

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016646.D
 Acq On : 01 Oct 2021 21:23
 Operator : CG/JU
 Sample : M3833-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 DUP01-20210920

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 1 % 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:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	5	9	12	rBV	1175899	1829703	100.00%	50.647%
2	3.825	77	81	97	rVB	9544	37285	2.04%	1.032%
3	4.821	185	189	203	rVB	44051	93854	5.13%	2.598%
4	6.831	403	407	421	rVB2	5761	19011	1.04%	0.526%
5	7.642	490	495	500	rBV	48233	97065	5.30%	2.687%
6	8.784	601	605	612	rBV	25213	49373	2.70%	1.367%
7	10.191	713	716	725	rBV	31544	54818	3.00%	1.517%
8	10.407	729	733	737	rBV	101029	173432	9.48%	4.801%
9	12.003	919	931	943	rBV2	43356	71079	3.88%	1.968%
10	12.886	1071	1074	1078	rBV	81130	151684	8.29%	4.199%
11	14.269	1180	1183	1186	rBV	128152	188162	10.28%	5.208%
12	17.018	1400	1403	1410	rBV	88595	153863	8.41%	4.259%
13	19.068	1689	1697	1720	rBV	111199	159205	8.70%	4.407%
14	19.678	1813	1820	1843	rBV	109140	138238	7.56%	3.827%
15	21.164	1993	1995	1998	rBV	28590	40966	2.24%	1.134%
16	21.238	1998	2002	2011	rVB2	108493	173515	9.48%	4.803%
17	23.484	2415	2427	2457	rVB	91315	181392	9.91%	5.021%

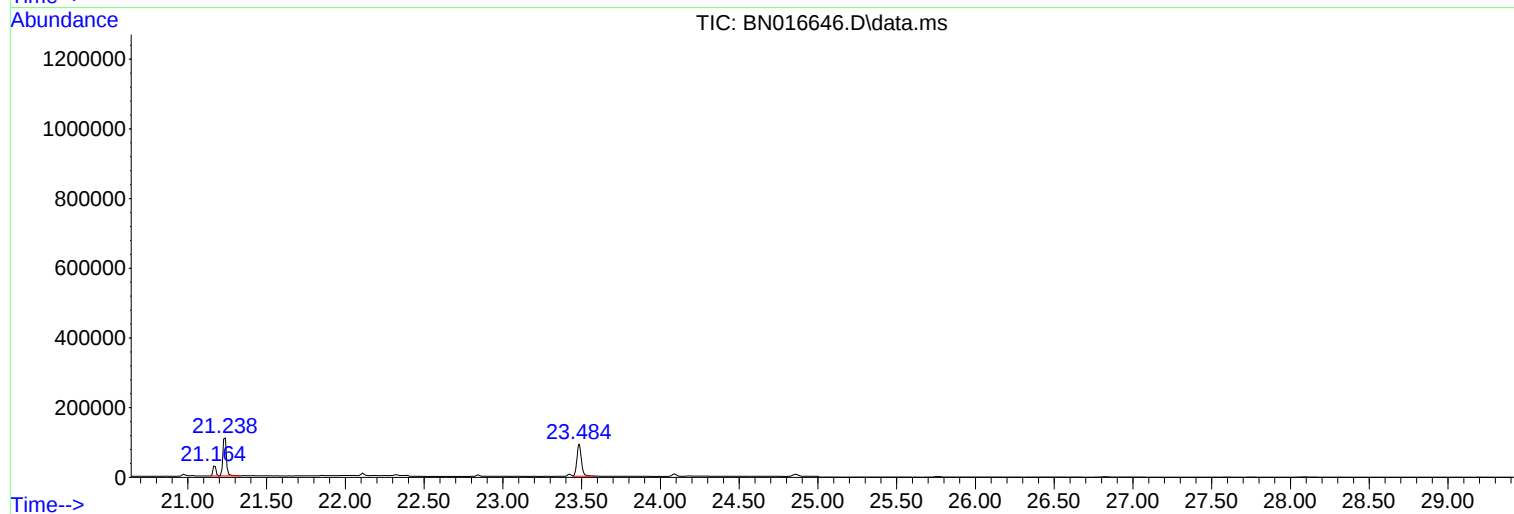
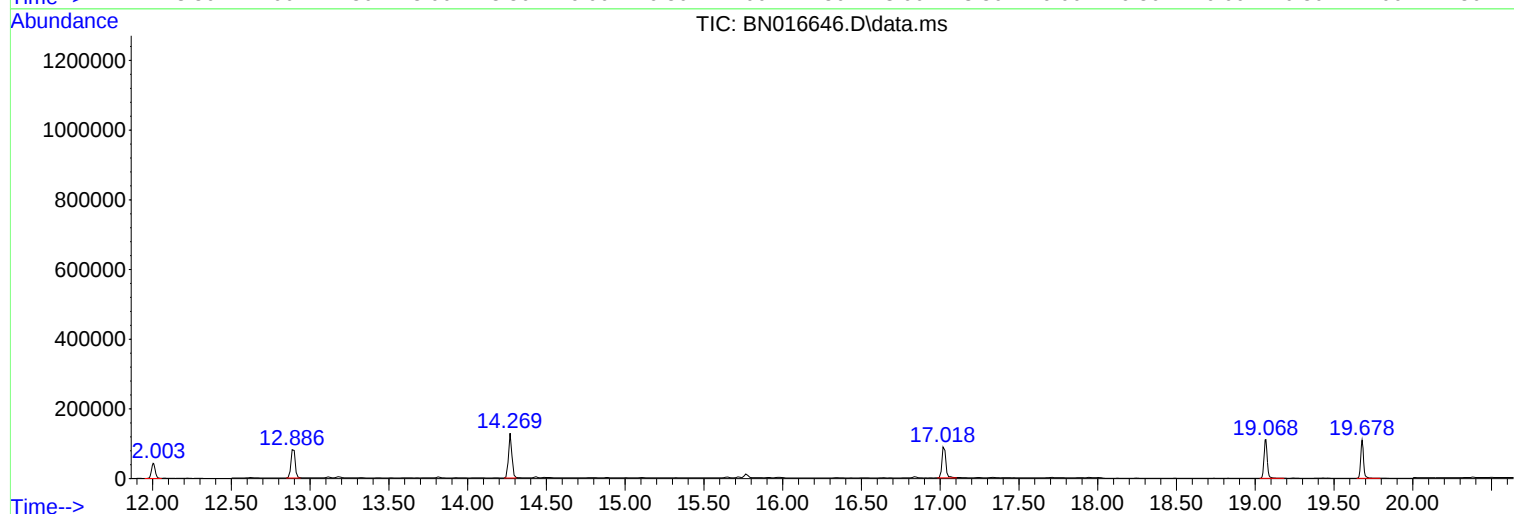
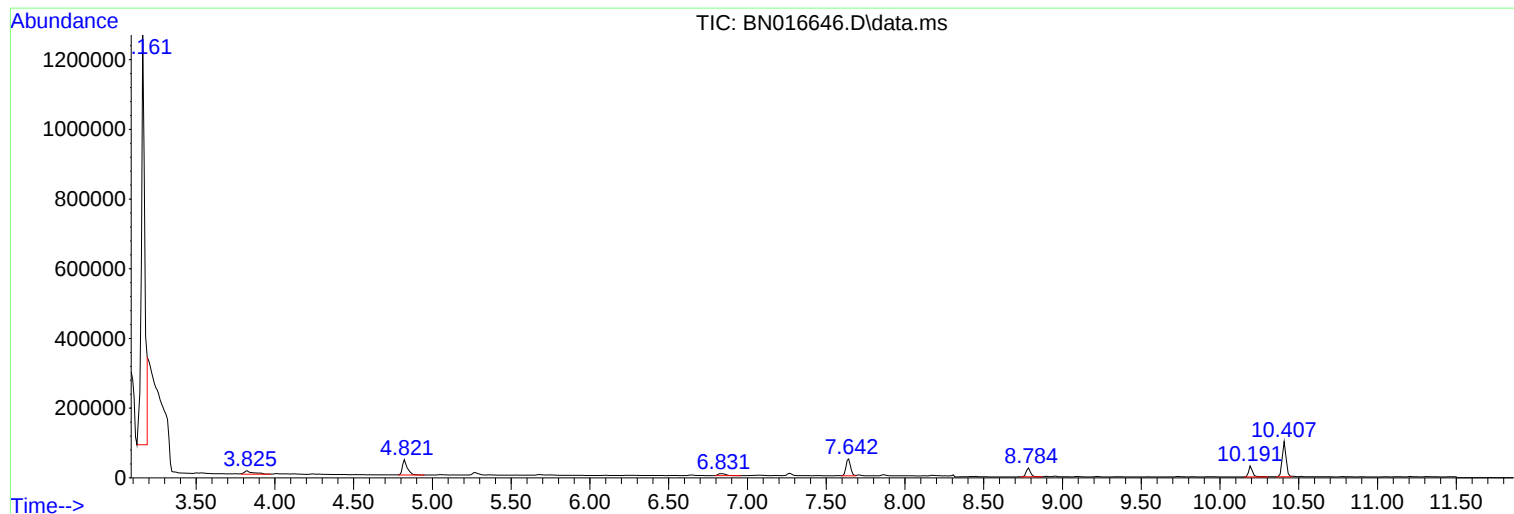
Sum of corrected areas: 3612645

