

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016625.D
 Acq On : 01 Oct 2021 07:47
 Operator : CG/JU
 Sample : M3833-15
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE122D1-20210920

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: BN016625.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	4	9	12	rBV	1059851	1923352	100.00%	48.607%
2	3.816	76	80	96	rVB	13749	53546	2.78%	1.353%
3	4.821	185	189	202	rVB	65198	139945	7.28%	3.537%
4	5.273	234	238	246	rVB	9233	22923	1.19%	0.579%
5	6.840	403	408	418	rVB2	6999	22993	1.20%	0.581%
6	7.633	490	494	499	rBV	48040	100177	5.21%	2.532%
7	8.785	601	605	610	rBV	28792	56582	2.94%	1.430%
8	10.191	713	716	721	rBV	32770	53004	2.76%	1.340%
9	10.407	729	733	736	rBV	101459	175184	9.11%	4.427%
10	12.003	921	931	943	rBV	50120	82561	4.29%	2.086%
11	12.886	1071	1074	1078	rBV	106055	187533	9.75%	4.739%
12	14.269	1180	1183	1186	rBV	130669	193500	10.06%	4.890%
13	15.766	1299	1301	1305	rVB2	13064	23389	1.22%	0.591%
14	17.018	1400	1403	1406	rBV	101731	161568	8.40%	4.083%
15	19.063	1689	1696	1721	rBV	134987	183371	9.53%	4.634%
16	19.679	1813	1820	1840	rBV	129984	166485	8.66%	4.207%
17	21.164	1993	1995	1998	rBV	24340	33528	1.74%	0.847%
18	21.228	1998	2001	2011	rVV	120482	185904	9.67%	4.698%
