

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050617\
 Data File : BM009936.D
 Acq On : 06 May 2017 11:49
 Operator : SJ/MA
 Sample : I2893-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3070-PA1

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	4.904	304	309	319	rBV	352800	505006	4.38%	1.113%
2	5.363	381	387	404	rBV	1152886	1761026	15.29%	3.880%
3	6.963	651	659	671	rBV	698297	1212081	10.52%	2.670%
4	7.310	710	718	734	rBV	2279409	3587907	31.15%	7.904%
5	7.775	791	797	803	rBV	406617	657141	5.71%	1.448%
6	8.092	843	851	862	rVB	1906264	3025032	26.27%	6.664%
7	8.951	989	997	1010	rBV	1903308	3240921	28.14%	7.140%
8	10.569	1266	1272	1279	rBV	531894	901694	7.83%	1.986%
9	11.239	1381	1386	1394	rBV2	80390	146968	1.28%	0.324%
10	13.039	1685	1692	1699	rBV	4160602	6155439	53.45%	13.561%
11	14.427	1921	1928	1935	rBV2	784495	1209899	10.51%	2.665%
12	15.933	2177	2184	2196	rBV	4163755	5792049	50.29%	12.760%
13	16.151	2216	2221	2227	rVB2	125487	188629	1.64%	0.416%
14	17.186	2391	2397	2403	rBV	1137499	1579333	13.71%	3.479%
15	18.062	2543	2546	2553	rBV3	96220	142199	1.23%	0.313%
16	19.350	2761	2765	2772	rBV9	94556	156391	1.36%	0.345%
17	19.809	2838	2843	2848	rBV	9169502	11516985	100.00%	25.372%
18	21.374	3105	3109	3116	rVB	1701335	2067168	17.95%	4.554%
19	23.680	3495	3501	3508	rVB	805584	1546385	13.43%	3.407%

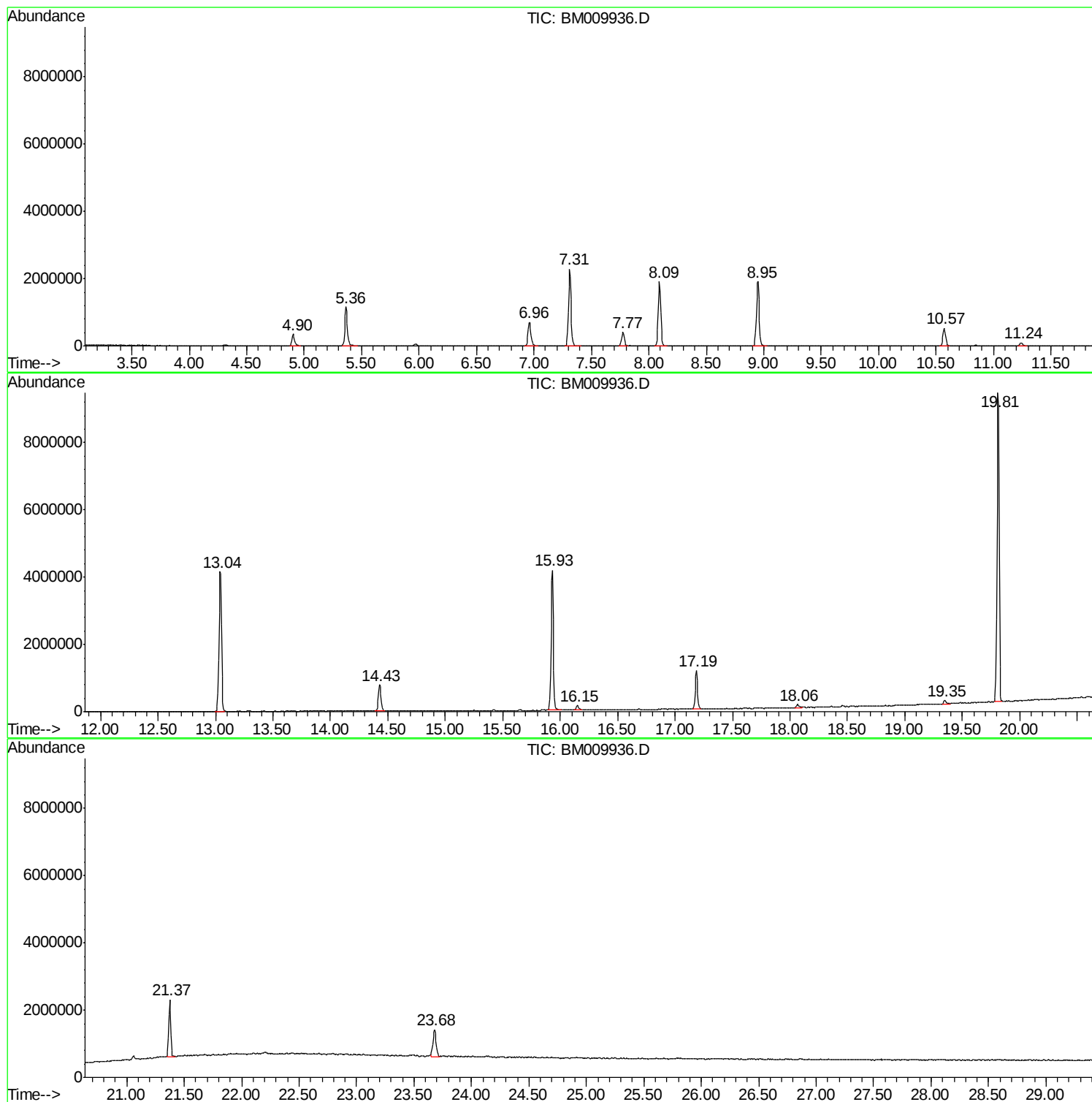
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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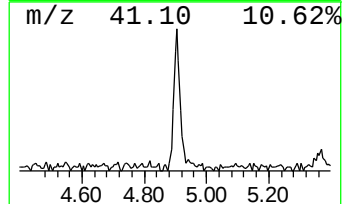
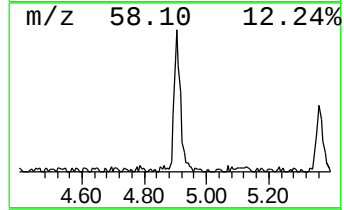
