

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099450.D
 Acq On : 13 Oct 2017 20:12
 Operator : SJ/JU
 Sample : I5819-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3902-PP1

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	16	rVB	169563	221013	7.55%	1.190%
2	3.928	308	313	321	rBV	88571	119682	4.09%	0.644%
3	5.075	505	508	520	rBV	166935	196808	6.73%	1.060%
4	5.475	572	576	593	rBV	1399044	1318788	45.07%	7.101%
5	6.481	744	747	759	rBV	865757	780352	26.67%	4.202%
6	6.628	767	772	775	rBV	2345928	2263578	77.36%	12.188%
7	6.851	807	810	817	rBV	647044	519198	17.74%	2.796%
8	7.010	833	837	840	rBV	2546226	2267454	77.49%	12.209%
9	7.422	902	907	910	rBV	1769388	1724277	58.93%	9.284%
10	8.134	1024	1028	1034	rBV	830168	662638	22.65%	3.568%
11	8.416	1072	1076	1093	rBV	259541	244694	8.36%	1.318%
12	9.210	1206	1211	1214	rBV	3247876	2925941	100.00%	15.755%
13	9.886	1323	1326	1335	rVB	712570	622188	21.26%	3.350%
14	10.680	1457	1461	1471	rBV	1368612	1258947	43.03%	6.779%
15	11.375	1575	1579	1583	rBV	591210	493408	16.86%	2.657%
16	12.957	1844	1848	1852	rBV	2101625	1941282	66.35%	10.453%
17	13.980	2019	2022	2025	rBV	60468	48900	1.67%	0.263%
18	14.016	2025	2028	2038	rVV	531035	456683	15.61%	2.459%
19	15.486	2273	2278	2285	rBV	389902	505984	17.29%	2.724%

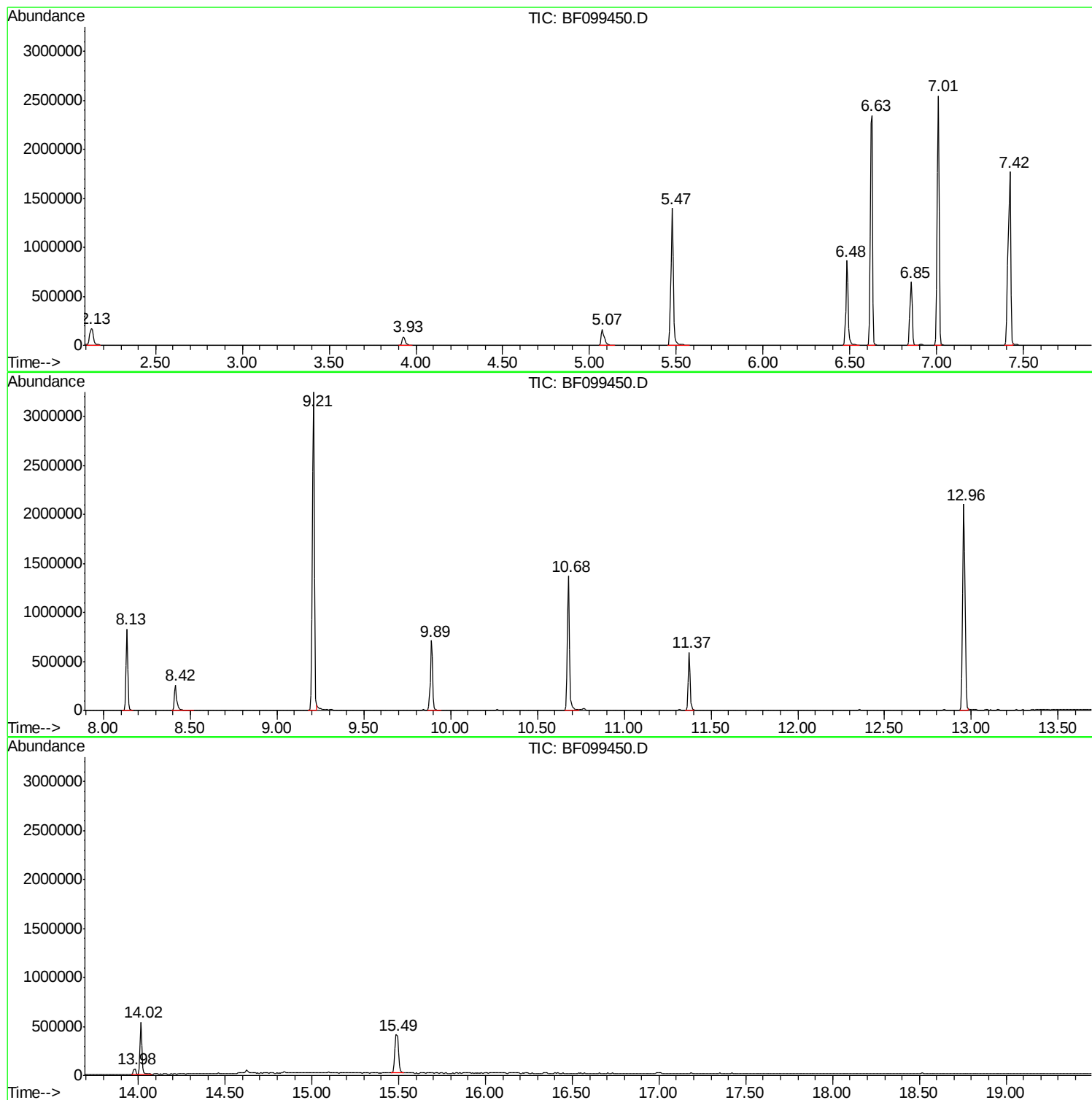
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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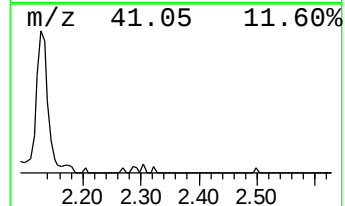
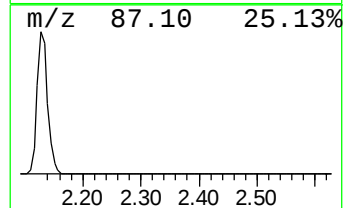
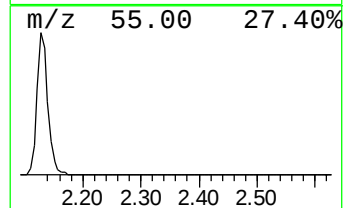
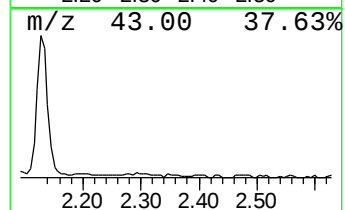
