

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099454.D
 Acq On : 13 Oct 2017 22:05
 Operator : SJ/JU
 Sample : I5819-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3906-PP4

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	2.134	3	8	21	rVB	170775	222330	7.49%	1.167%
2	5.075	505	508	519	rBV	167684	203029	6.84%	1.066%
3	5.475	573	576	589	rBV	1461357	1401486	47.22%	7.356%
4	6.487	744	748	759	rBV	906091	860921	29.00%	4.518%
5	6.628	767	772	775	rBV	2504367	2360656	79.53%	12.390%
6	6.851	807	810	816	rBV	707909	566735	19.09%	2.974%
7	7.010	833	837	840	rBV	2602931	2299312	77.46%	12.068%
8	7.422	902	907	910	rBV	1833637	1760826	59.32%	9.241%
9	8.134	1024	1028	1036	rBV	912759	726191	24.47%	3.811%
10	8.416	1073	1076	1086	rBV	78687	74158	2.50%	0.389%
11	9.210	1206	1211	1214	rBV	3331295	2968247	100.00%	15.578%
12	9.886	1323	1326	1338	rBV	819674	699337	23.56%	3.670%
13	10.680	1457	1461	1475	rBV	1481596	1361513	45.87%	7.146%
14	11.374	1576	1579	1583	rBV	668610	565199	19.04%	2.966%
15	12.957	1844	1848	1852	rBV	2028525	1955702	65.89%	10.264%
16	14.015	2024	2028	2034	rBV	541186	490459	16.52%	2.574%
17	15.492	2274	2279	2284	rBV	428660	537468	18.11%	2.821%

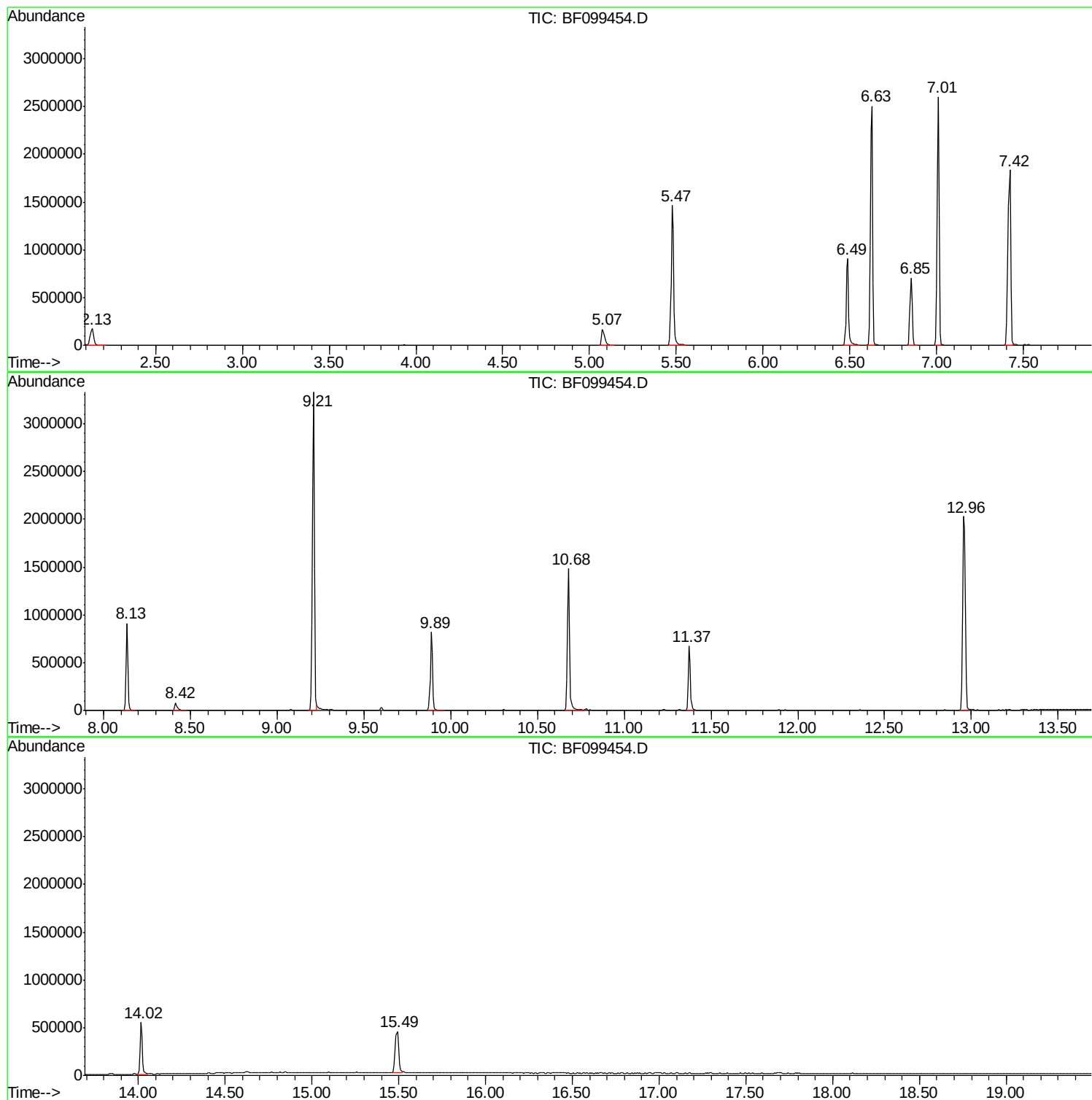
Sum of corrected areas: 19053569

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ClientSampled :
3906-PP4

