

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
 Data File : BM011385.D
 Acq On : 31 Aug 2017 23:09
 Operator : SJ/JU
 Sample : I4963-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3824-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_M\METHODS\8270-BM083117.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	3.058	41	46	56	rBV	1043387	1876104	5.26%	1.106%
2	3.134	56	59	75	rVB	490787	668168	1.87%	0.394%
3	5.081	383	390	398	rBV	350758	568199	1.59%	0.335%
4	5.546	462	469	478	rBV	5107277	7378930	20.70%	4.351%
5	7.134	732	739	747	rBV	2990785	4621715	12.97%	2.725%
6	7.516	793	804	815	rBV	8862990	14455564	40.56%	8.524%
7	7.987	878	884	891	rBV	1845747	2967053	8.33%	1.750%
8	8.316	931	940	952	rBV	7582613	12843876	36.04%	7.574%
9	9.151	1072	1082	1091	rBV	6482136	10692231	30.00%	6.305%
10	10.798	1352	1362	1373	rBV	2651271	4439130	12.46%	2.618%
11	11.445	1466	1472	1482	rVB	445257	823718	2.31%	0.486%
12	13.245	1767	1778	1786	rBV	16912545	24850896	69.73%	14.654%
13	14.621	2004	2012	2022	rBV2	3949538	5827421	16.35%	3.436%
14	16.104	2257	2264	2283	rBV	12964367	18443134	51.75%	10.875%
15	17.357	2471	2477	2484	rBV2	4611602	6861241	19.25%	4.046%
16	19.509	2839	2843	2856	rBV	272344	398448	1.12%	0.235%
17	19.968	2915	2921	2927	rBV	28859065	35639346	100.00%	21.015%
18	21.521	3180	3185	3190	rBV	6979893	8563310	24.03%	5.049%
19	23.903	3583	3590	3600	rVB2	3850272	7671204	21.52%	4.523%

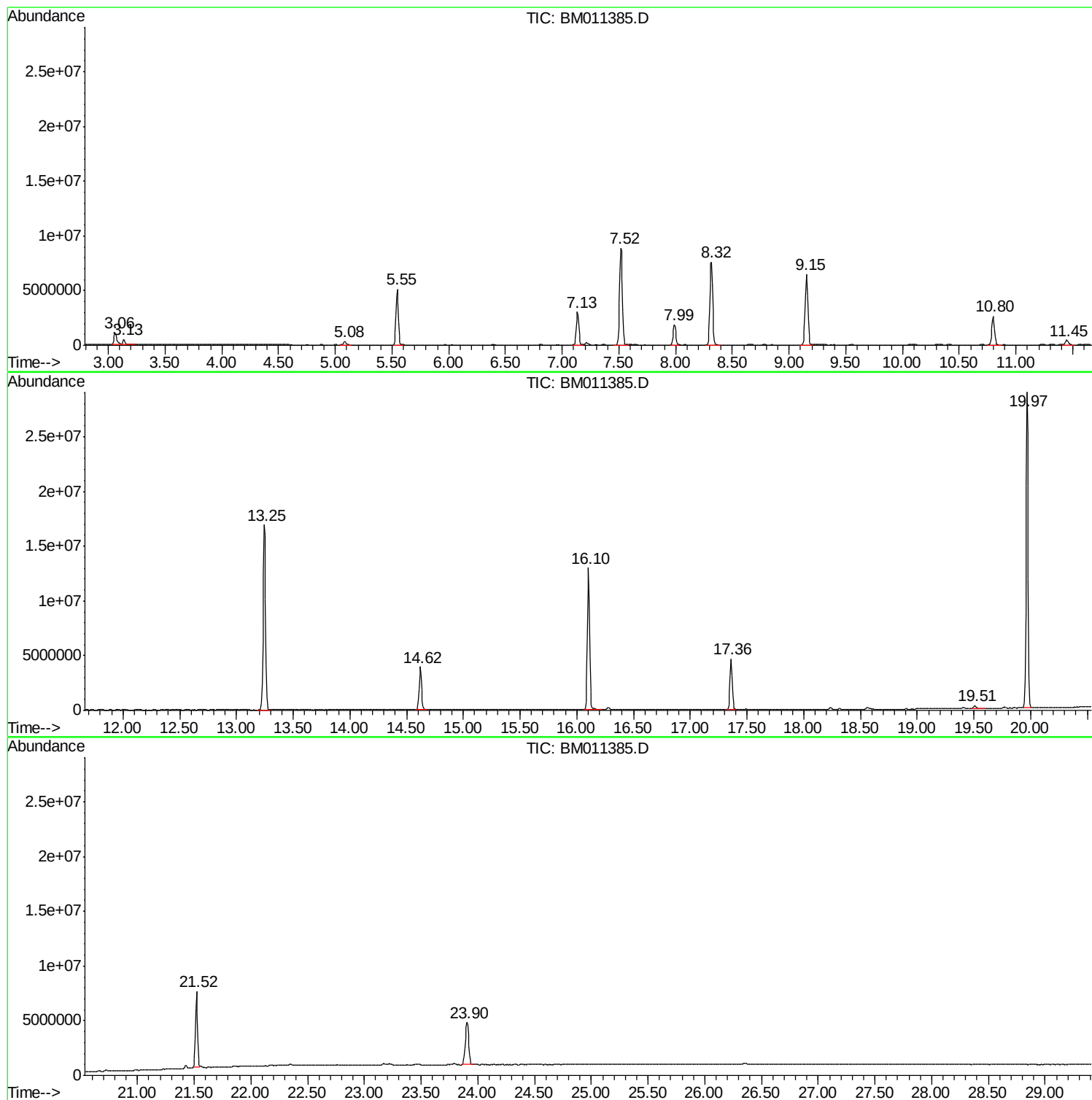
