

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099455.D
 Acq On : 13 Oct 2017 22:33
 Operator : SJ/JU
 Sample : I5819-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3907-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_F\METHODS\8270-BF092317.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	2.128	3	7	17	rVB	185404	265499	8.95%	1.372%
2	5.075	505	508	521	rBV	166337	188107	6.34%	0.972%
3	5.475	572	576	592	rBV	1451463	1384731	46.67%	7.154%
4	6.486	744	748	762	rBV	899392	835359	28.16%	4.316%
5	6.628	767	772	775	rBV	2469442	2307441	77.78%	11.921%
6	6.851	807	810	814	rBV	681429	549044	18.51%	2.836%
7	7.010	833	837	840	rBV	2545229	2264339	76.32%	11.698%
8	7.422	902	907	910	rBV	1846035	1726017	58.18%	8.917%
9	8.133	1024	1028	1035	rBV	890968	708305	23.87%	3.659%
10	8.416	1072	1076	1082	rBV	512525	441105	14.87%	2.279%
11	9.210	1206	1211	1214	rBV	3200750	2966773	100.00%	15.327%
12	9.886	1323	1326	1332	rVB	780211	677726	22.84%	3.501%
13	10.680	1457	1461	1464	rBV	1484302	1329087	44.80%	6.866%
14	10.792	1477	1480	1487	rBV	64335	69482	2.34%	0.359%
15	10.921	1500	1502	1505	rBV	36122	31969	1.08%	0.165%
16	11.374	1576	1579	1583	rBV	651799	552778	18.63%	2.856%
17	12.962	1844	1849	1852	rBV	2000585	2005090	67.58%	10.359%
18	14.015	2025	2028	2038	rBV	504227	491784	16.58%	2.541%
19	15.492	2274	2279	2290	rVB	444015	561801	18.94%	2.902%

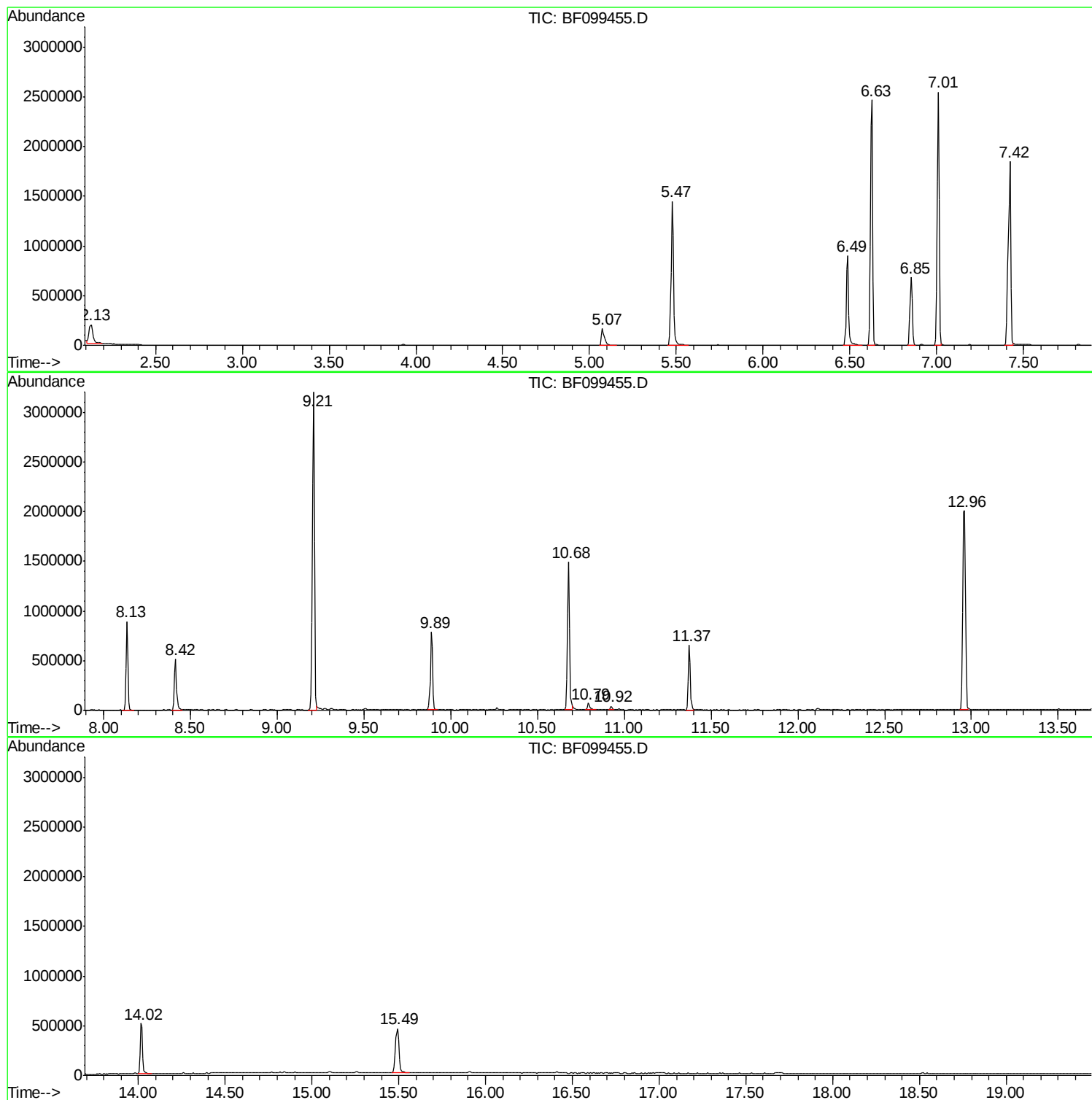
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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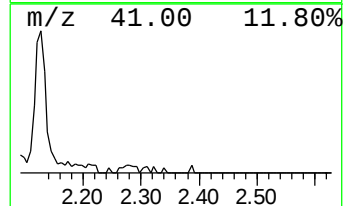
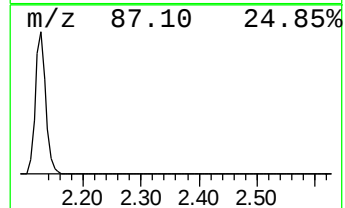