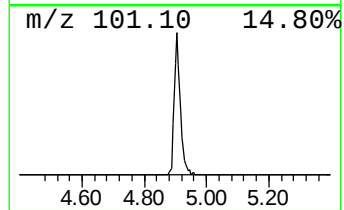
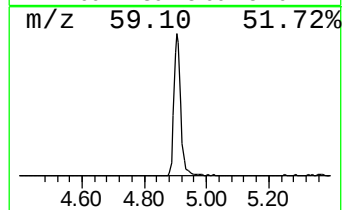
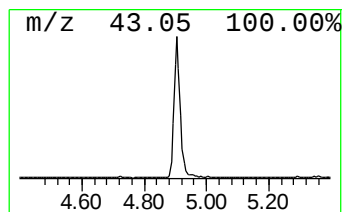
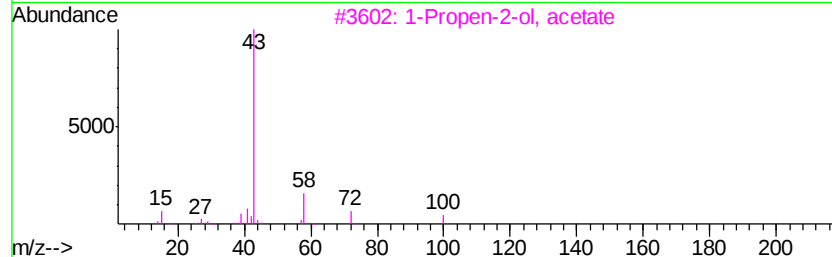
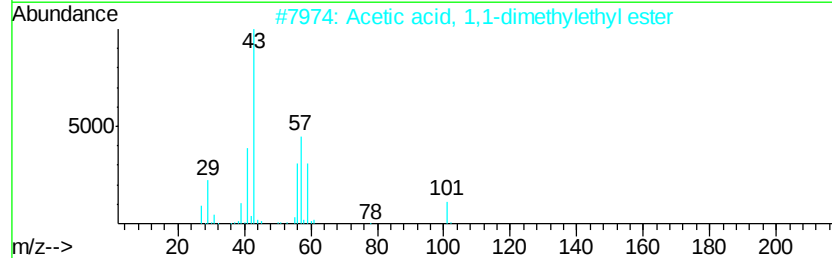
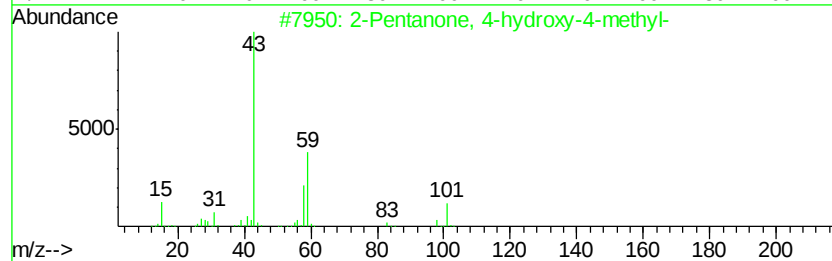
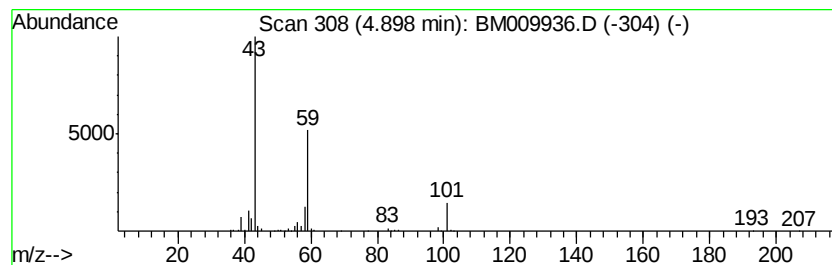
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	15.37 ng	505006	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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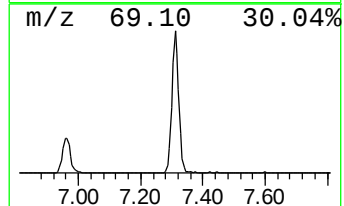
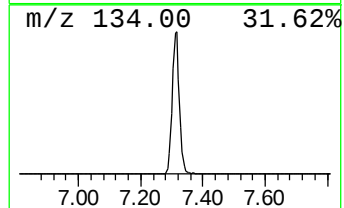
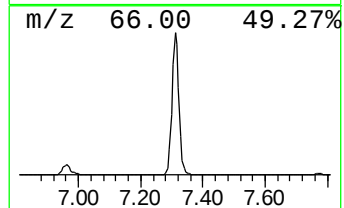
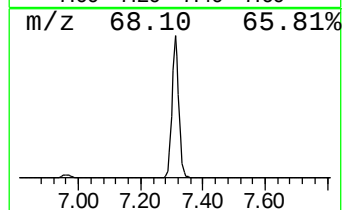
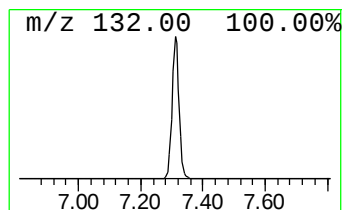
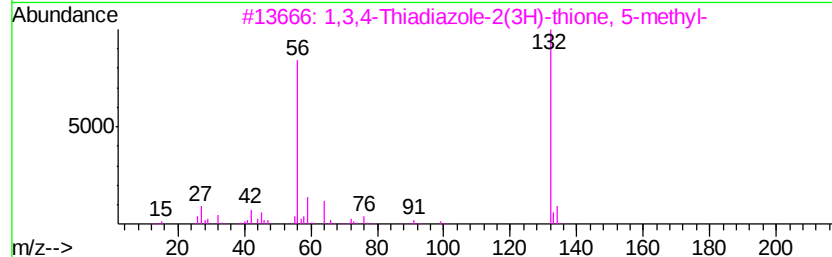
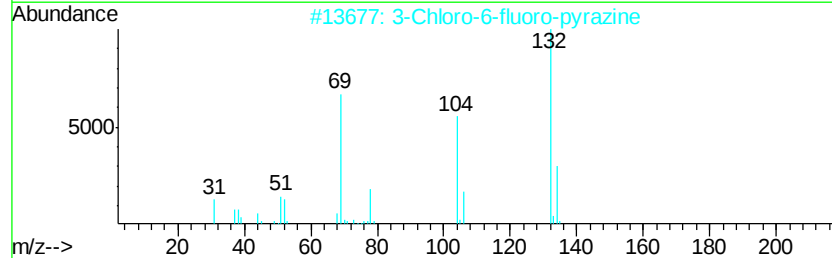
