

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099456.D
 Acq On : 13 Oct 2017 23:01
 Operator : SJ/JU
 Sample : I5819-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3908-SPP2

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	29	rVB	228739	415981	15.36%	2.290%
2	5.075	505	508	520	rBV	175719	197825	7.31%	1.089%
3	5.475	573	576	591	rBV	1355163	1285063	47.46%	7.075%
4	6.487	744	748	761	rBV	823874	775679	28.65%	4.271%
5	6.628	767	772	775	rBV	2251784	2148896	79.37%	11.831%
6	6.851	807	810	815	rBV	654070	516763	19.09%	2.845%
7	7.010	833	837	840	rBV	2351408	2087503	77.10%	11.493%
8	7.422	902	907	910	rBV	1649676	1589555	58.71%	8.752%
9	8.134	1024	1028	1035	rBV	834892	669258	24.72%	3.685%
10	8.416	1072	1076	1084	rBV	504722	461007	17.03%	2.538%
11	9.210	1206	1211	1214	rBV	3062974	2707528	100.00%	14.907%
12	9.886	1323	1326	1331	rVB2	721483	623777	23.04%	3.434%
13	10.680	1457	1461	1470	rBV	1388554	1239591	45.78%	6.825%
14	10.792	1476	1480	1489	rVB	43950	56107	2.07%	0.309%
15	10.922	1499	1502	1505	rBV	33724	33145	1.22%	0.182%
16	11.374	1576	1579	1583	rBV	587829	509525	18.82%	2.805%
17	12.957	1844	1848	1852	rBV	1900604	1855296	68.52%	10.215%
18	14.015	2025	2028	2036	rBV	503221	462341	17.08%	2.546%
19	15.492	2273	2279	2290	rVB	417709	527713	19.49%	2.906%

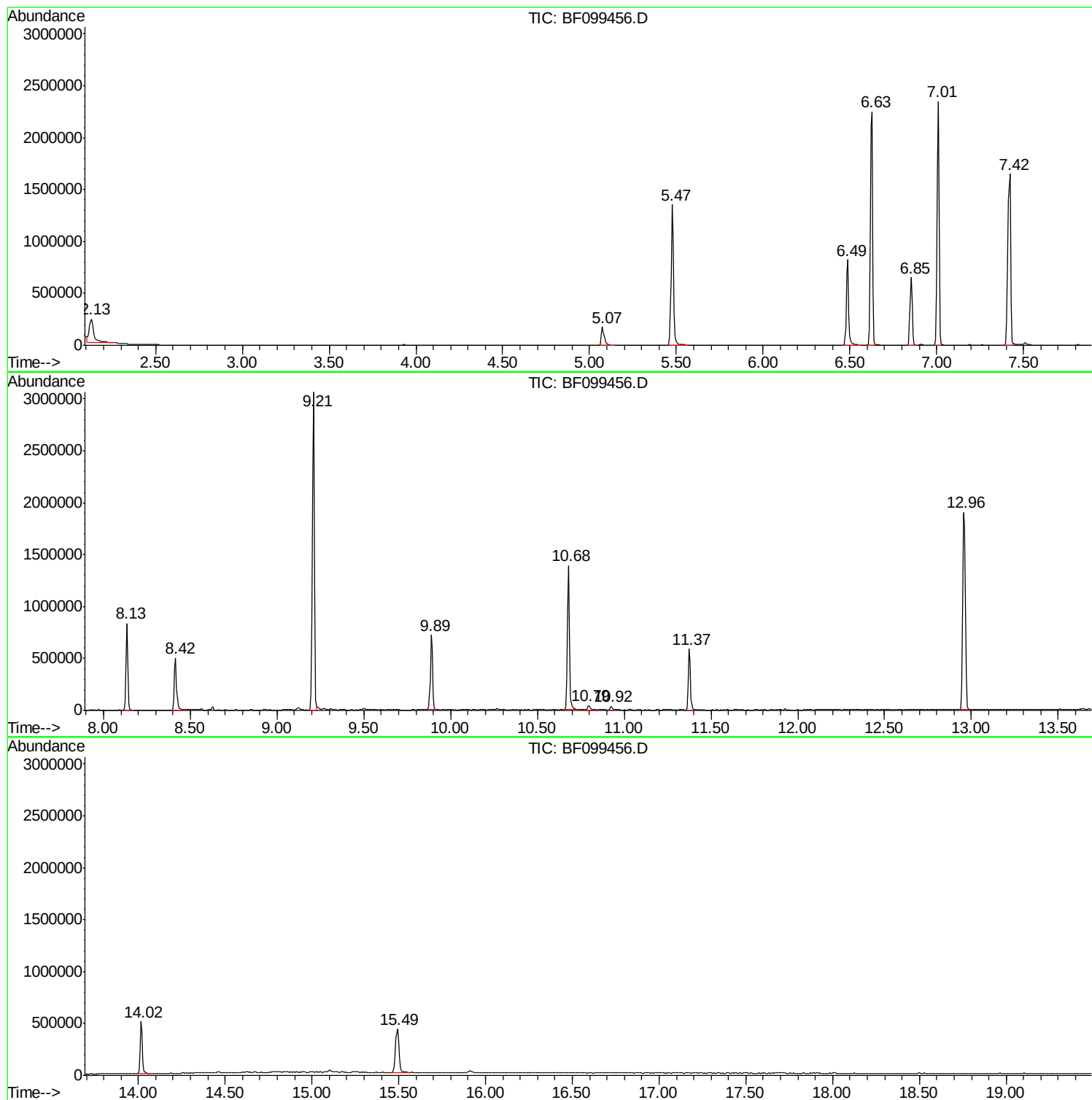
Sum of corrected areas: 18162553

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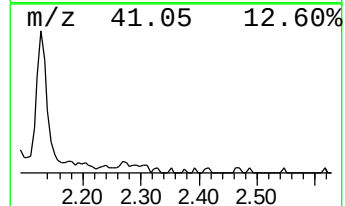