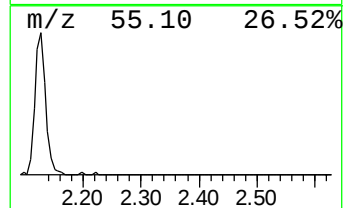
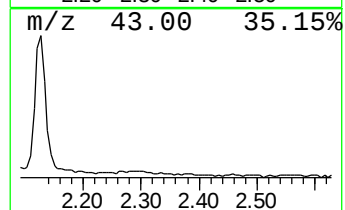
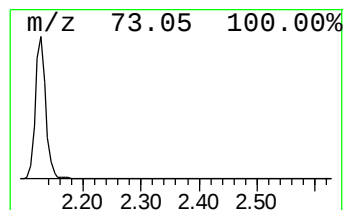
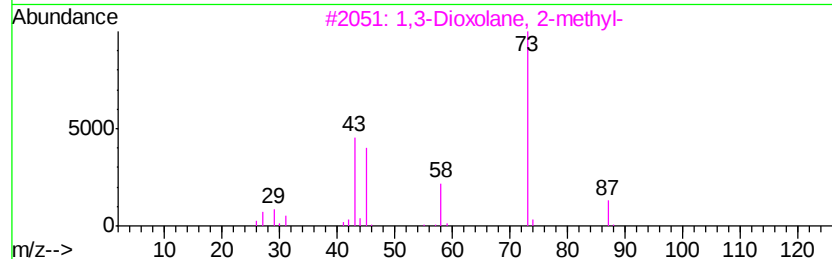
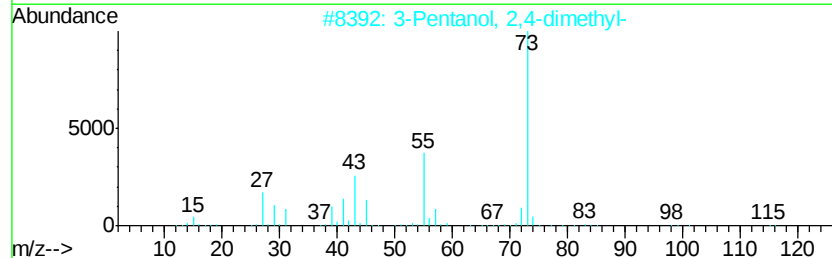
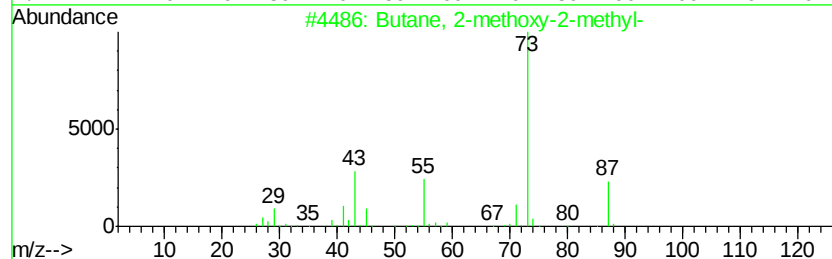
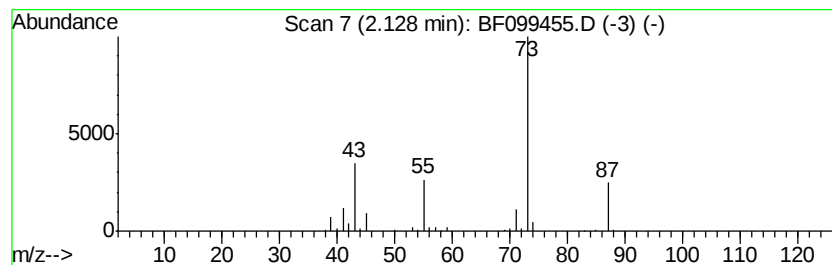
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	9.67 ng	265499	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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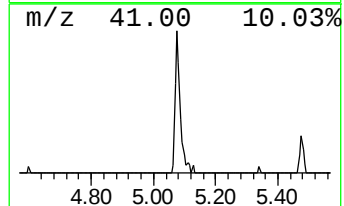
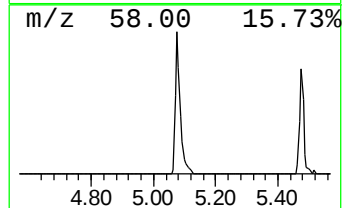
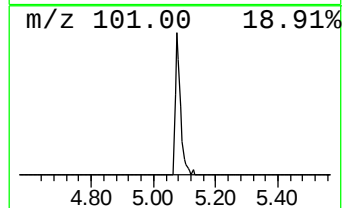
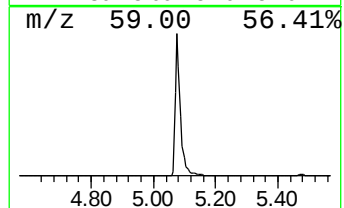
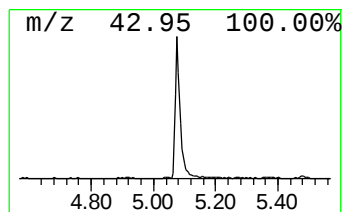
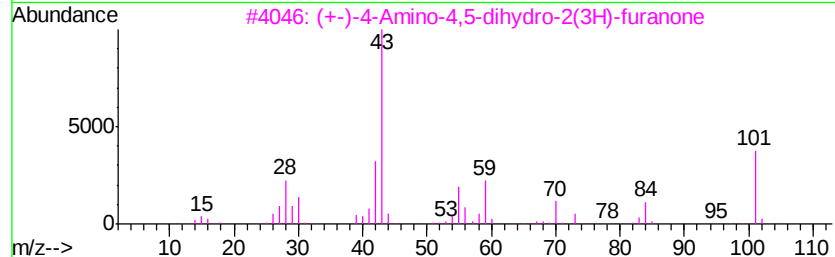
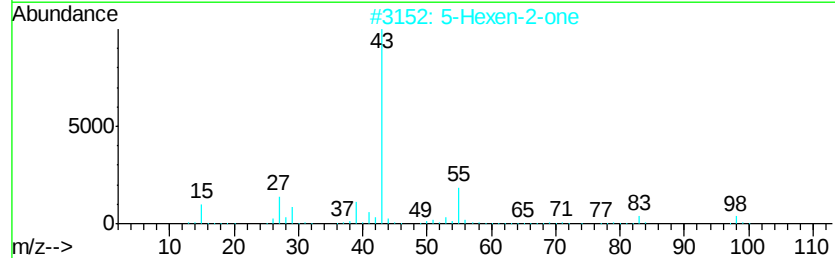
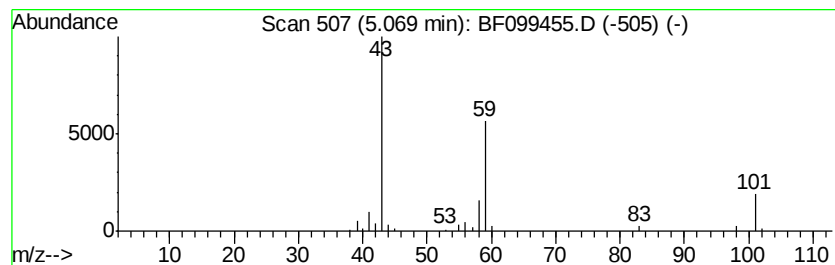