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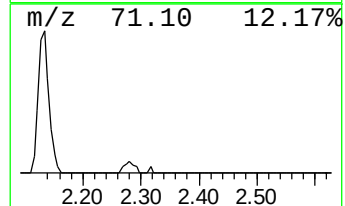
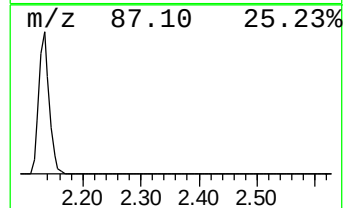
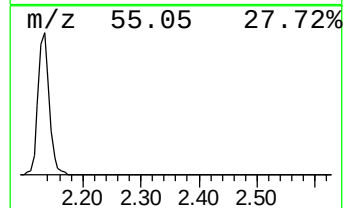
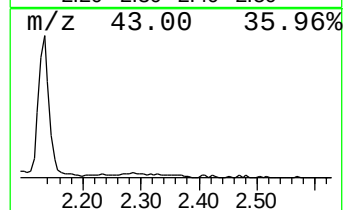
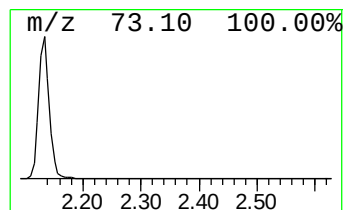
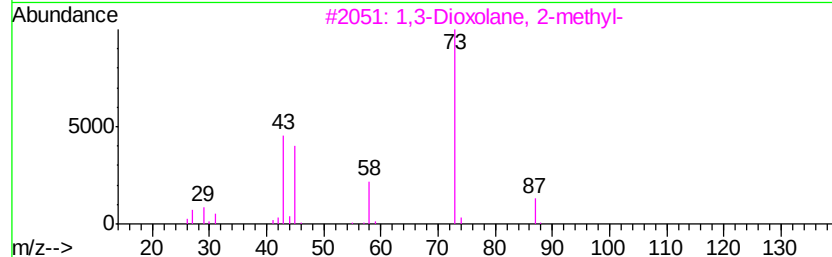
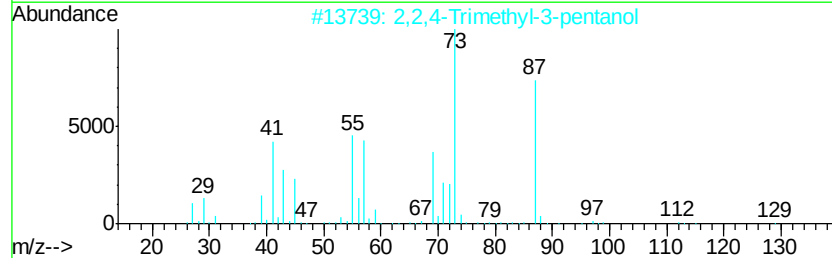
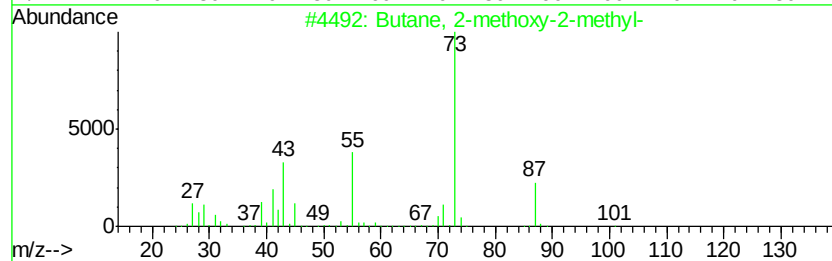
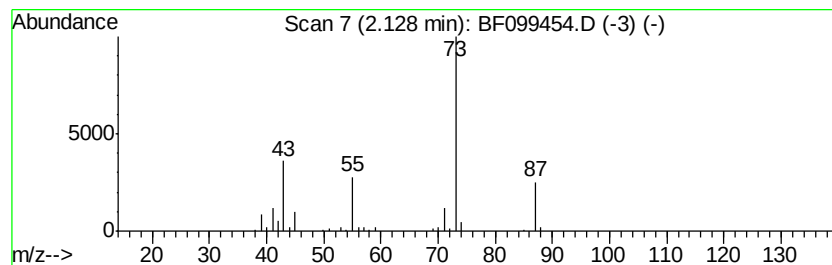
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	7.85 ng	222330	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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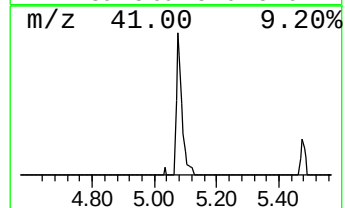
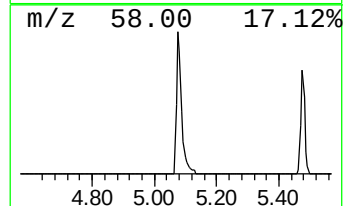