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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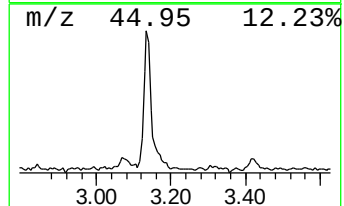
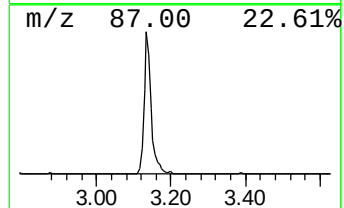
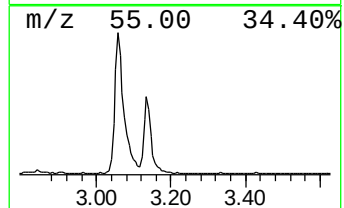
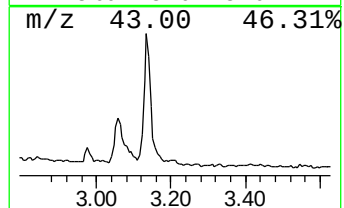
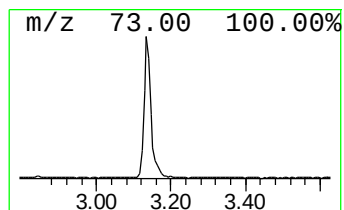
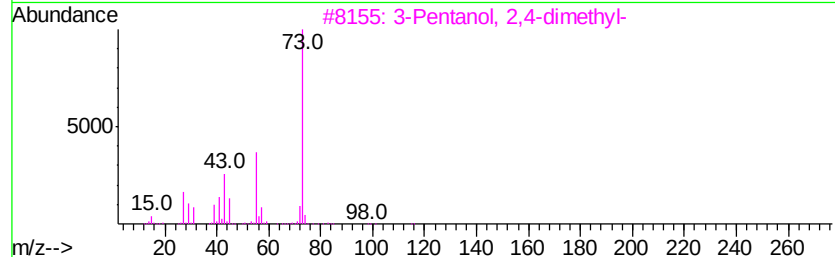
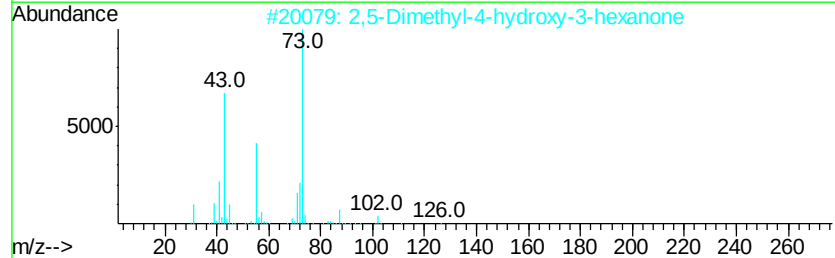
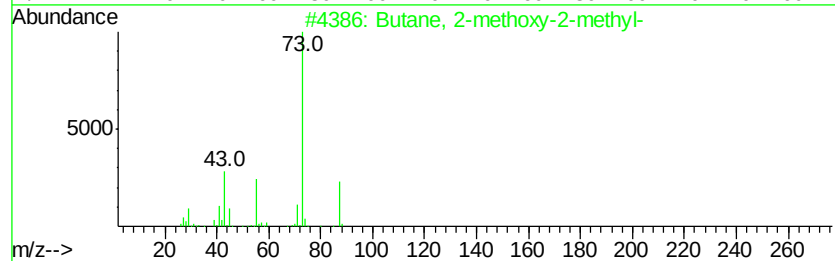
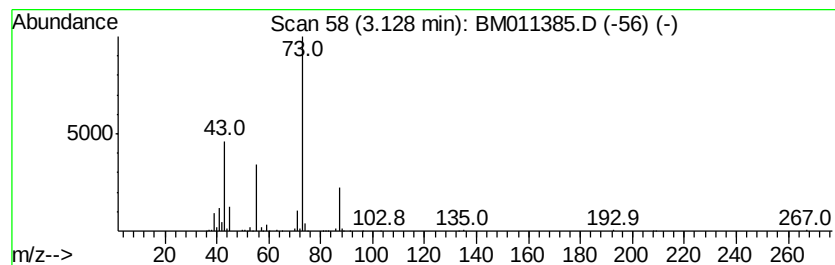
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	4.50 ng	668168	1,4-Dichlorobenzene-d4	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32



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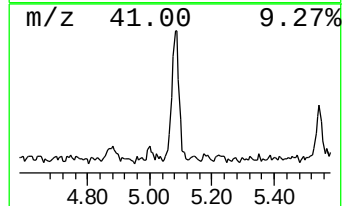
