

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
 Data File : BM010885.D
 Acq On : 18 Jul 2017 23:54
 Operator : SJ/JU
 Sample : I4199-13
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3575-DB

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	291	297	303	rVB2	197021	316184	1.26%	0.271%
2	5.081	366	373	381	rVB	3175127	4385543	17.54%	3.758%
3	6.634	630	637	646	rVB	1996917	3011479	12.04%	2.581%
4	6.981	688	696	708	rBV	6160538	9172622	36.68%	7.860%
5	7.440	768	774	781	rVB	1323852	1960057	7.84%	1.680%
6	7.757	820	828	838	rBV	5305839	8478913	33.91%	7.266%
7	8.587	961	969	978	rBV	4835895	7685191	30.73%	6.586%
8	9.728	1156	1163	1169	rBV2	190546	328873	1.32%	0.282%
9	10.198	1236	1243	1251	rBV	1703288	2691208	10.76%	2.306%
10	10.845	1344	1353	1361	rVB	175202	343997	1.38%	0.295%
11	12.704	1659	1669	1679	rBV	12346087	17834450	71.32%	15.283%
12	14.092	1899	1905	1914	rVB2	2407812	3633222	14.53%	3.113%
13	15.592	2153	2160	2169	rBV	10887341	14927406	59.70%	12.792%
14	15.804	2188	2196	2206	rVB	2298270	3795135	15.18%	3.252%
15	16.845	2367	2373	2382	rVB2	3140739	4408001	17.63%	3.777%
16	19.509	2820	2826	2831	rBV	19957042	25004816	100.00%	21.428%
17	21.062	3085	3090	3095	rBV	3775401	4646887	18.58%	3.982%
18	21.903	3231	3233	3239	rVB5	229979	290430	1.16%	0.249%
19	23.191	3446	3452	3459	rVB2	2102096	3778668	15.11%	3.238%

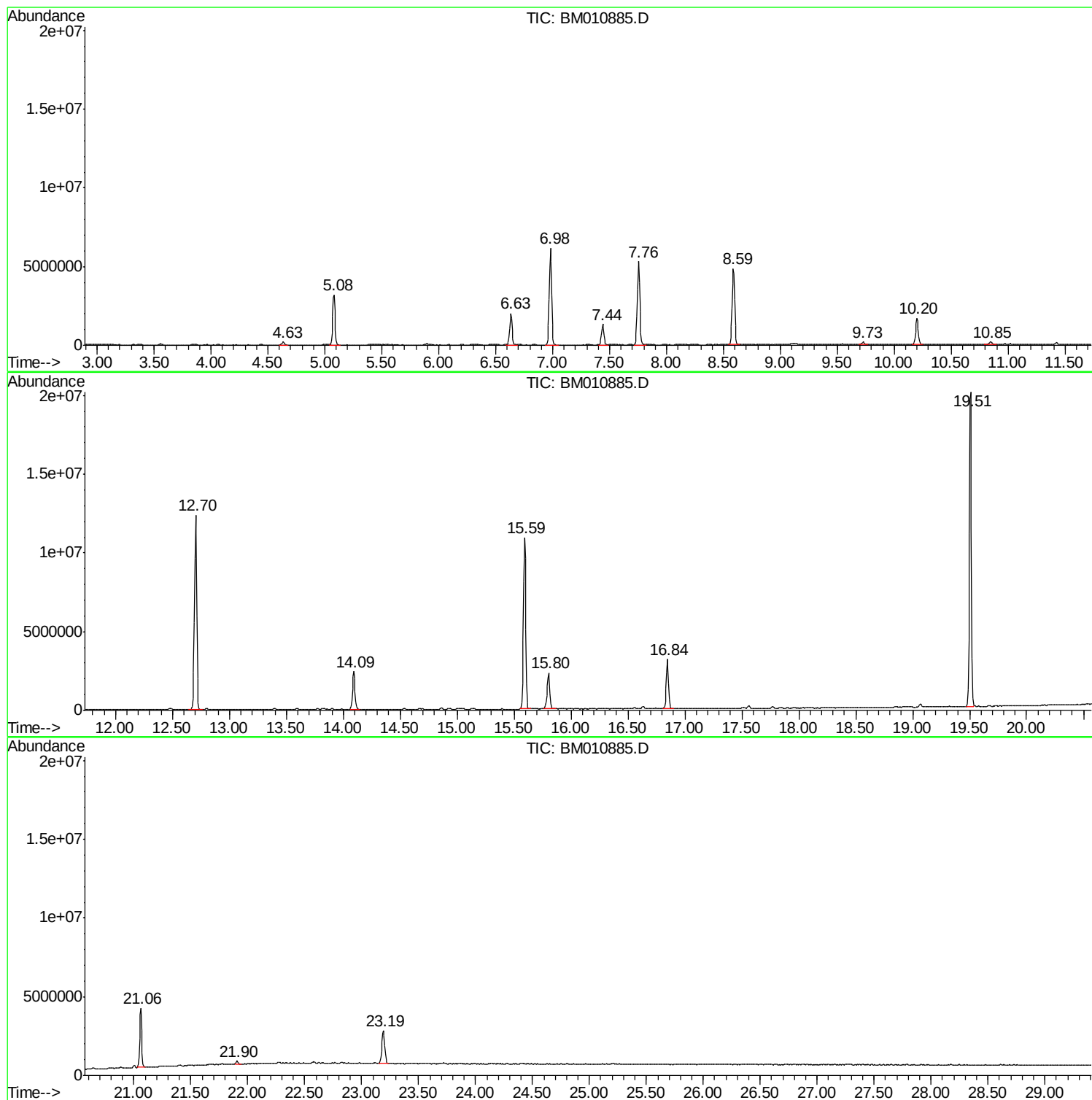
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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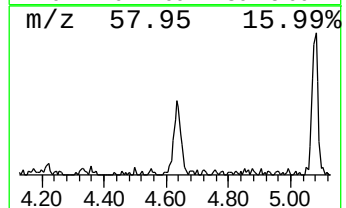
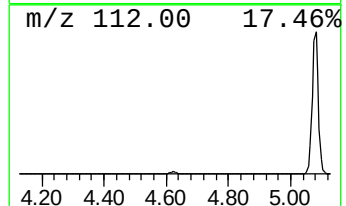
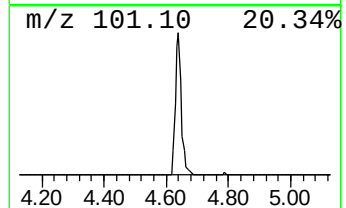