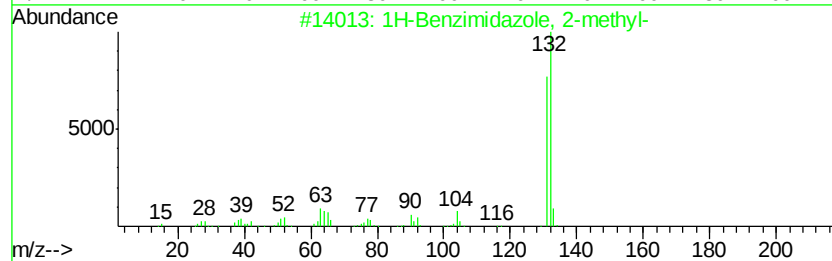
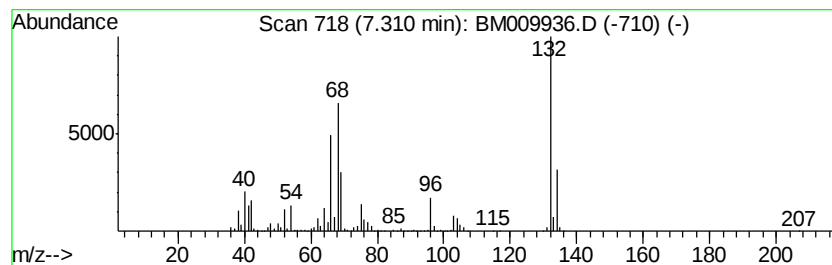
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Peak Number 2 unknown7.31 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	109.20 ng	3587910	1,4-Dichlorobenzene-d4	7.77

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		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14



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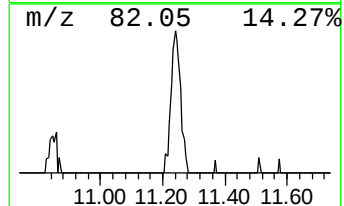
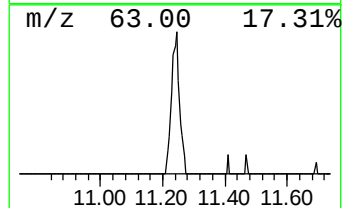
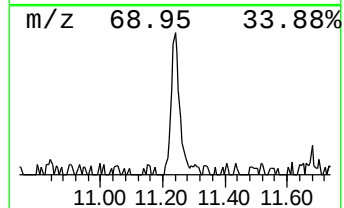
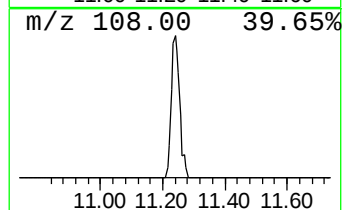
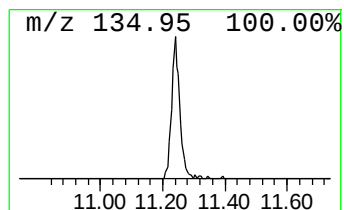
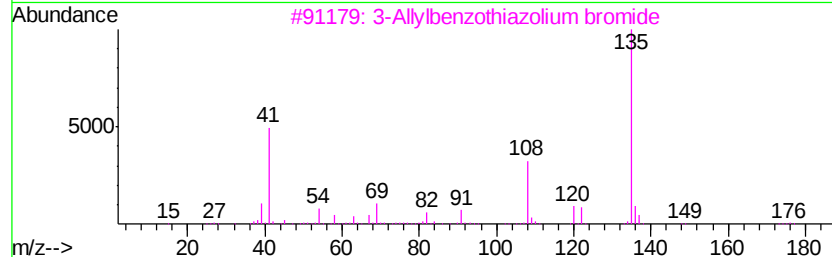
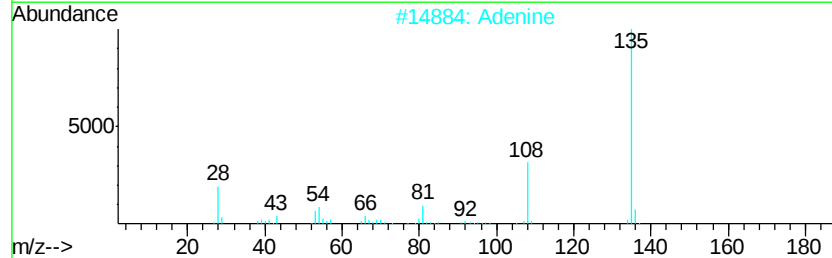
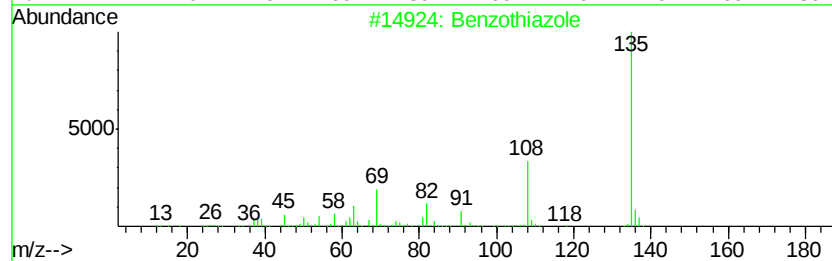
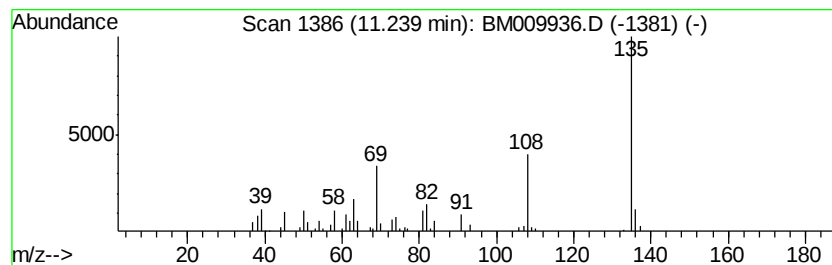