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.85 ng	188107	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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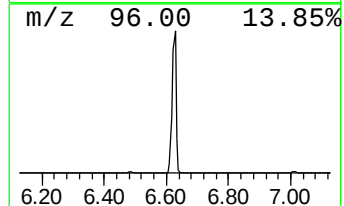
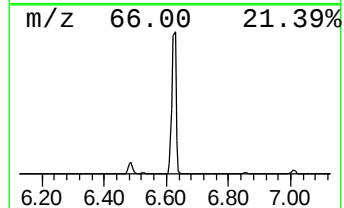
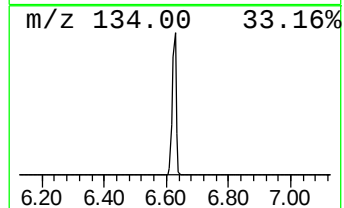
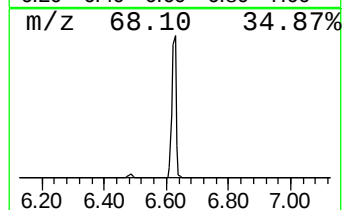
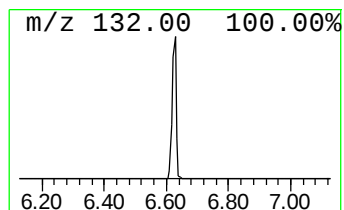
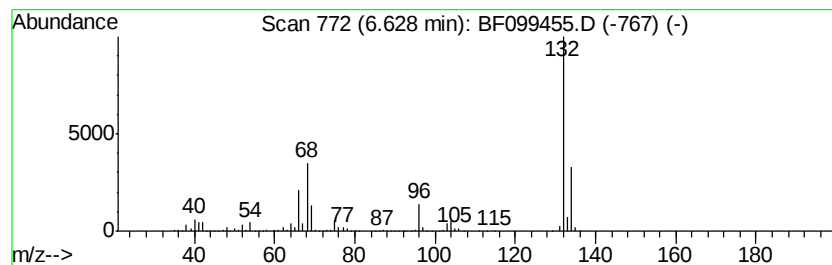
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.05 ng	2307440	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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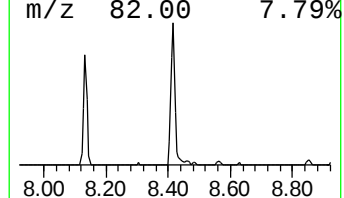
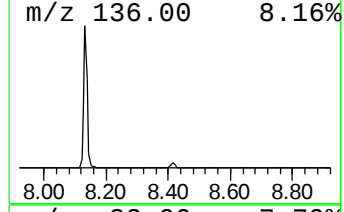
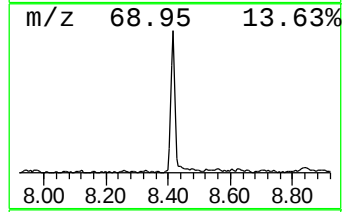
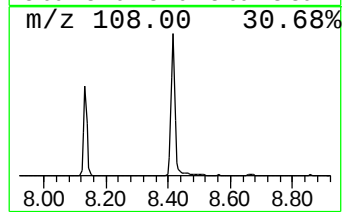
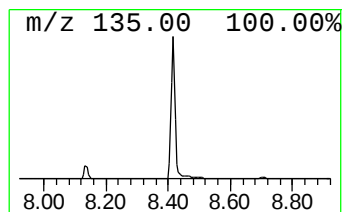
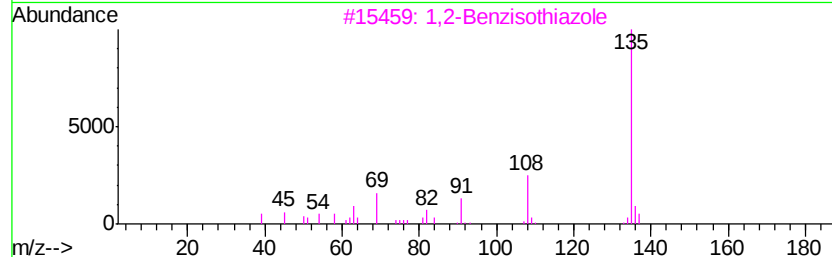