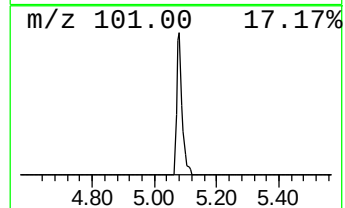
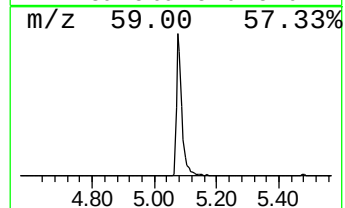
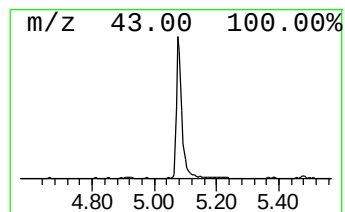
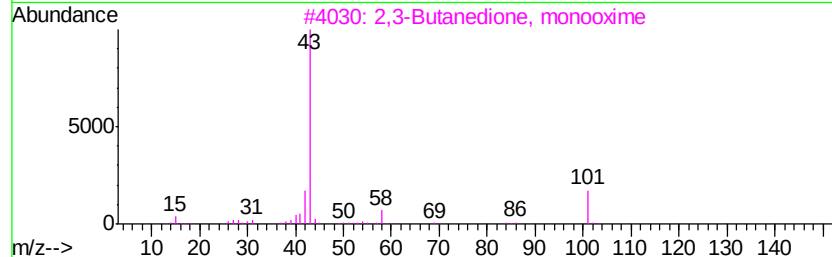
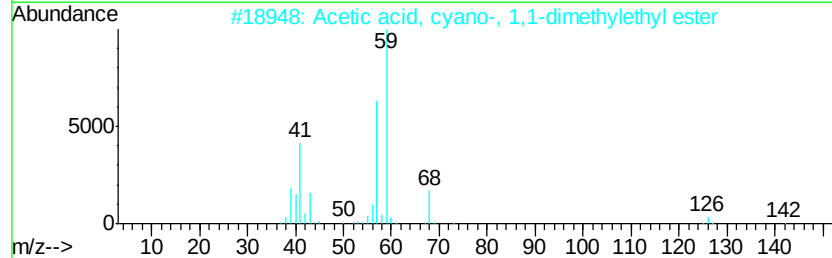
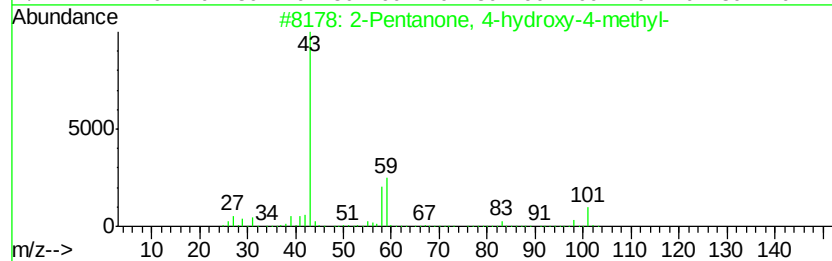
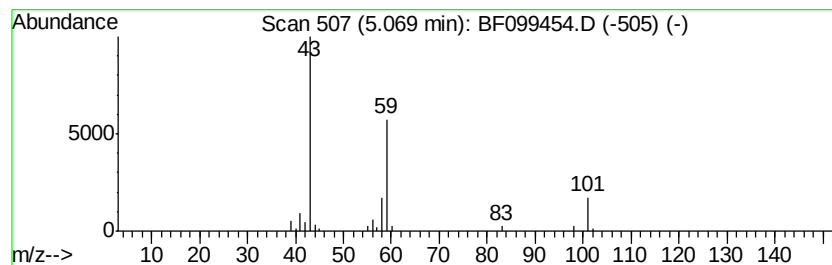
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.16 ng	203029	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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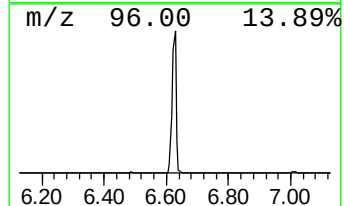
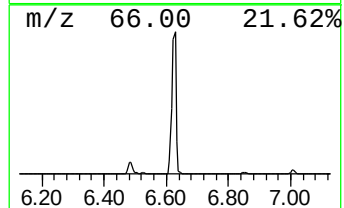
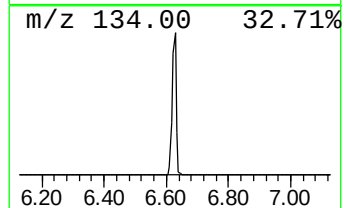
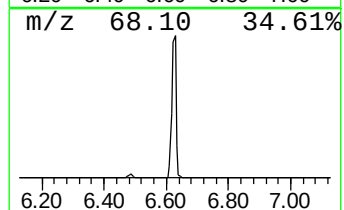
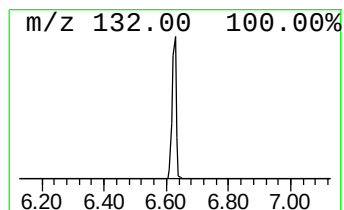