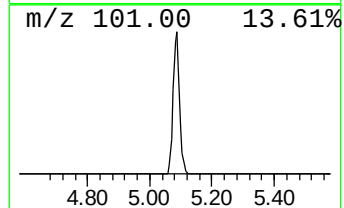
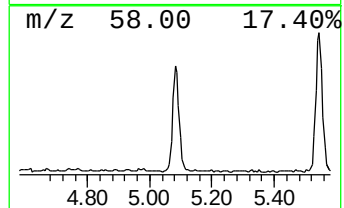
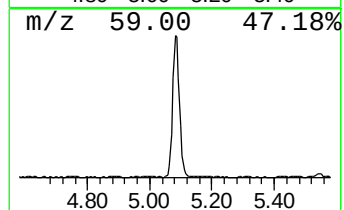
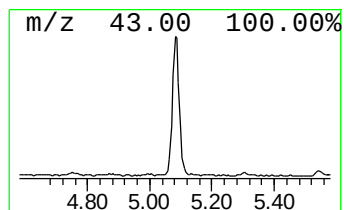
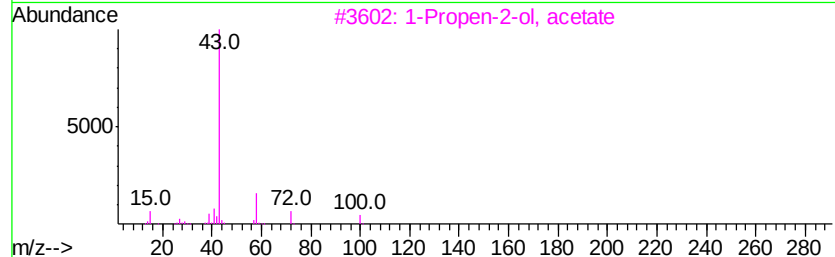
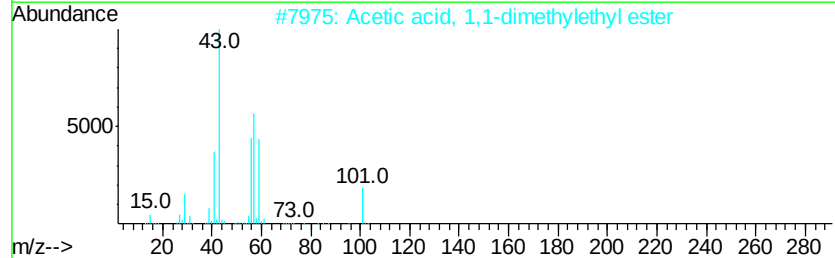
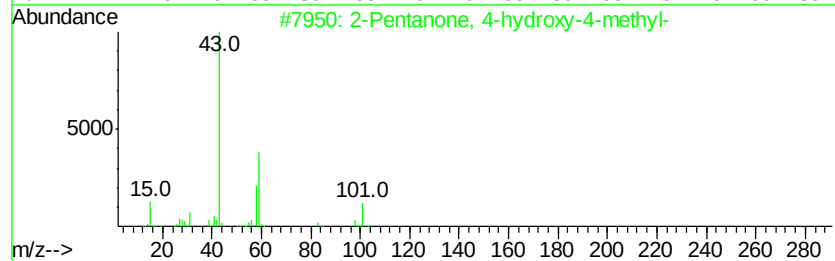
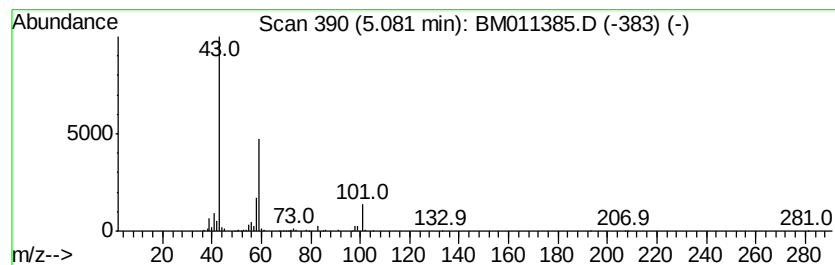
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	3.83 ng	568199	1,4-Dichlorobenzene-d4	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		Acetone	58	C3H6O	000067-64-1	9



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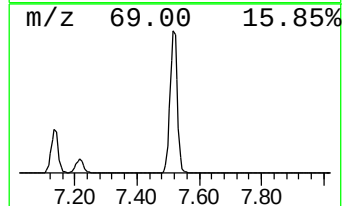
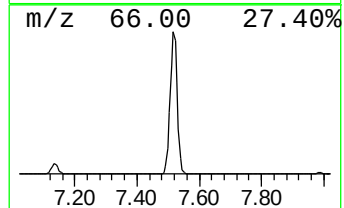
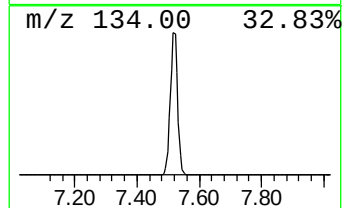