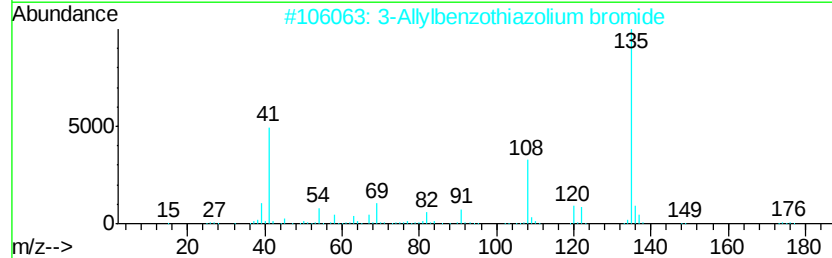
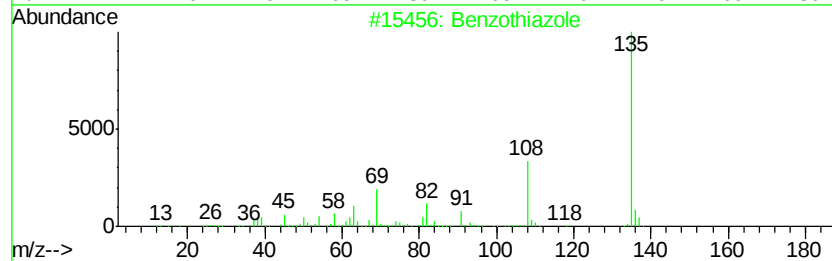
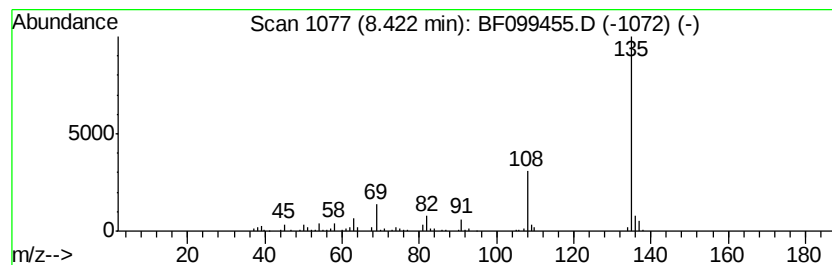
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Peak Number 5 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	12.46 ng	441105	Naphthalene-d8	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	94
2		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
3		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86
4		Adenine	135	C5H5N5	000073-24-5	64
5		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64



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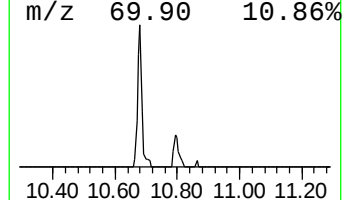
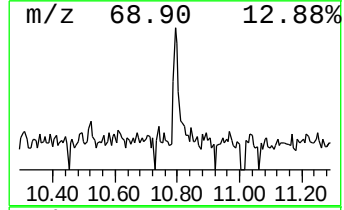
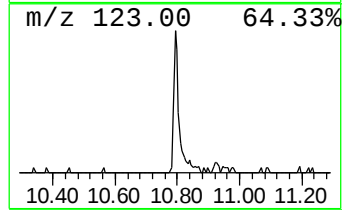
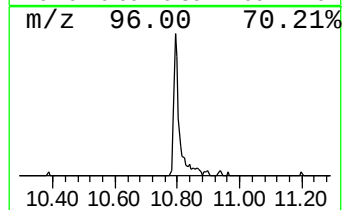
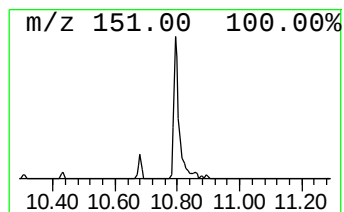