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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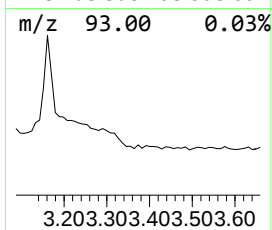
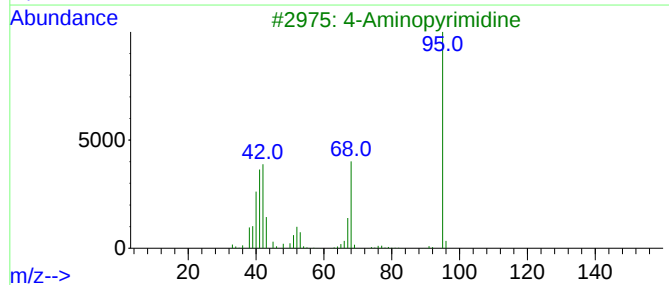
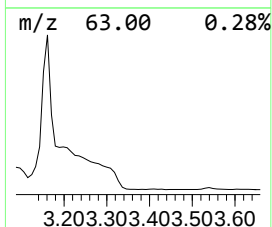
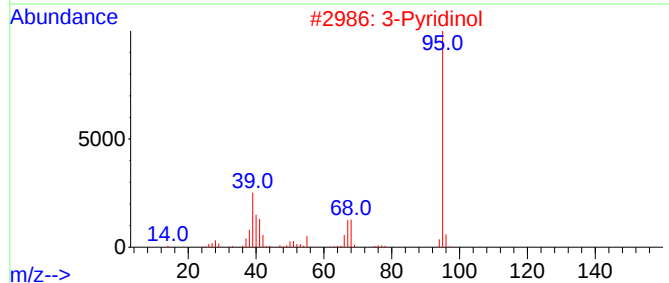
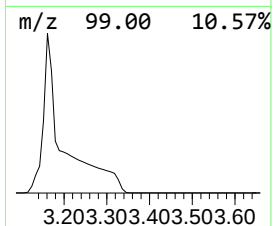
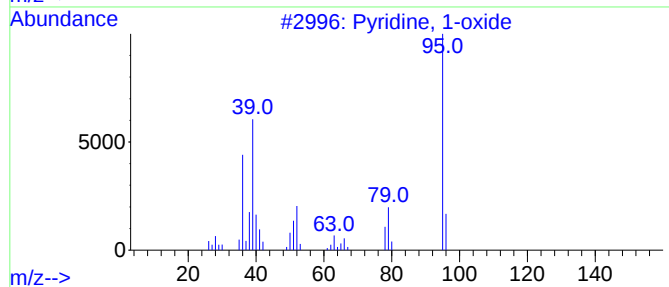
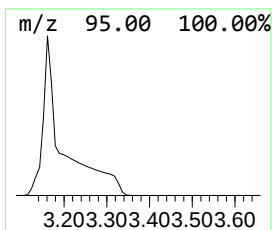
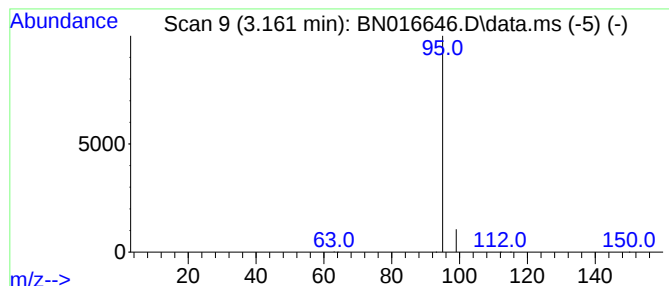
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	7.54 ng	1829700	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4			4-Pyridinol	95	C5H5NO	000626-64-2	2
5			2-(Aminomethylene)aminoacrylonitrile	95	C4H5N3	167320-31-2	2



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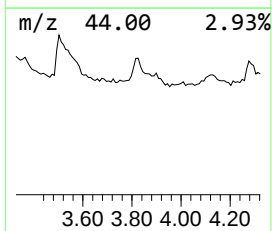
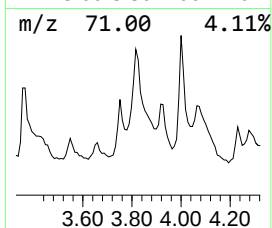