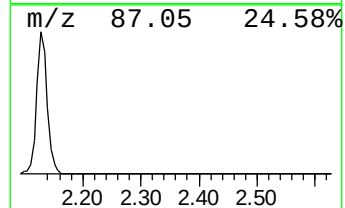
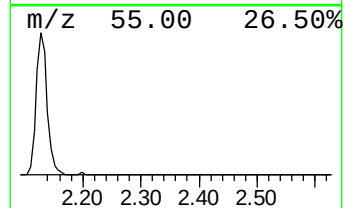
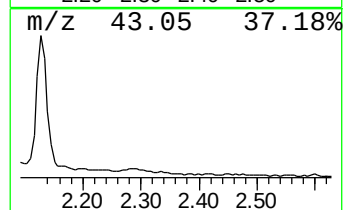
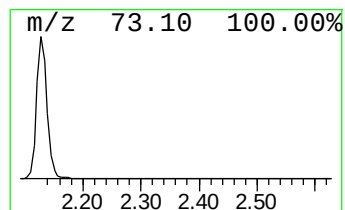
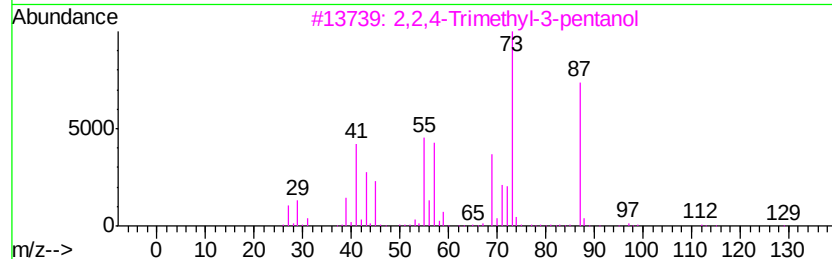
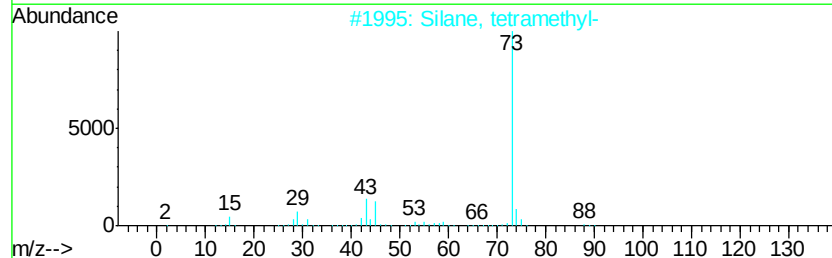
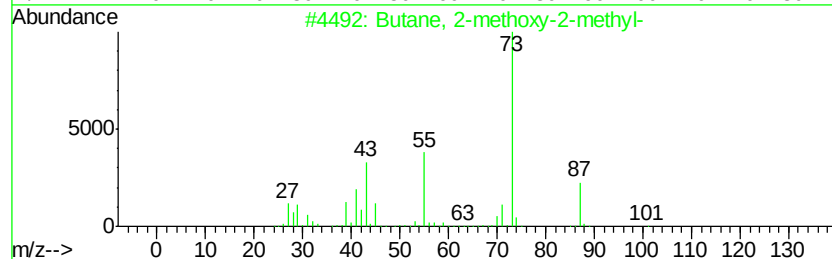
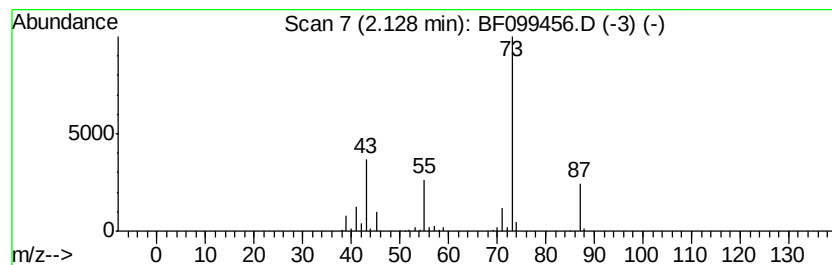
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	16.10 ng	415981	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	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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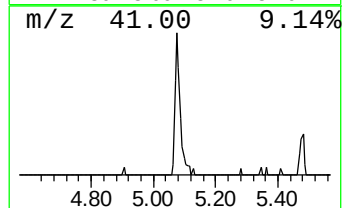
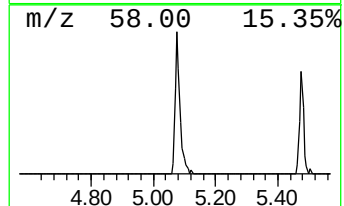
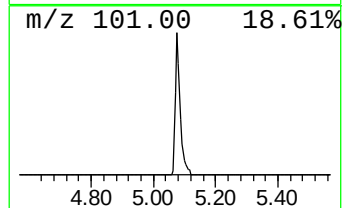