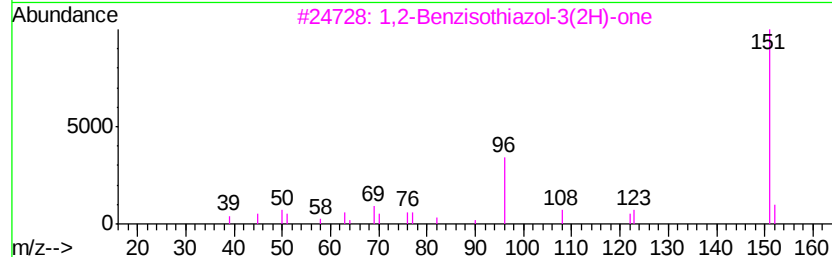
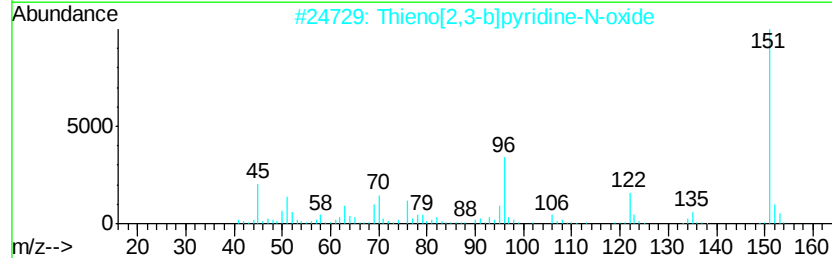
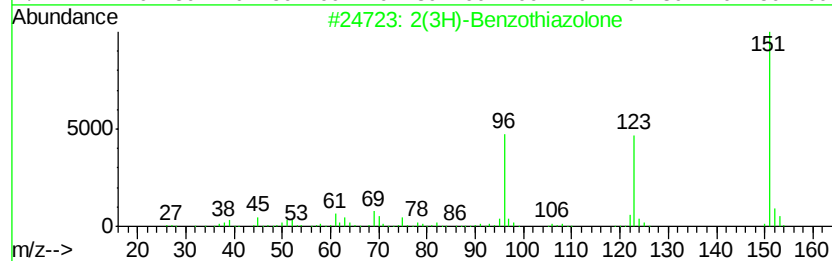
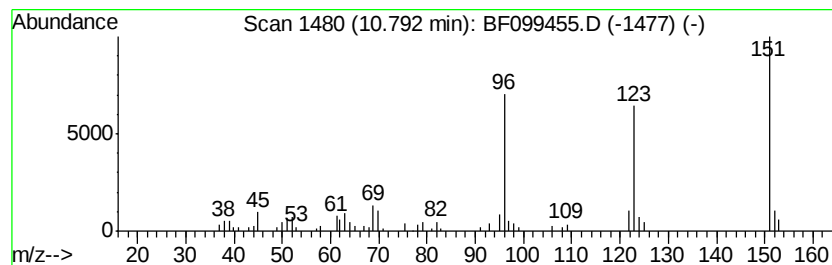
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Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.79	2.51 ng	69482	Phenanthrene-d10	11.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	50
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	49
4	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	45
5	4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	9.7	ng	265499	1	6.85	549044	20.0
2-Pentanone, 4-hy...	5.07	6.8	ng	188107	1	6.85	549044	20.0
unknown6.63	6.63	84.0	ng	2307440	1	6.85	549044	20.0
Benzothiazole	8.42	12.5	ng	441105	2	8.13	708305	20.0
2(3H)-Benzothiazo...	10.79	2.5	ng	69482	4	11.37	552778	20.0