19	23.481	2414	2426	2469	rVB	97059	191390	9.95%	4.837%

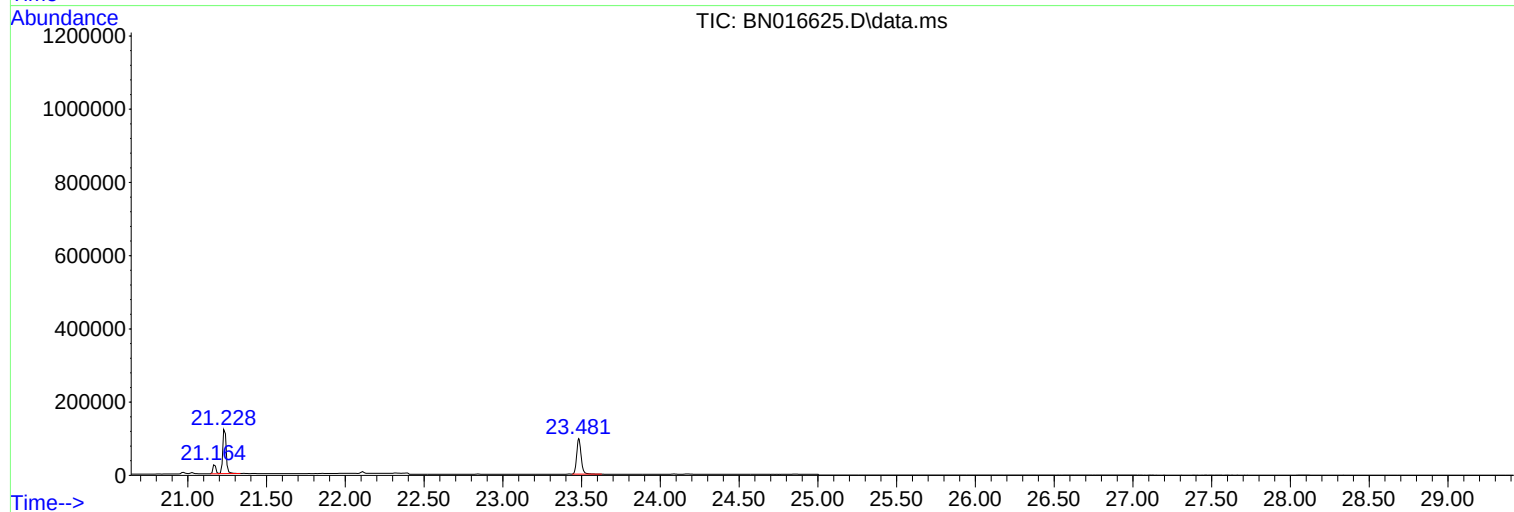
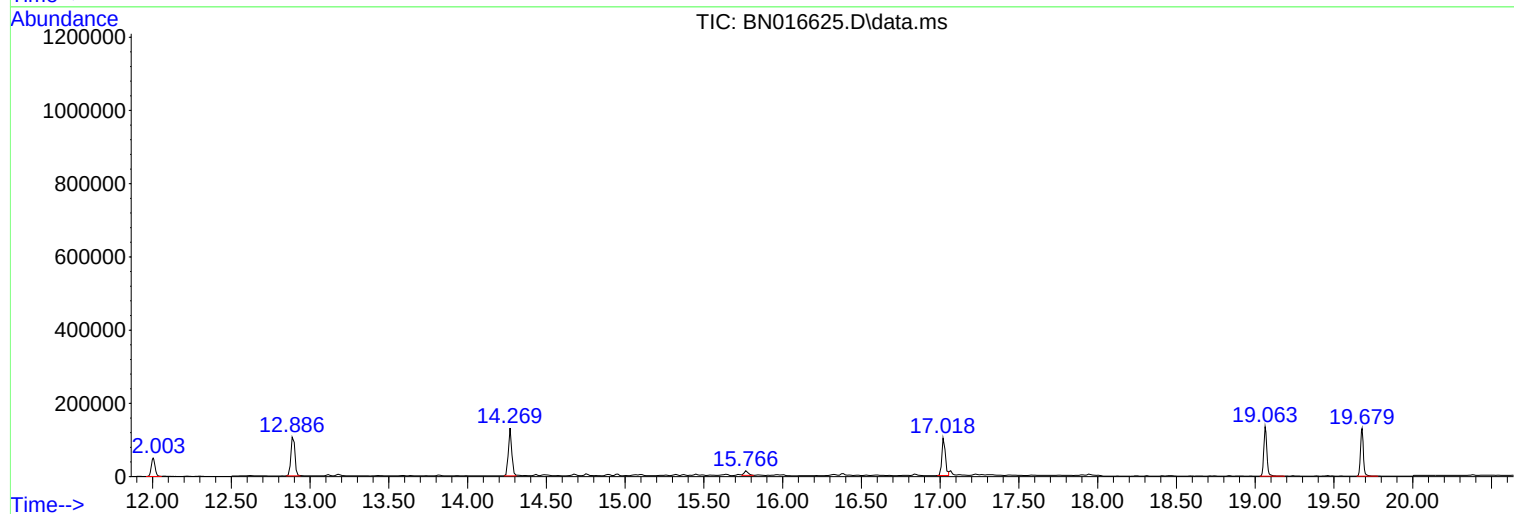
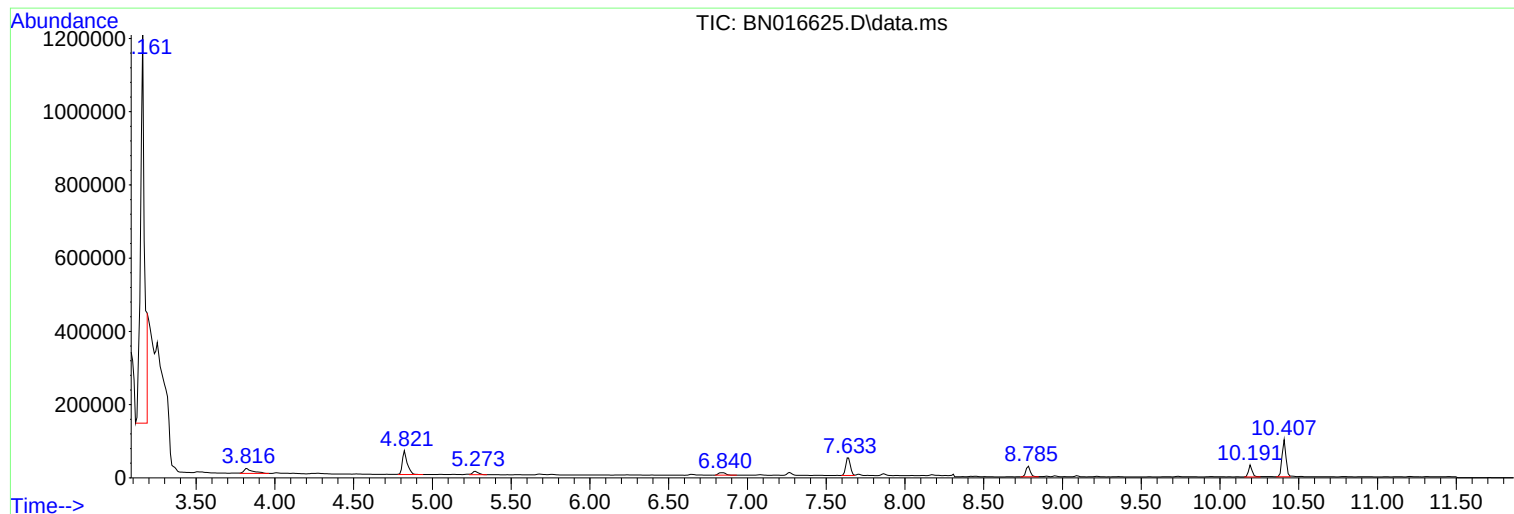
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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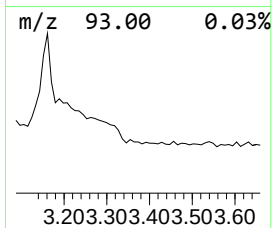
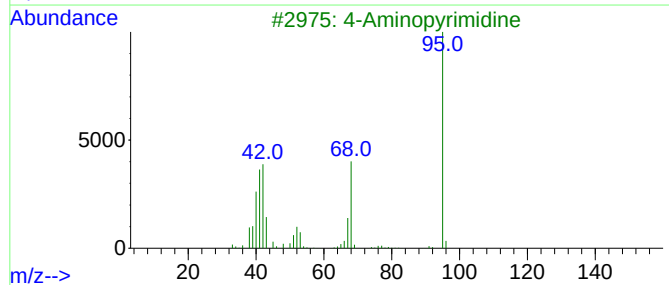
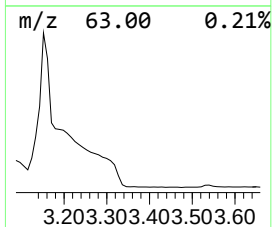
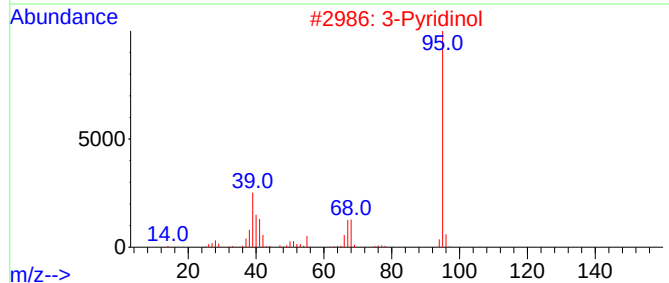
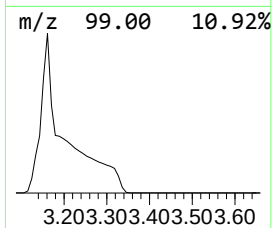
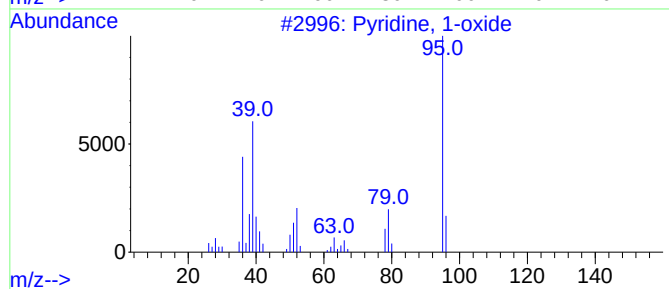
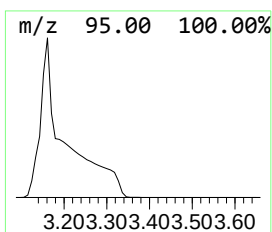
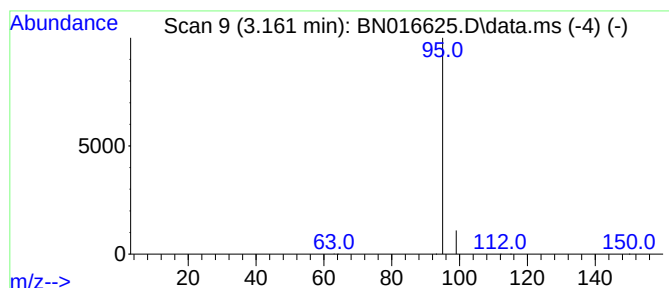