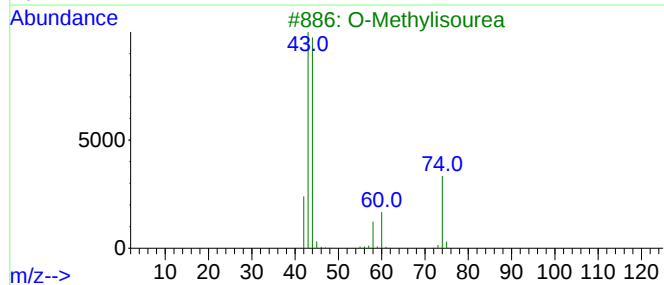
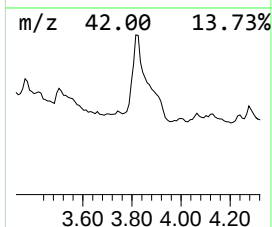
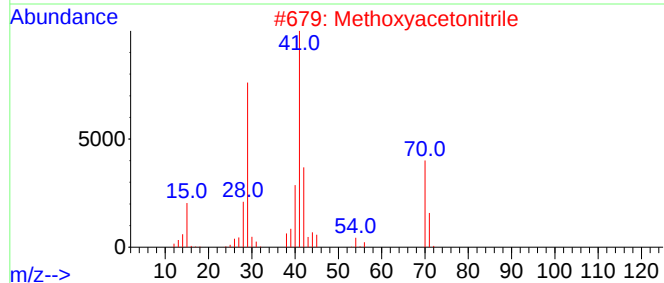
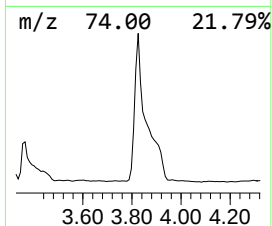
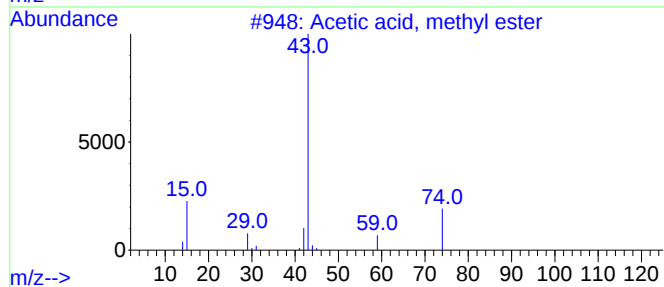
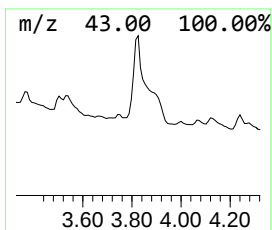
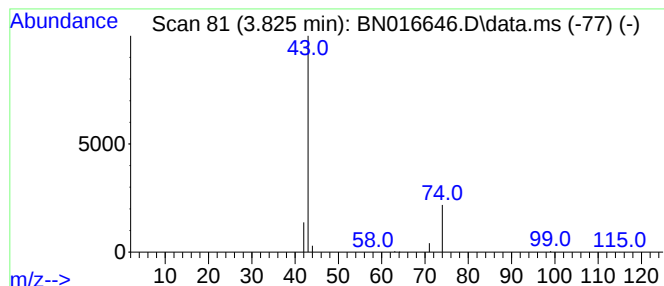
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Peak Number 2 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.15 ng	37285	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2			Methoxyacetoneitrile	71	C3H5NO	001738-36-9	4
3			O-Methylisourea	74	C2H6N2O	002440-60-0	4
4			Hydrogen azide	43	HN3	007782-79-8	4
5			1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3



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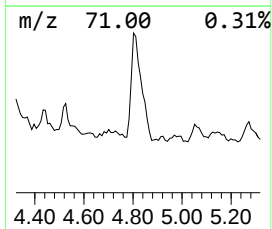