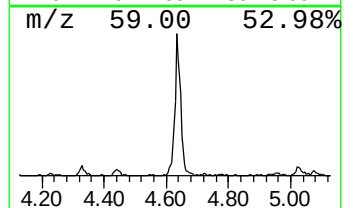
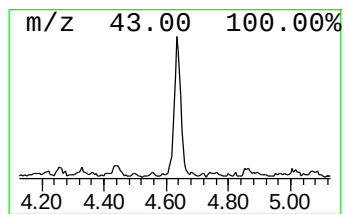
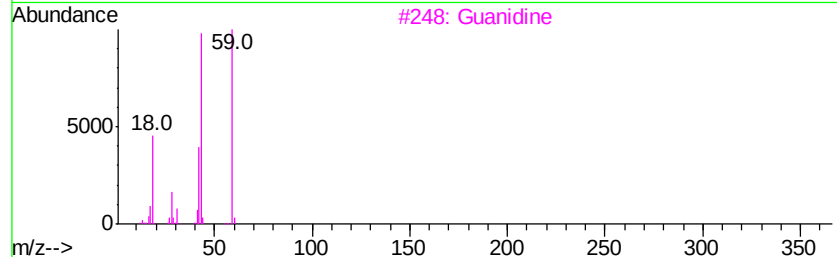
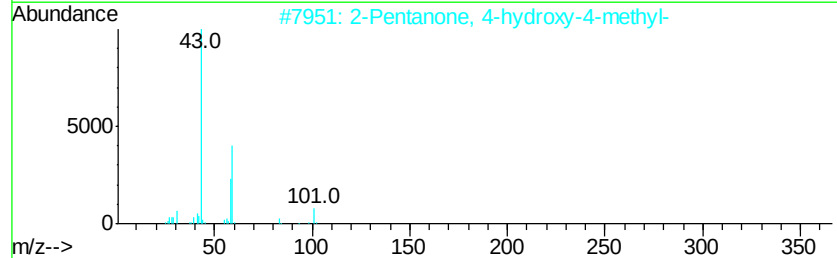
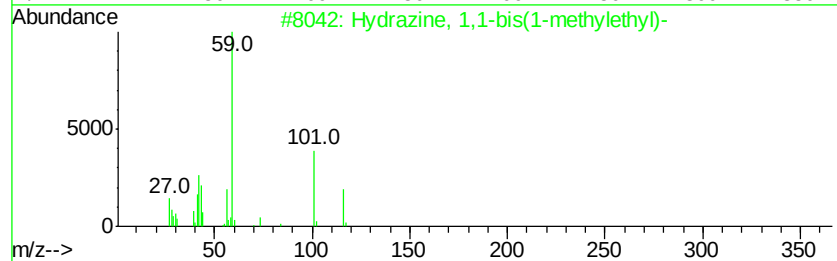
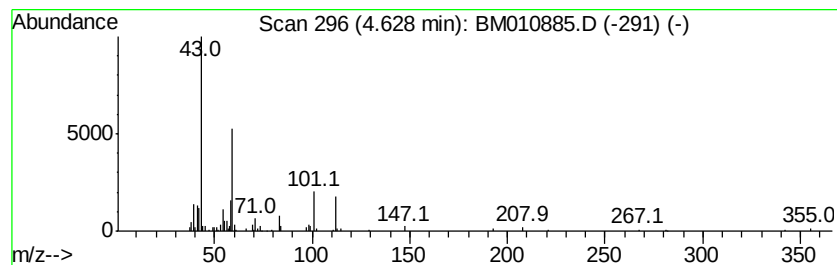
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hydrazine, 1,1-bis(1-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	3.23 ng	316184	1,4-Dichlorobenzene-d4	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	53
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			Guanidine	59	CH5N3	000113-00-8	47
4			2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	38
5			Dimethadione	129	C5H7NO3	000695-53-4	36



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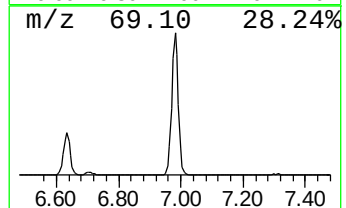
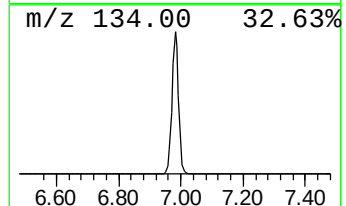
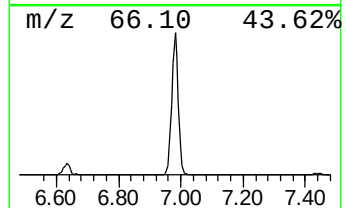
