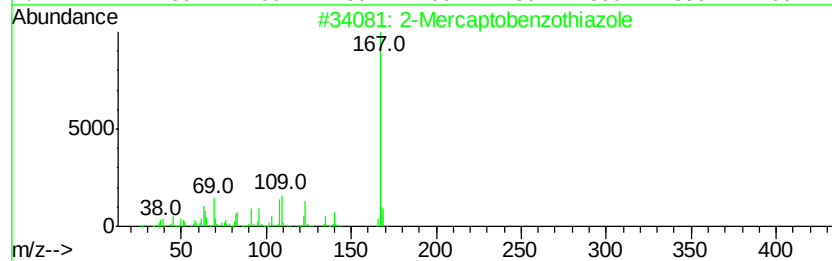
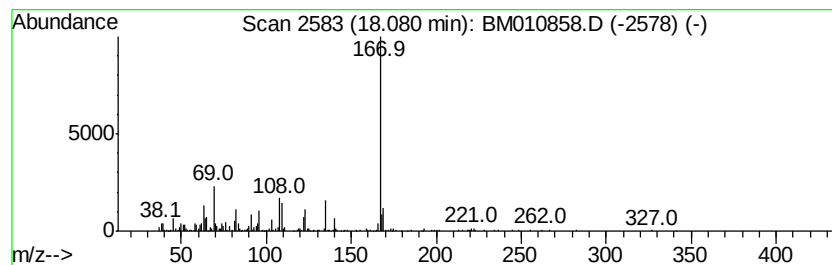
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Peak Number 5 2-Mercaptobenzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	2.54 ng	563615	Phenanthrene-d10	16.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2		1,3-Di(2-benzothiazolyl)-1,3-bis...	418	C17H14N4OS4	064216-20-2	80
3		S-(2-Benzothiazolyl)cysteine	254	C10H10N2O2S2	000399-82-6	78
4		Benzothiazole, 2-(2-hydroxyethyl...	211	C9H9NOS2	004665-63-8	56
5		Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.98	6.98	87.2	ng	8889700	1	7.45	2038500	20.0
Benzothiazole	10.85	21.4	ng	3070260	2	10.20	2871880	20.0
2(3H)-Benzothiazo...	15.79	2.9	ng	652435	4	16.84	4436870	20.0
2-Mercaptobenzoth...	18.08	2.5	ng	563615	4	16.84	4436870	20.0