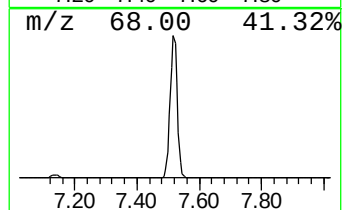
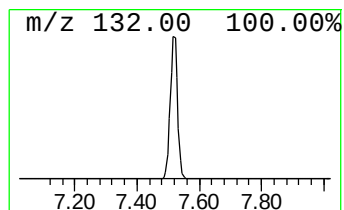
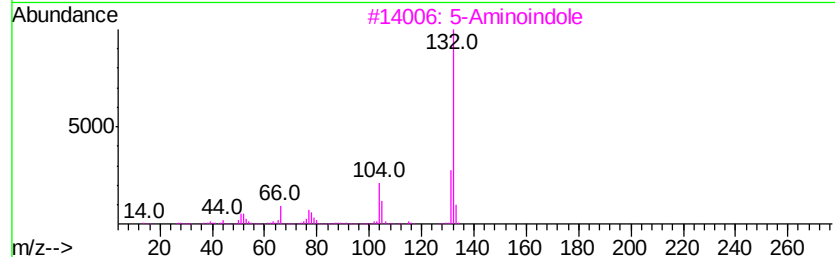
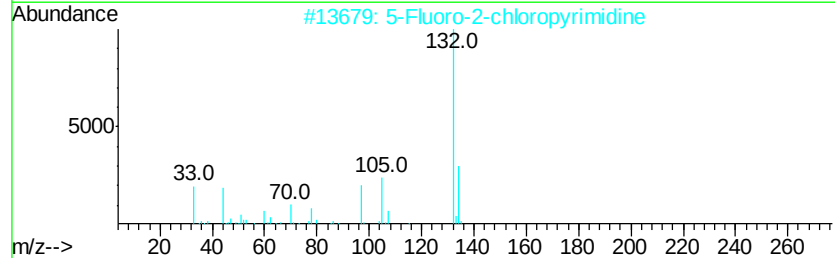
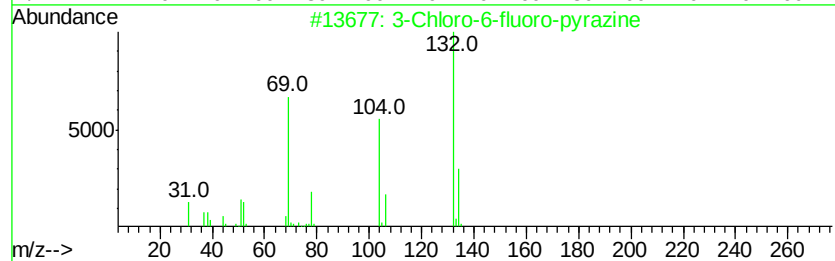
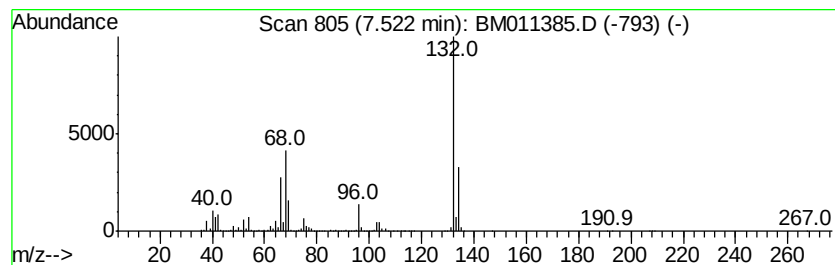
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Peak Number 4 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	97.44 ng	14455600	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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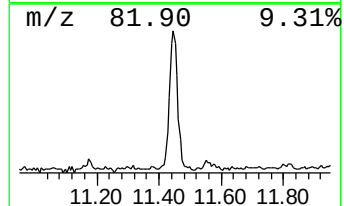
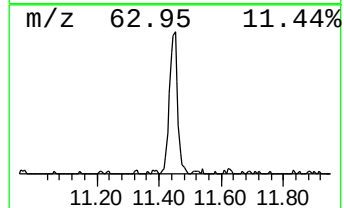
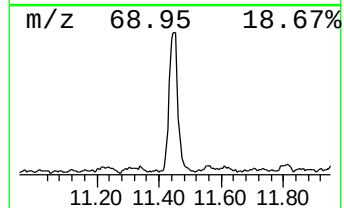
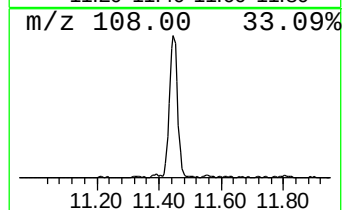
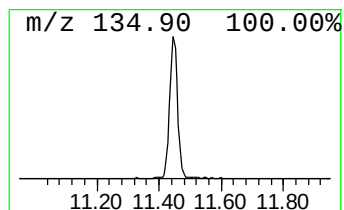
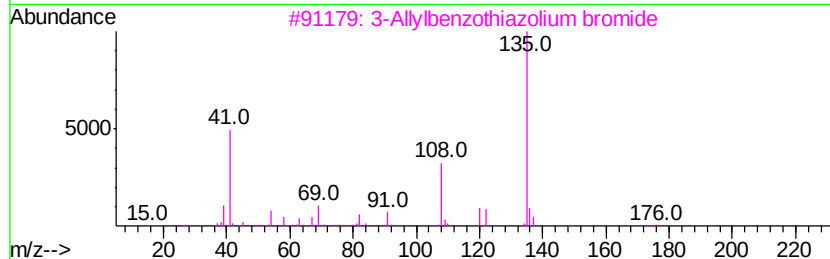