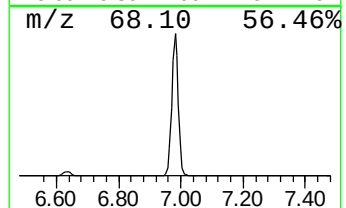
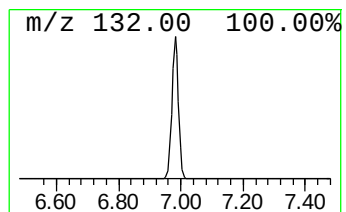
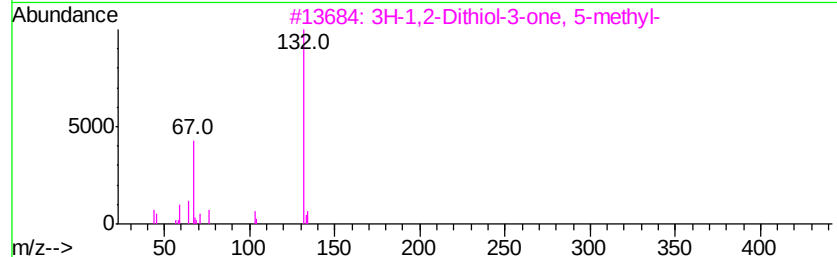
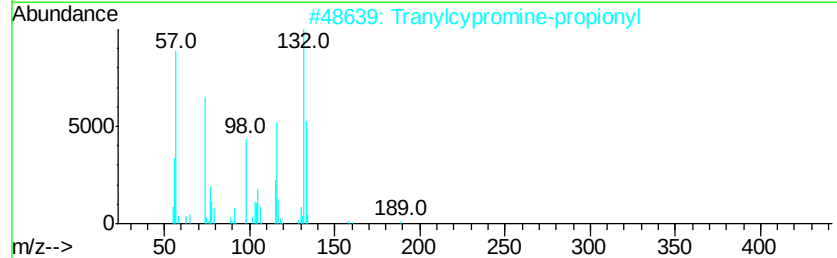
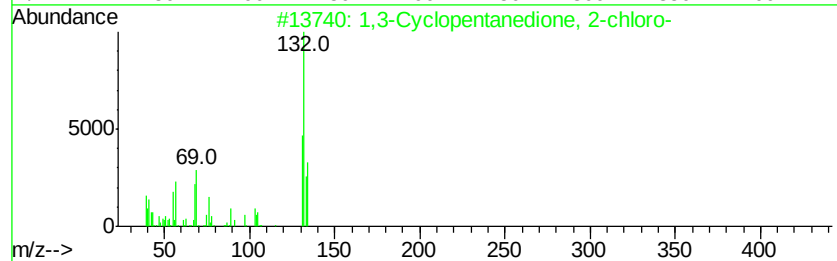
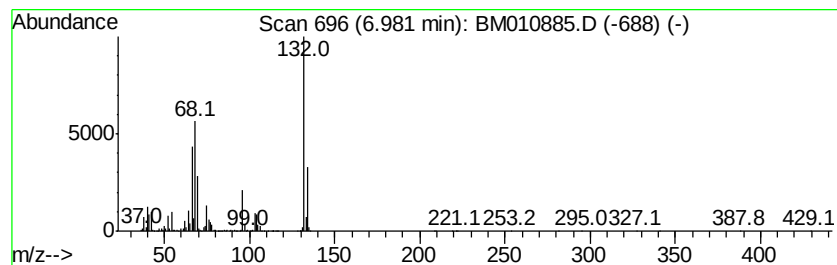
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	93.60 ng	9172620	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10



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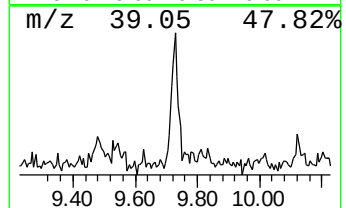
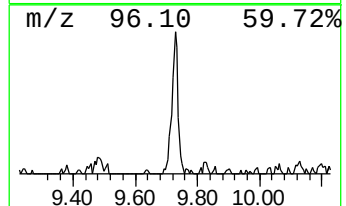
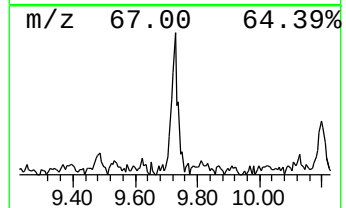
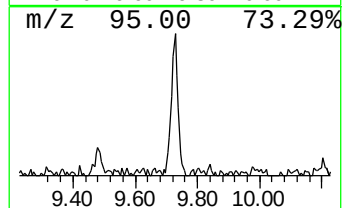
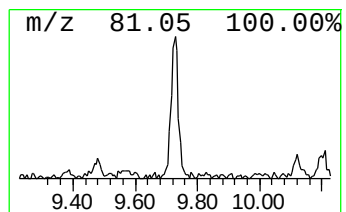
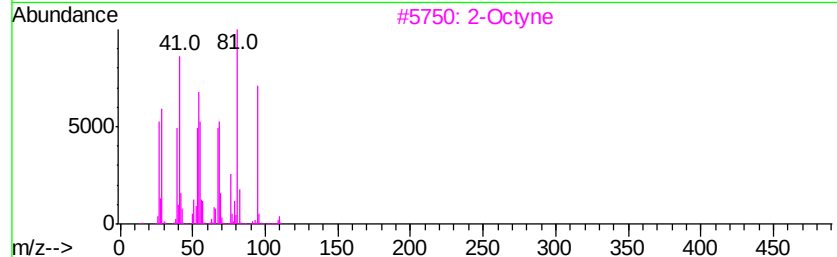
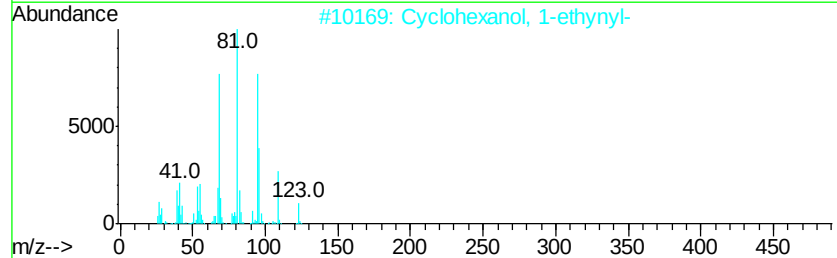
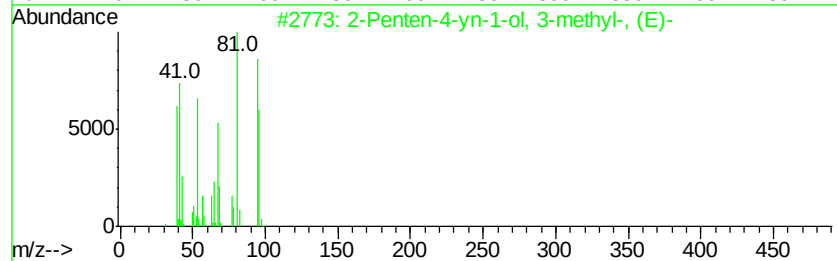
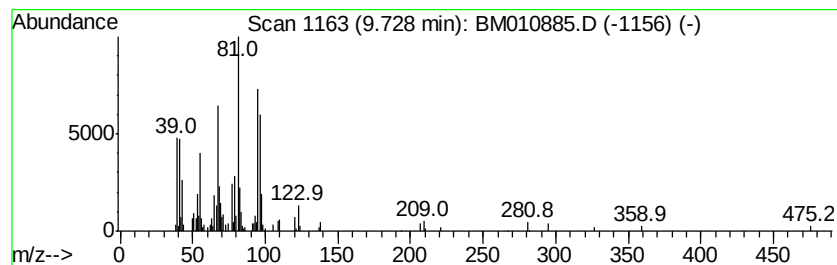