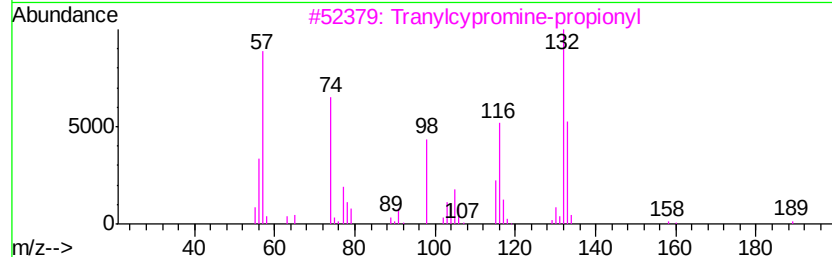
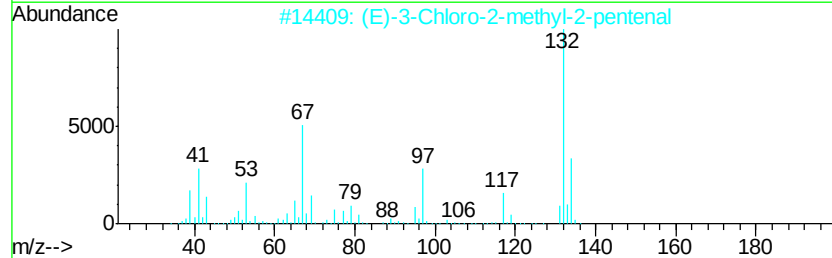
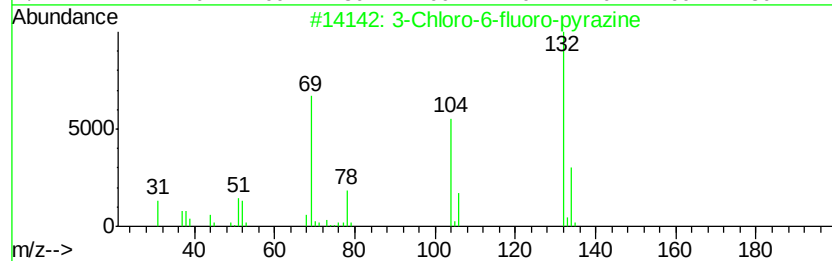
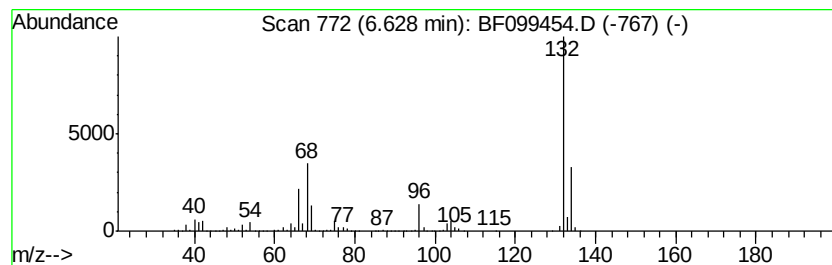
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	83.31 ng	2360660	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		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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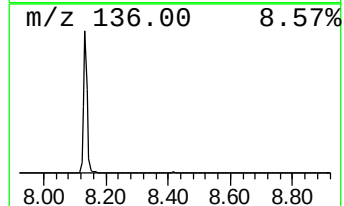
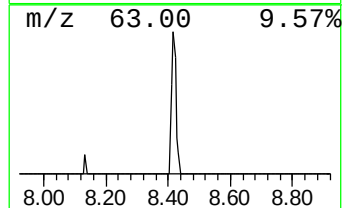
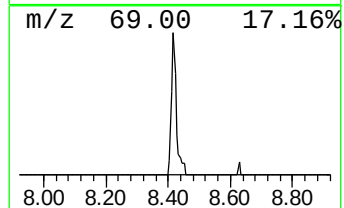
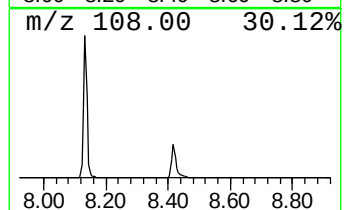
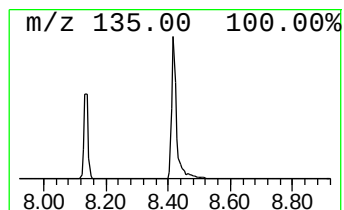
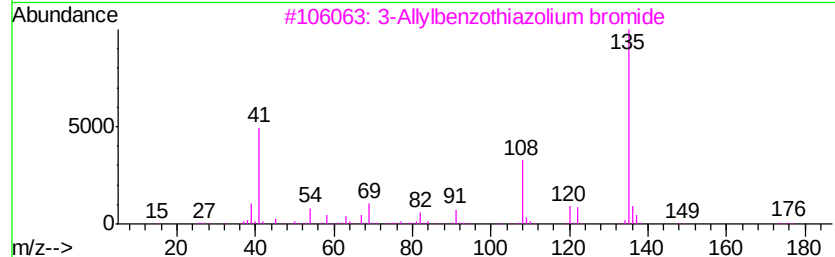