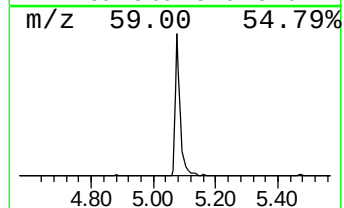
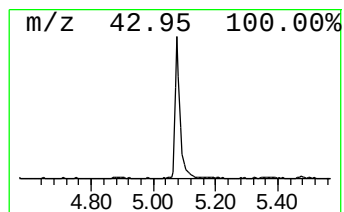
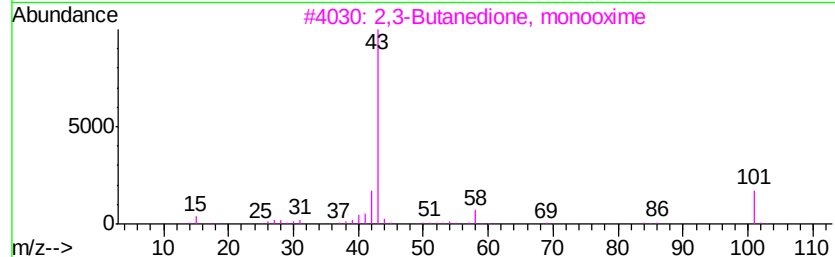
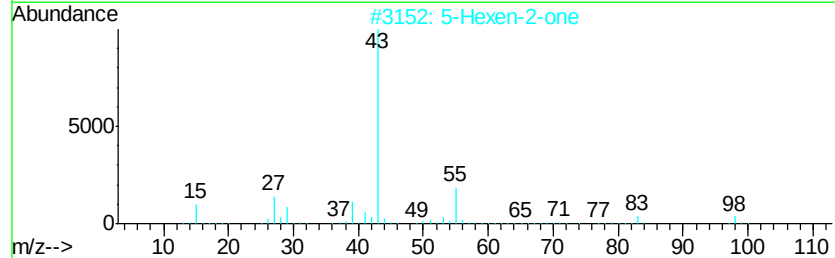
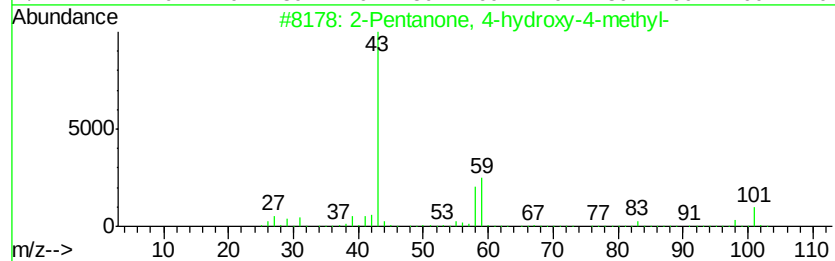
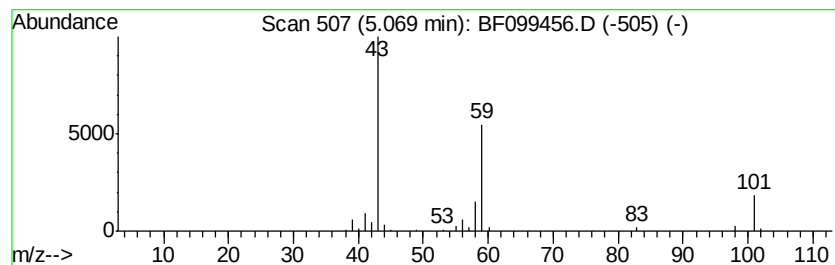
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.66 ng	197825	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		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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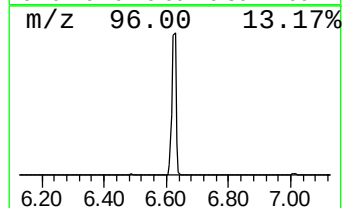
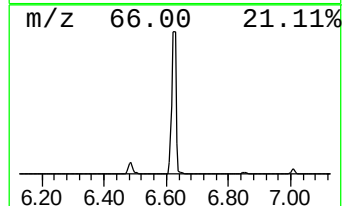
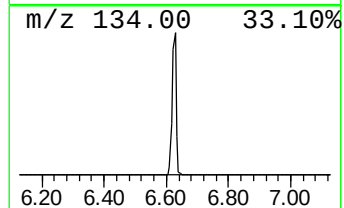
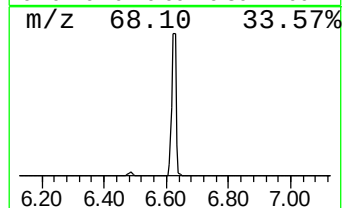
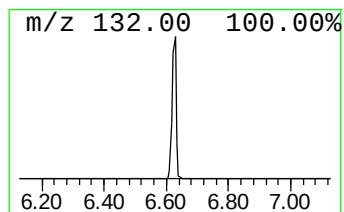
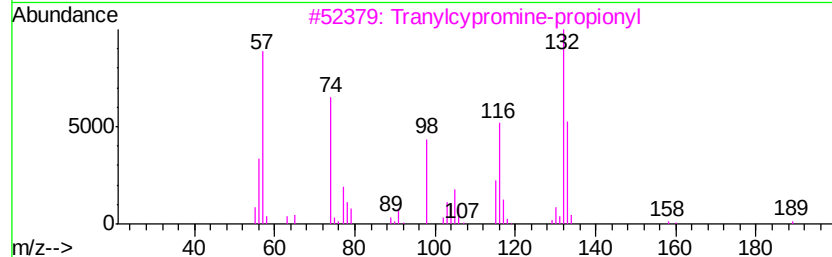