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Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	7.68 ng	1923350	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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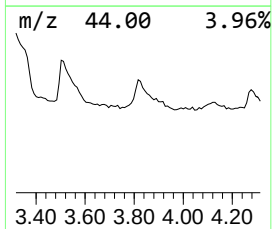
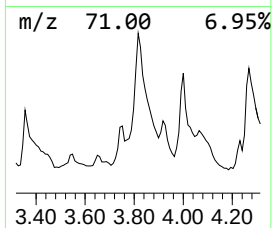
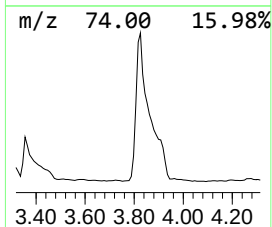
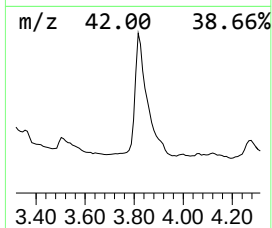
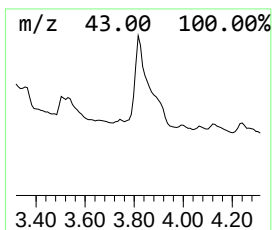
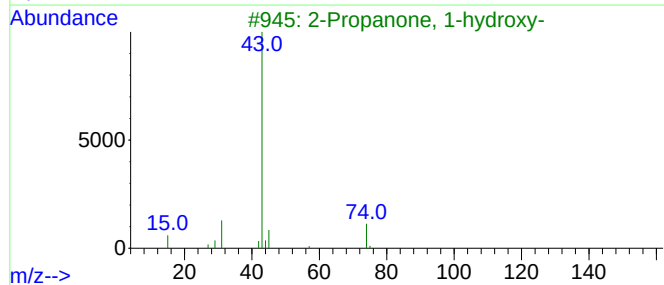
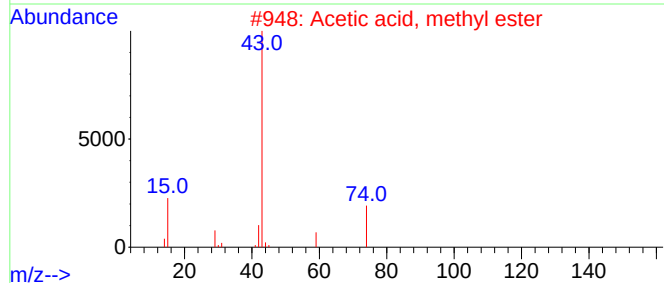
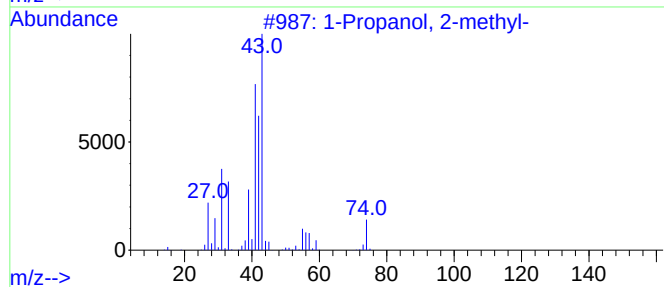
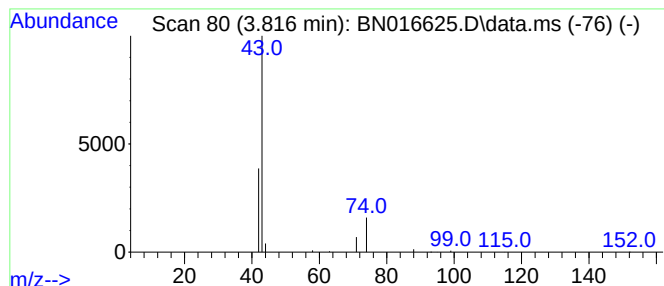