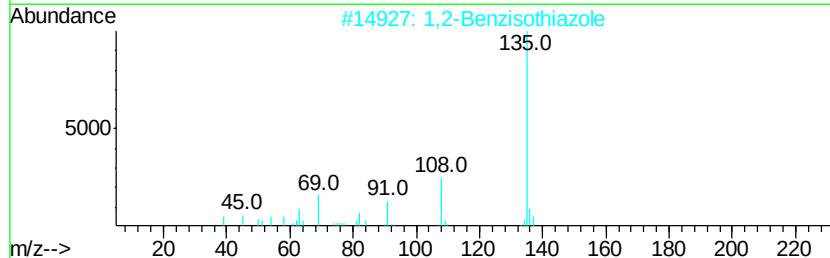
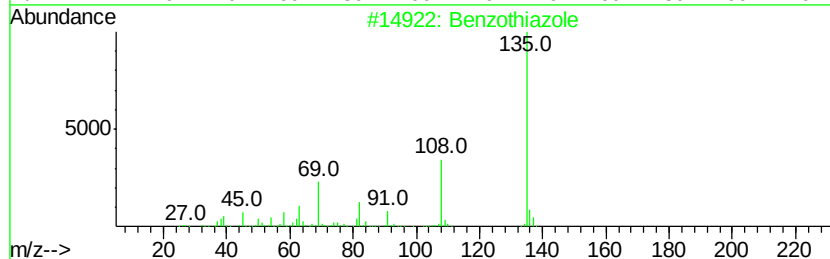
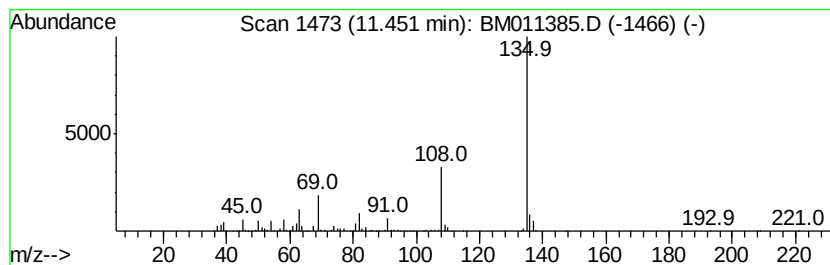
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Peak Number 6 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	3.71 ng	823718	Naphthalene-d8	10.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	97
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
4		2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5		Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	4.5	ng	668168	1	7.99	2967050	20.0
2-Pentanone, 4-hy...	5.08	3.8	ng	568199	1	7.99	2967050	20.0
unknown7.52	7.52	97.4	ng	14455600	1	7.99	2967050	20.0
Benzothiazole	11.45	3.7	ng	823718	2	10.80	4439130	20.0