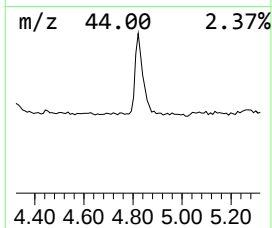
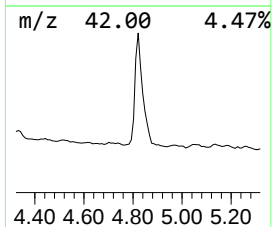
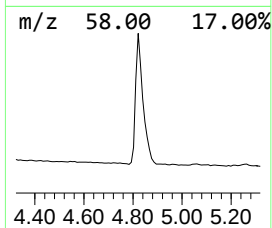
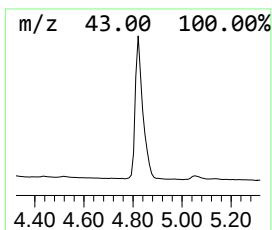
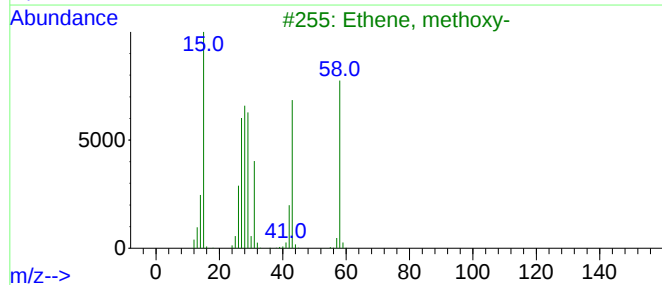
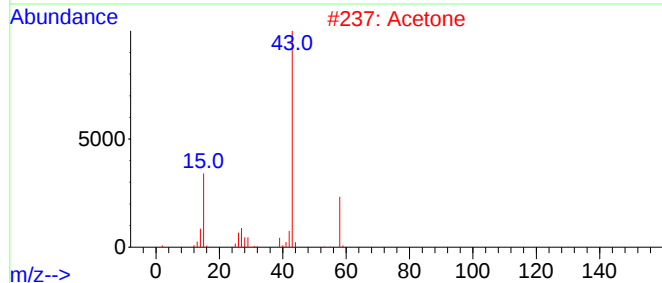
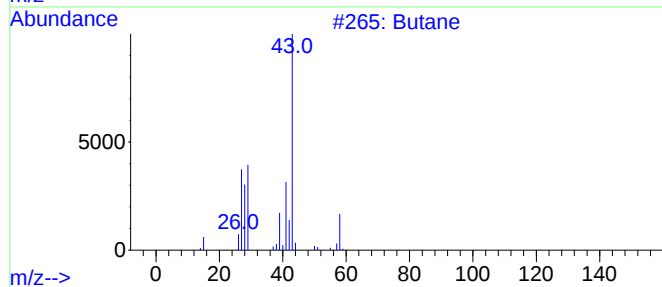
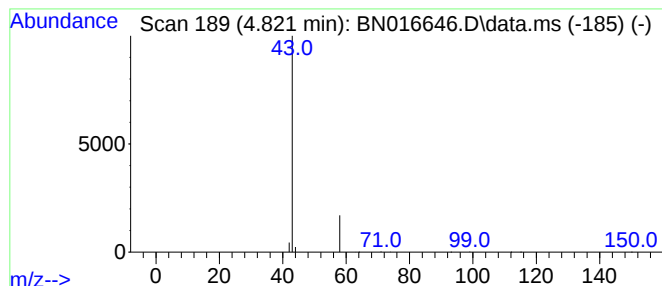
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Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.39 ng	93854	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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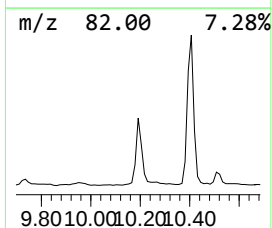
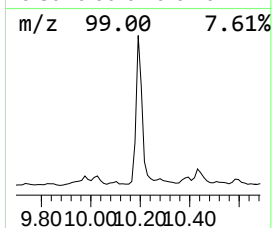
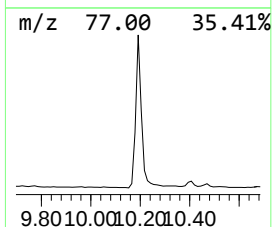
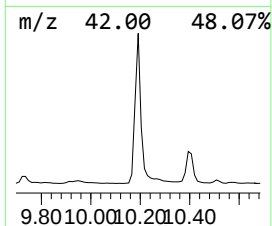