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Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.21 ng	53546	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
2		Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
3		2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
4		Hydrogen isocyanate	43	CHNO	000075-13-8	3
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	3



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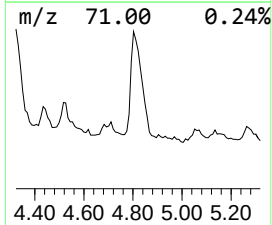
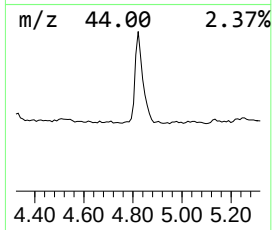
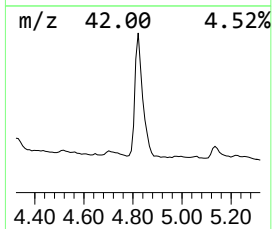
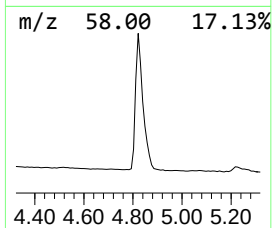
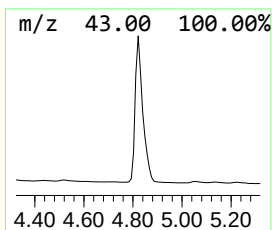
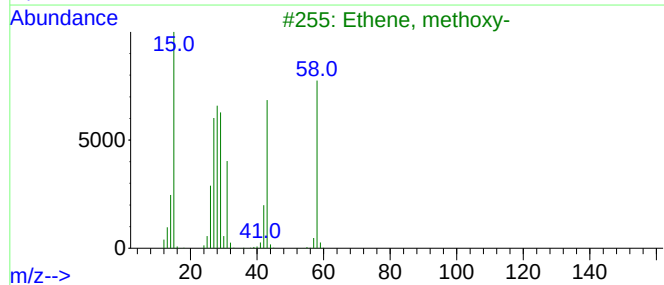