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Peak Number 4 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	3.26 ng	146968	Naphthalene-d8	10.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	90
2		Adenine	135	C5H5N5	000073-24-5	64
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64
4		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	58
5		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	58



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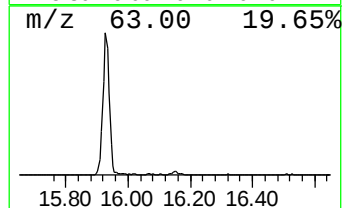
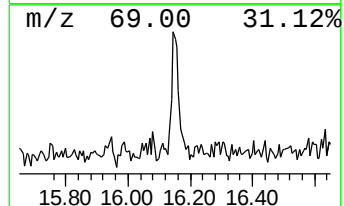
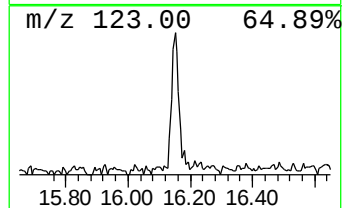
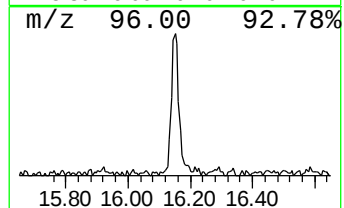
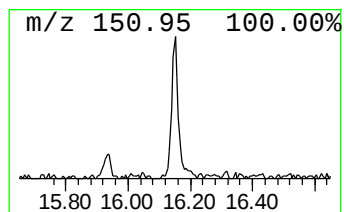
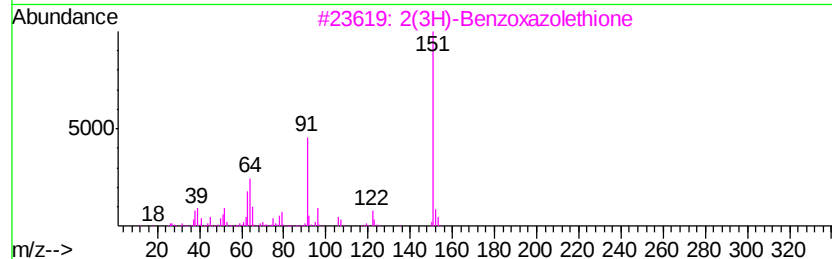
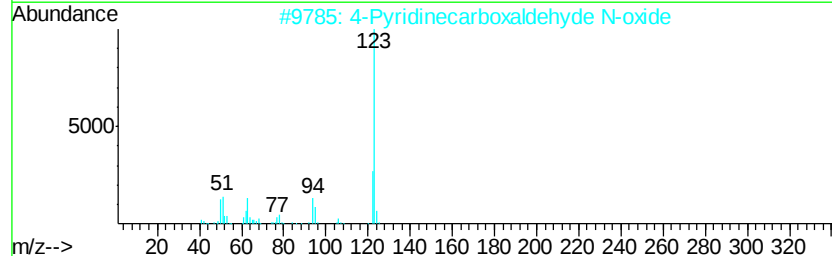