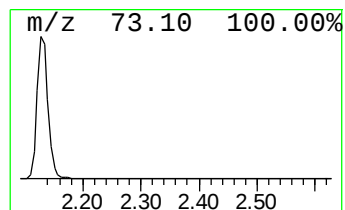
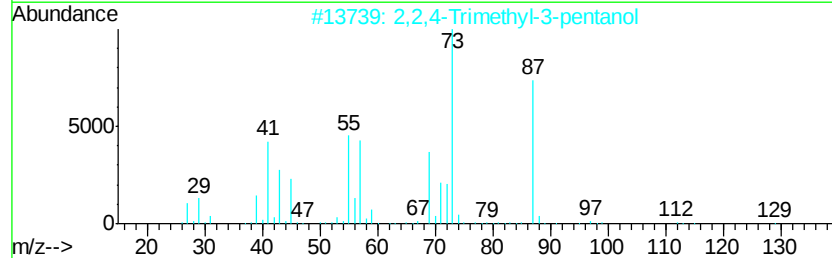
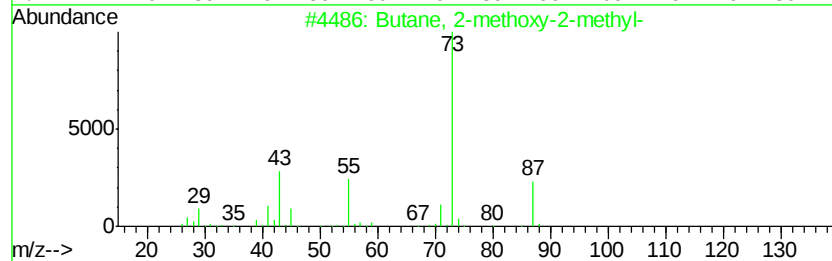
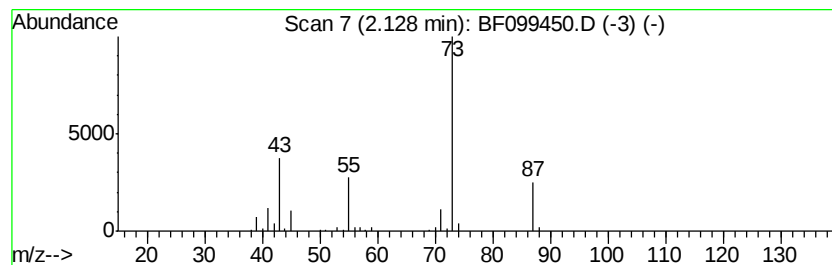
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	8.51 ng	221013	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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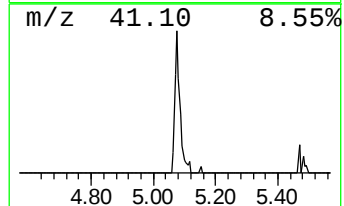
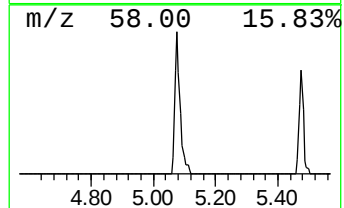
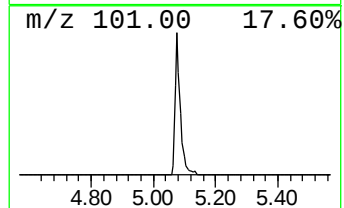
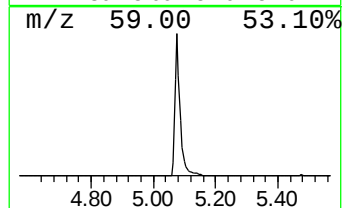
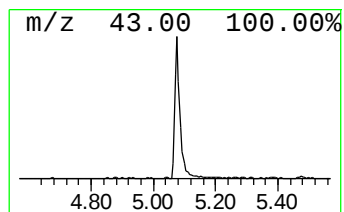
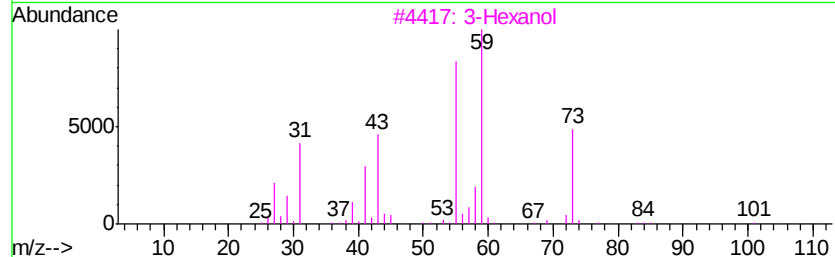
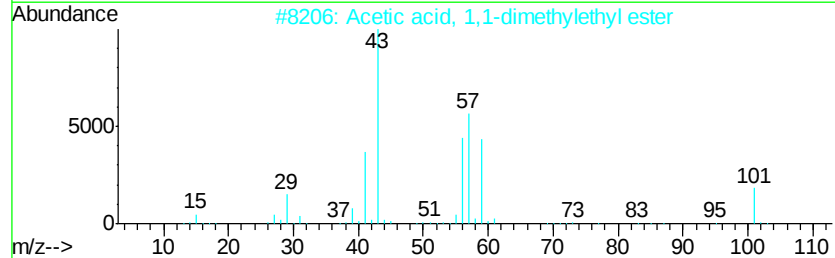
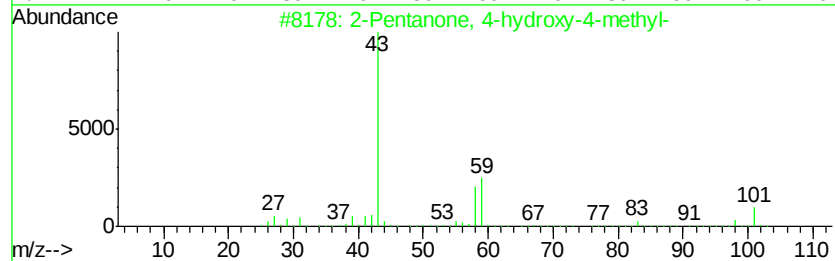
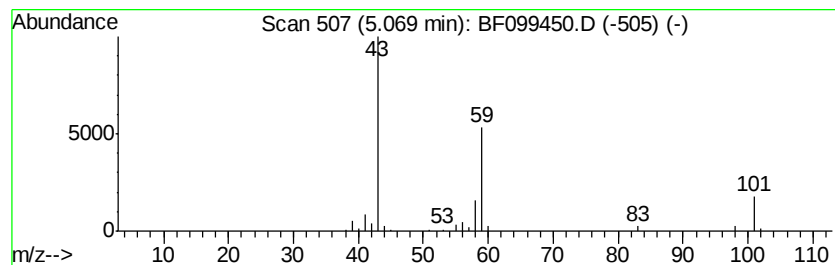