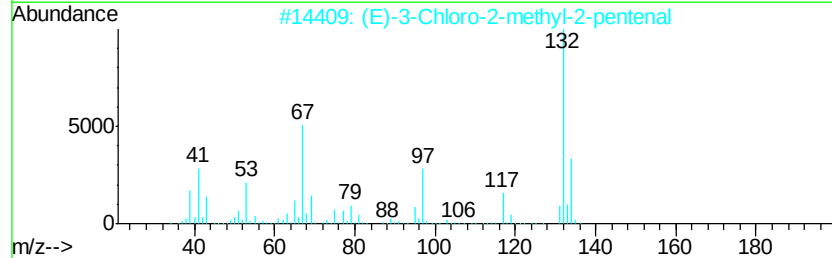
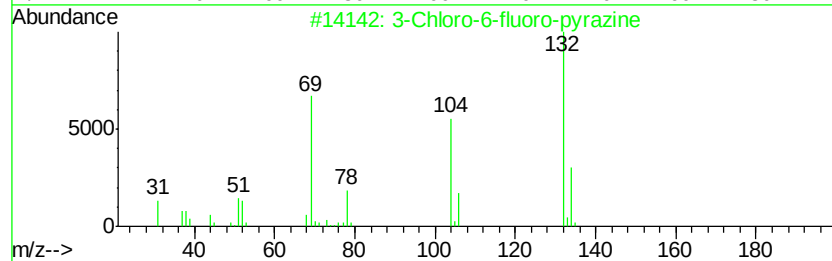
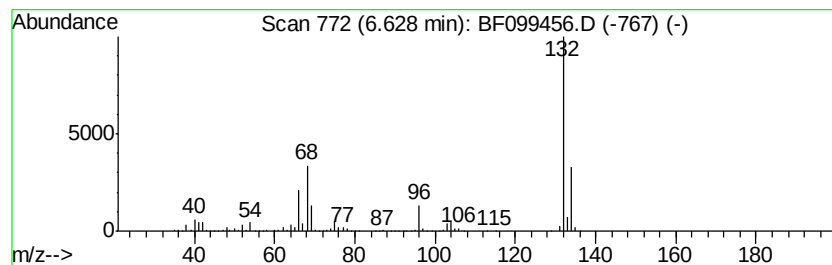
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	83.17 ng	2148900	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		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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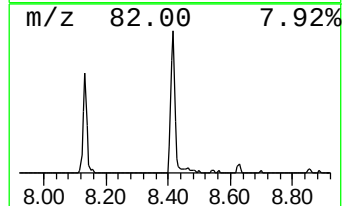
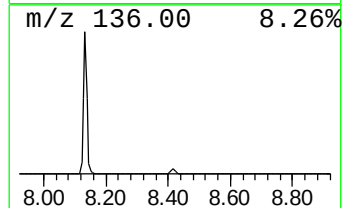
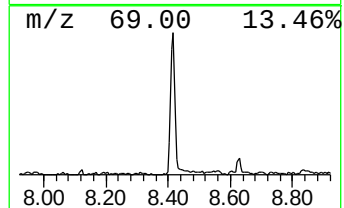
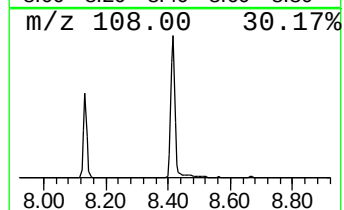
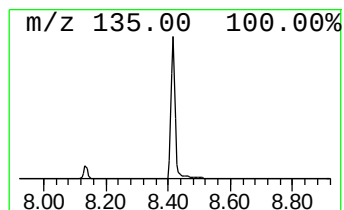
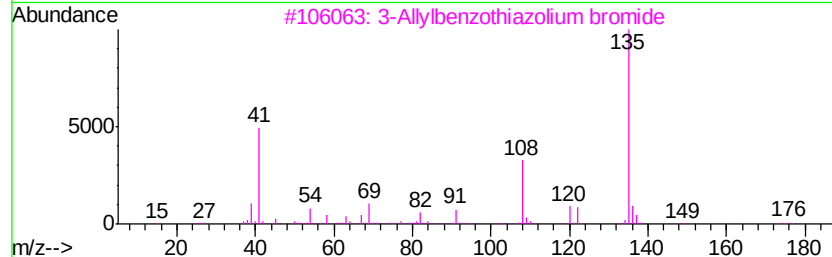
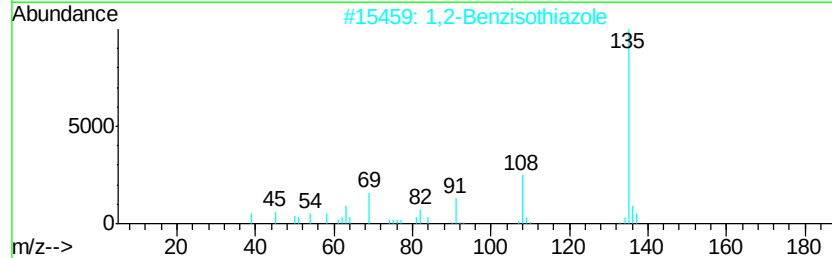
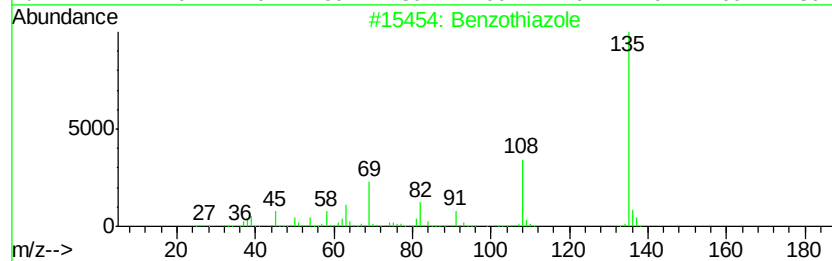
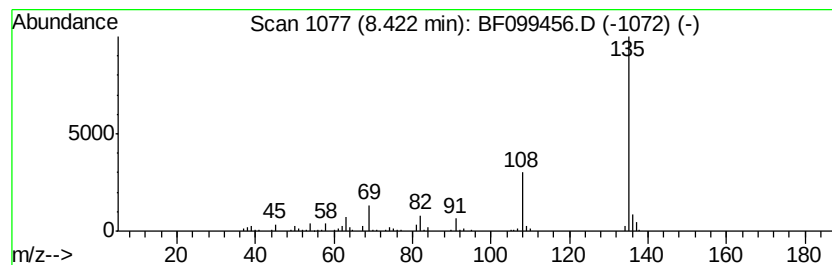