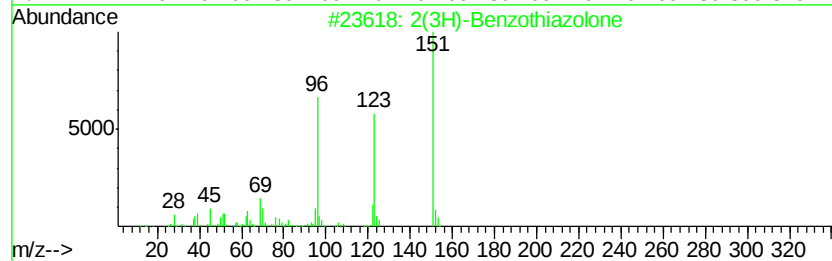
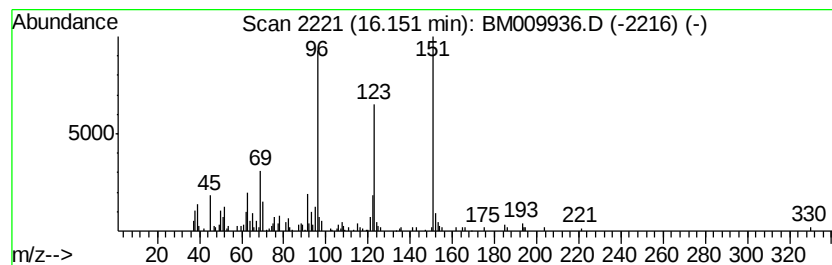
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Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.15	2.39 ng	188629	Phenanthrene-d10		17.19	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2		4-Pyridinecarboxaldehyde N-oxide	123	C6H5NO2	007216-42-4	53
3		2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	46
4		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	38
5		2H-Pyran-2-carboxylic acid, 5-et...	196	C10H12O4	019776-81-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	15.4	ng	505006	1	7.77	657141	20.0
unknown7.31	7.31	109.2	ng	3587910	1	7.77	657141	20.0
Benzothiazole	11.24	3.3	ng	146968	2	10.57	901694	20.0
2(3H)-Benzothiazo...	16.15	2.4	ng	188629	4	17.19	1579330	20.0