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Peak Number 4 2-Penten-4-yn-1-ol, 3-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.73	2.44 ng	328873	Naphthalene-d8	10.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Penten-4-yn-1-ol, 3-methyl-, (E)-	96	C6H8O	006153-06-6	74
2		Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	64
3		2-Octyne	110	C8H14	002809-67-8	59
4		4-Decyne	138	C10H18	002384-86-3	52
5		3-Hexyne, 2-methyl-	96	C7H12	036566-80-0	46



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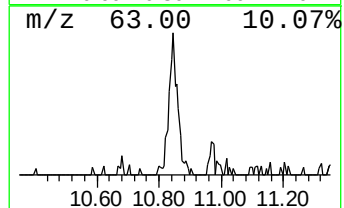
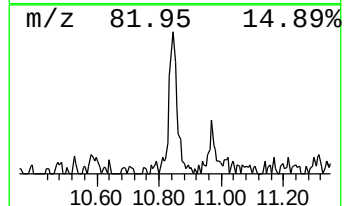
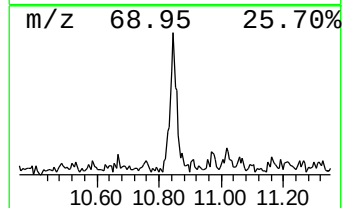
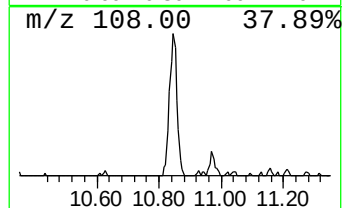
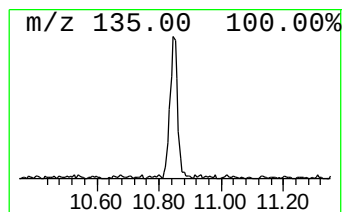
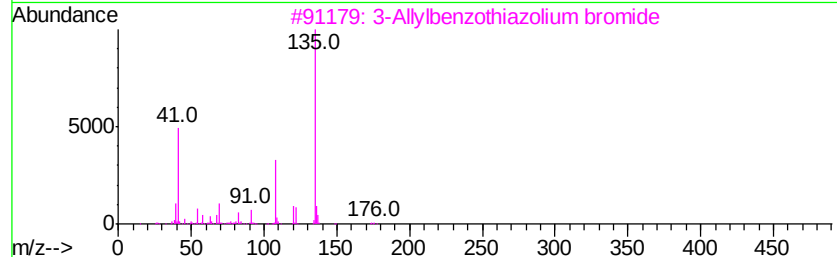
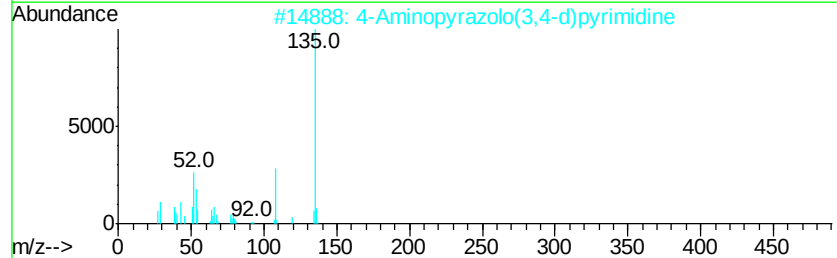