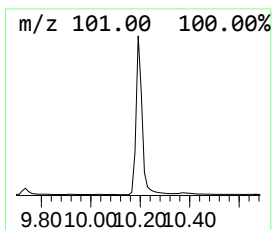
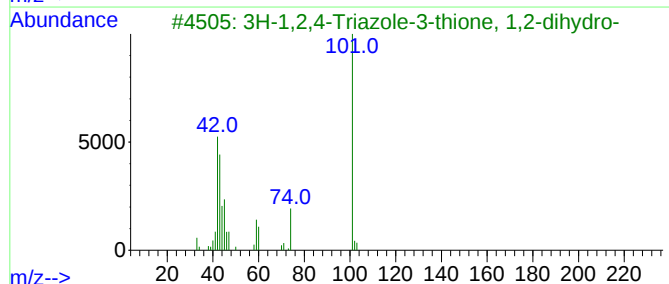
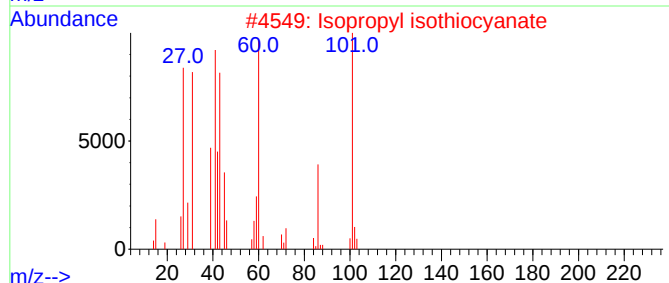
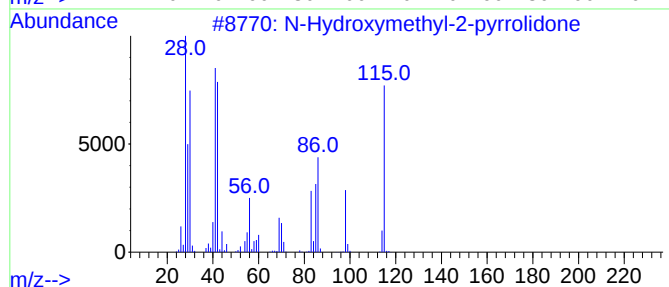
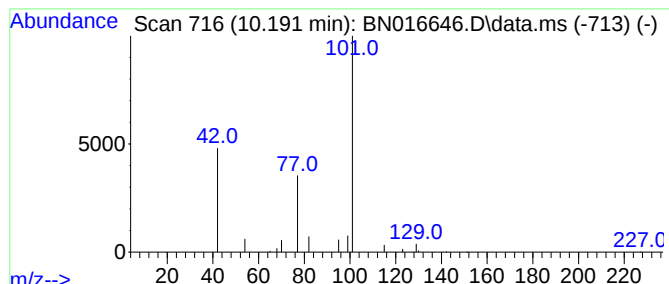
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Peak Number 4 N-Hydroxymethyl-2-pyrrolidone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.13 ng	54818	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Hydroxymethyl-2-pyrrolidone	115	C5H9NO2	1000426-51-3	7
2			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	7.5	ng	1829700	1	7.642	97065	0.4
Acetic acid, me...	3.825	0.2	ng	37285	1	7.642	97065	0.4
Butane	4.821	0.4	ng	93854	1	7.642	97065	0.4
N-Hydroxymethyl...	10.191	0.1	ng	54818	2	10.407	173432	0.4