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.58 ng	196808	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	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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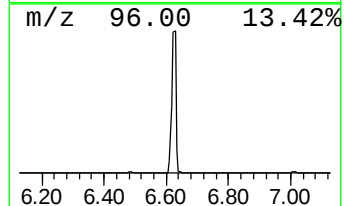
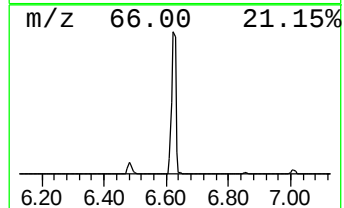
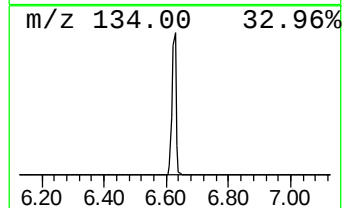
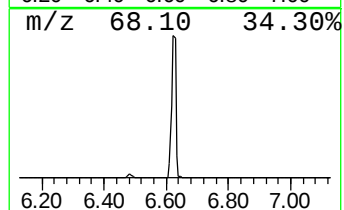
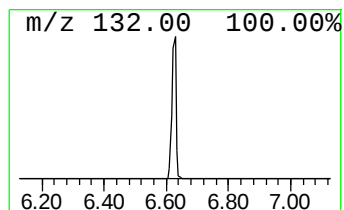
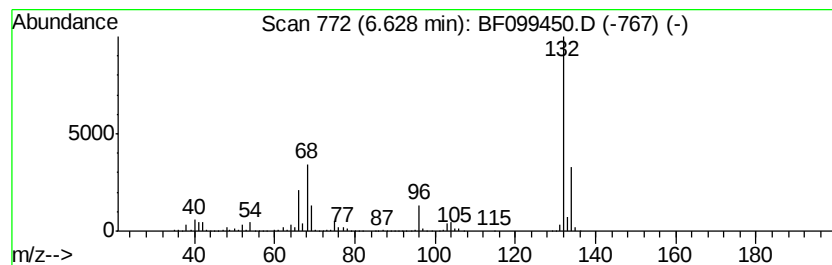
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Peak Number 4 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	87.20 ng	2263580	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	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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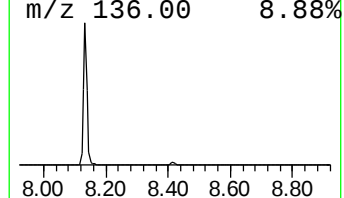
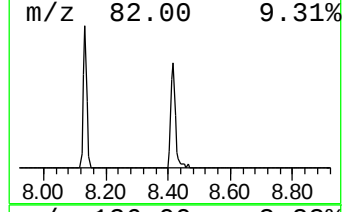
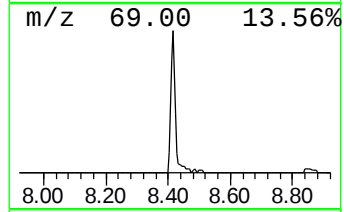