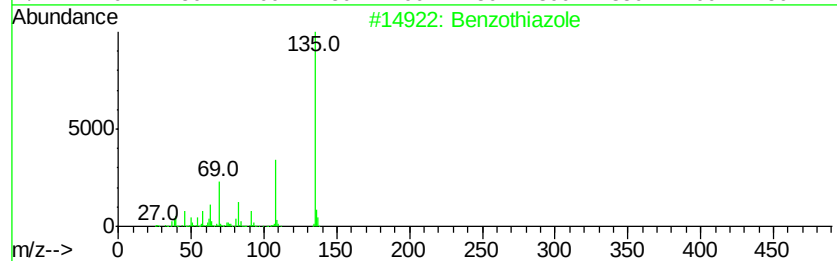
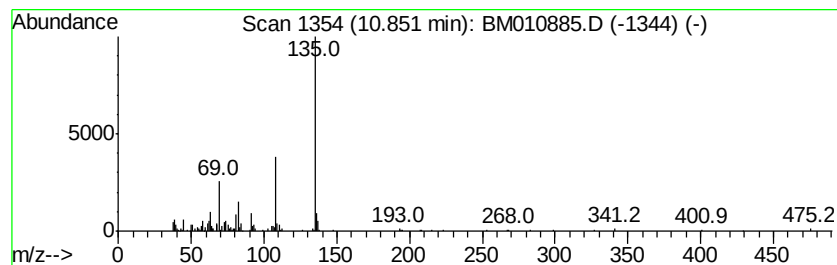
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Peak Number 5 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.85	2.56 ng	343997	Naphthalene-d8	10.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	90
2	4-Aminopyrazolo(3,4-d)pyrimidine	135	C5H5N5	020289-44-5	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	59
5	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	59



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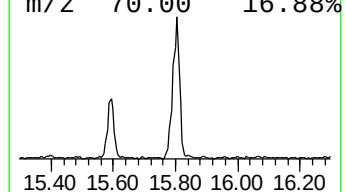
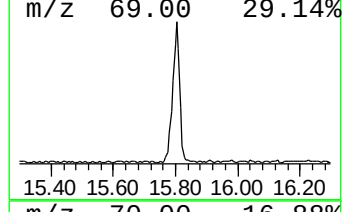
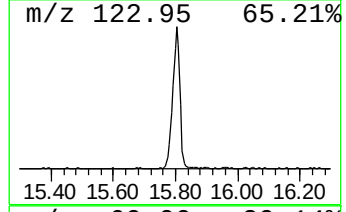
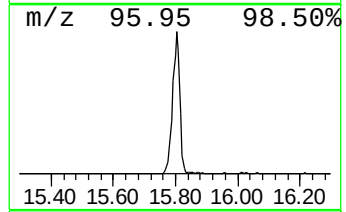
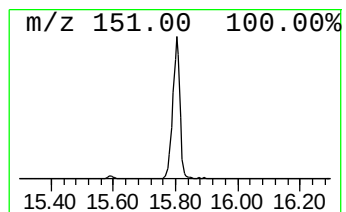
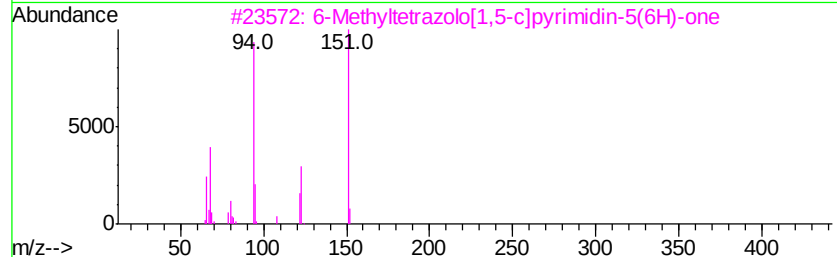
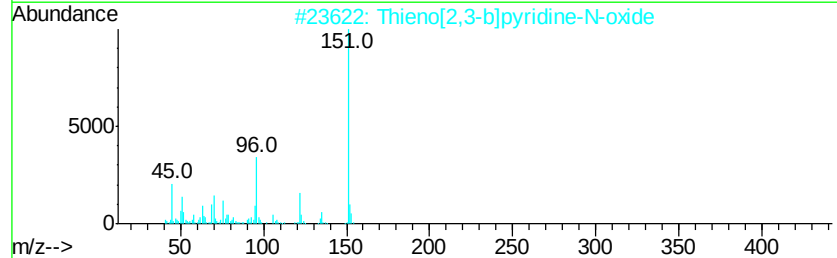