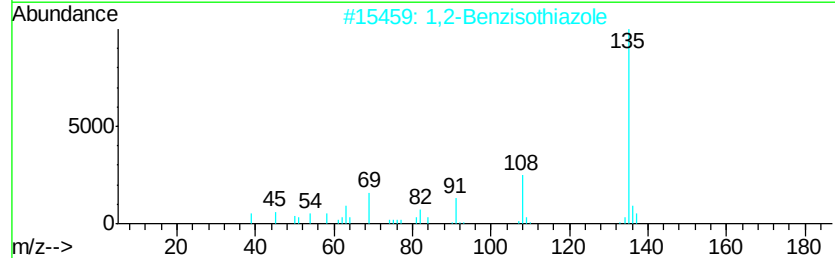
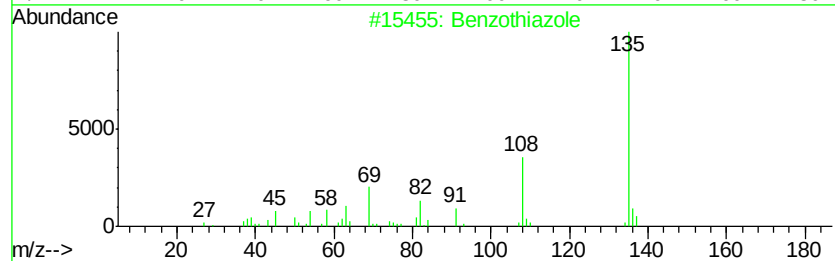
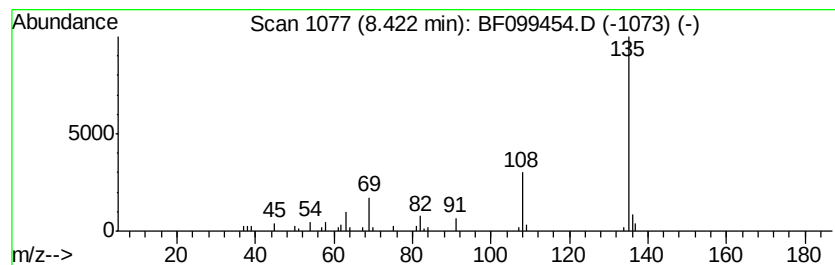
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Peak Number 5 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	2.04 ng	74158	Naphthalene-d8	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
4		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	78
5		Adenine	135	C5H5N5	000073-24-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	7.8	ng	222330	1	6.85	566735	20.0
2-Pentanone, 4-hy...	5.07	7.2	ng	203029	1	6.85	566735	20.0
unknown6.63	6.63	83.3	ng	2360660	1	6.85	566735	20.0
Benzothiazole	8.42	2.0	ng	74158	2	8.13	726191	20.0