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	13.78 ng	461007	Naphthalene-d8	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	91
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
4		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
5		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	59



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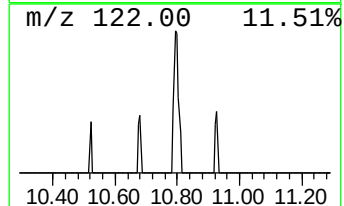
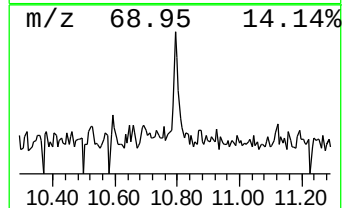
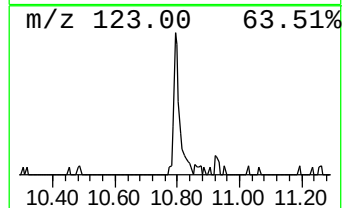
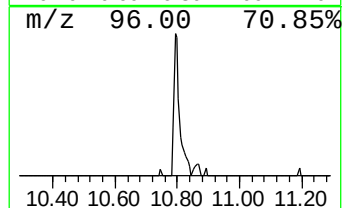
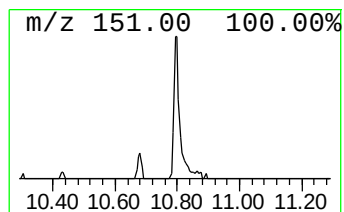
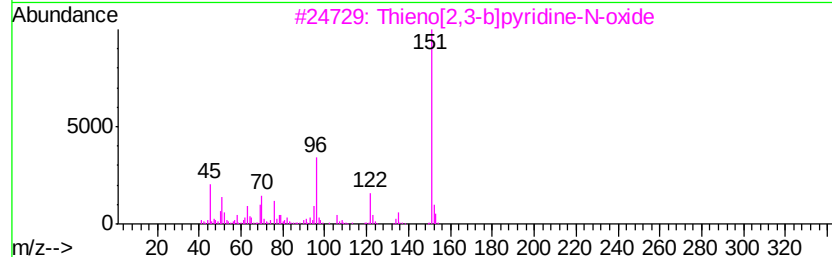
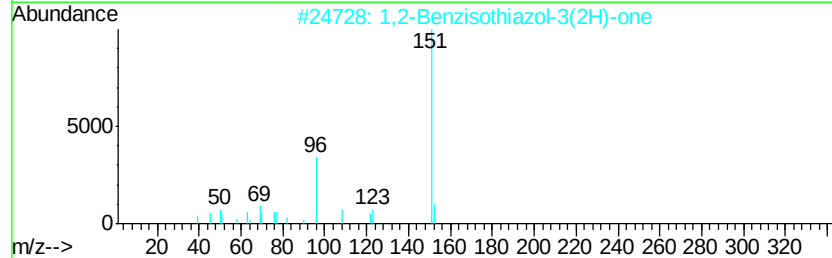
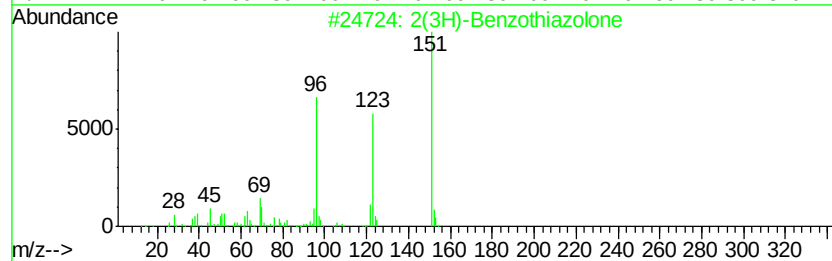