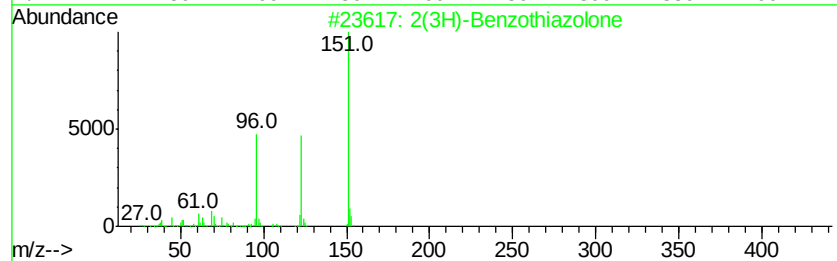
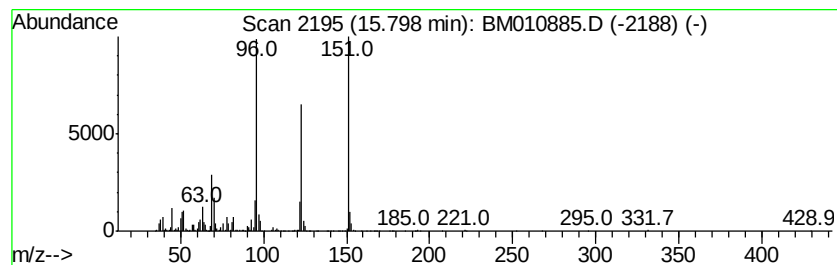
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Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.80	17.22 ng	3795140	Phenanthrene-d10	16.84		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	43
3		6-Methyltetrazolo[1,5-c]pyrimidin...	151	C5H5N5O	144877-40-7	38
4		5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	30
5		2,5-Pyridinedicarboxylic acid, 2...	181	C8H7NO4	017874-76-9	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hydrazine, 1,1-bi...	4.63	3.2	ng	316184	1	7.44	1960060	20.0
unknown6.98	6.98	93.6	ng	9172620	1	7.44	1960060	20.0
2-Penten-4-yn-1-o...	9.73	2.4	ng	328873	2	10.20	2691210	20.0
Benzothiazole	10.85	2.6	ng	343997	2	10.20	2691210	20.0
2(3H)-Benzothiazo...	15.80	17.2	ng	3795140	4	16.84	4408000	20.0