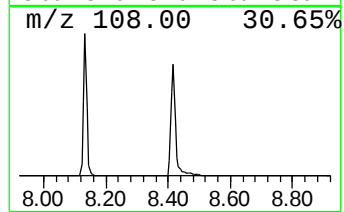
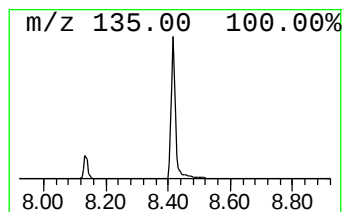
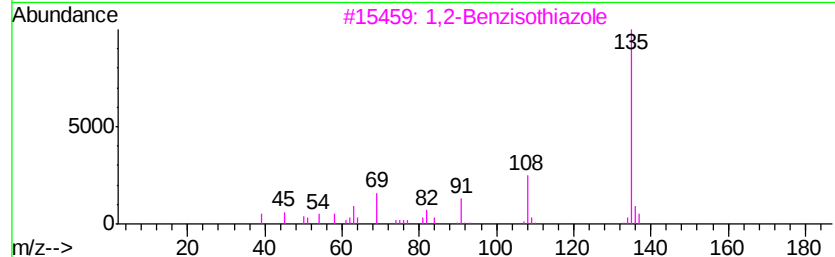
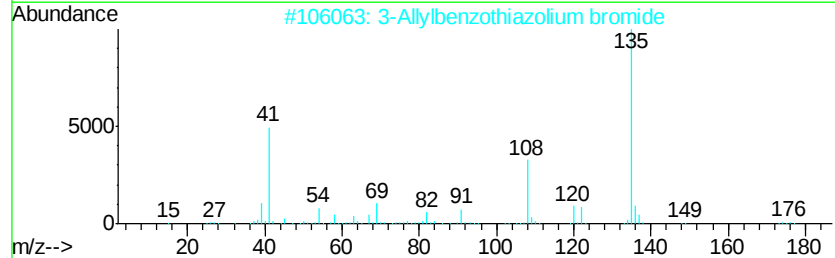
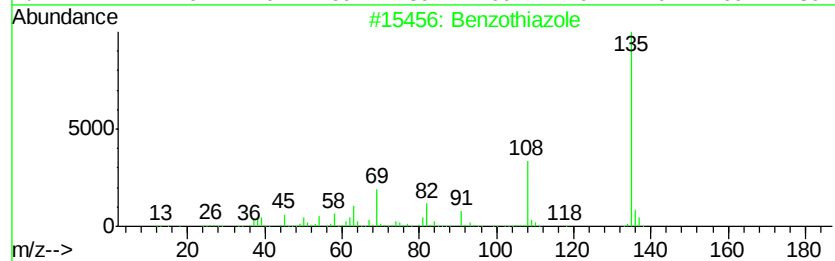
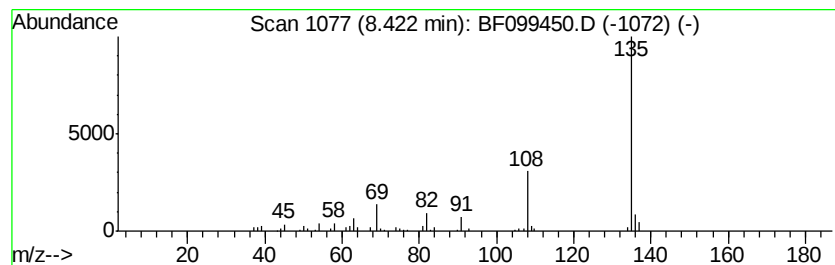
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Peak Number 6 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	7.39 ng	244694	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
3	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	78
4	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
5	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	8.5	ng	221013	1	6.85	519198	20.0
2-Pentanone, 4-hy...	5.07	7.6	ng	196808	1	6.85	519198	20.0
unknown6.63	6.63	87.2	ng	2263580	1	6.85	519198	20.0
Benzothiazole	8.42	7.4	ng	244694	2	8.13	662638	20.0