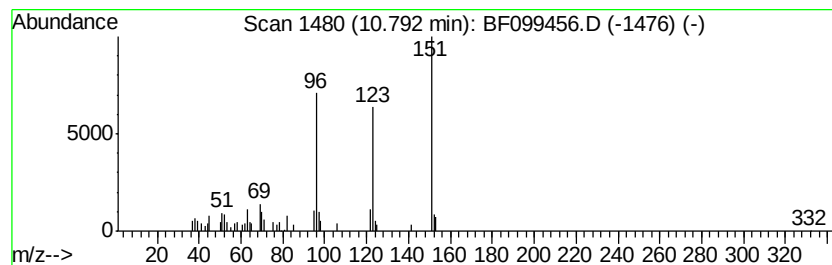
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Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.79	2.20 ng	56107	Phenanthrene-d10		11.37	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	58
3		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	52
4		6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	47
5		4-Methoxyformanilide	151	C8H9NO2	005470-34-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	16.1	ng	415981	1	6.85	516763	20.0
2-Pentanone, 4-hy...	5.07	7.7	ng	197825	1	6.85	516763	20.0
unknown6.63	6.63	83.2	ng	2148900	1	6.85	516763	20.0
Benzothiazole	8.42	13.8	ng	461007	2	8.13	669258	20.0
2(3H)-Benzothiazo...	10.79	2.2	ng	56107	4	11.37	509525	20.0