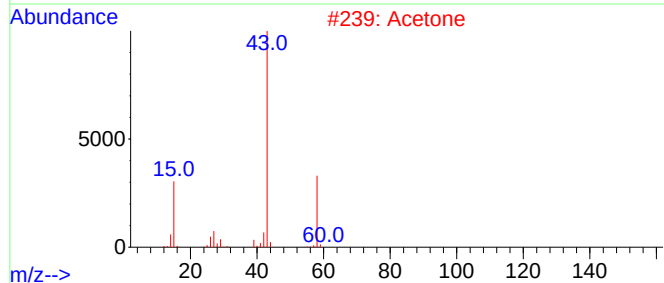
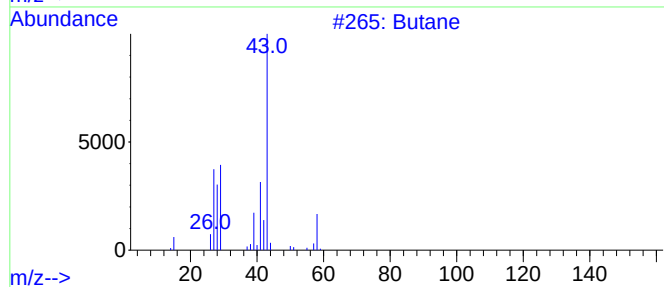
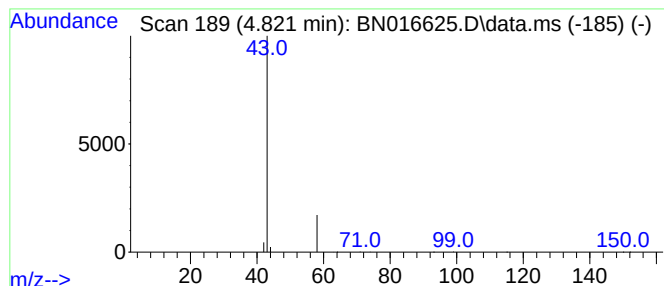
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Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.56 ng	139945	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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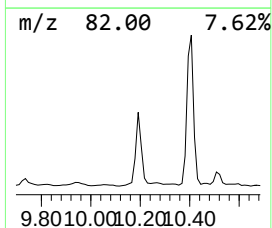
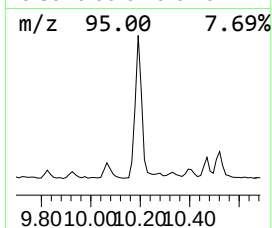
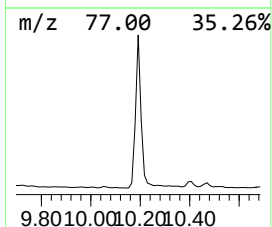
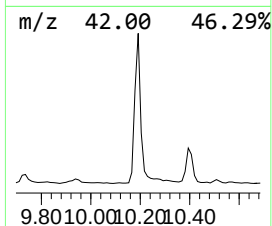
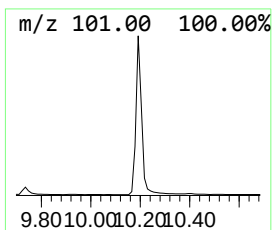
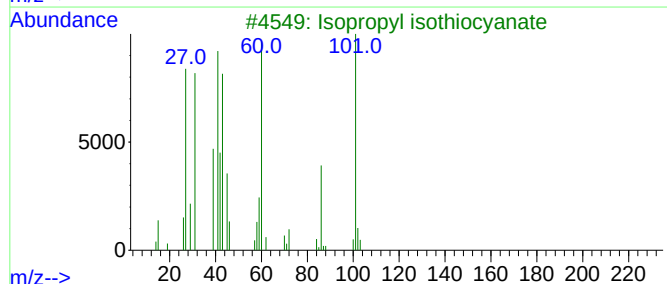
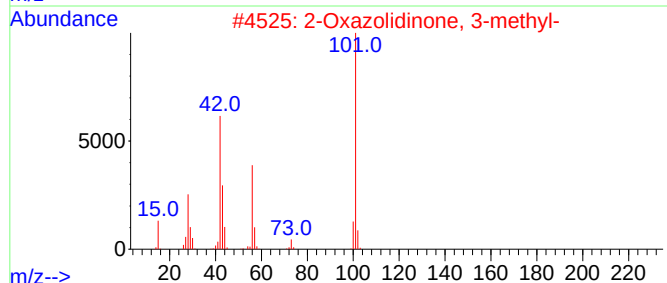
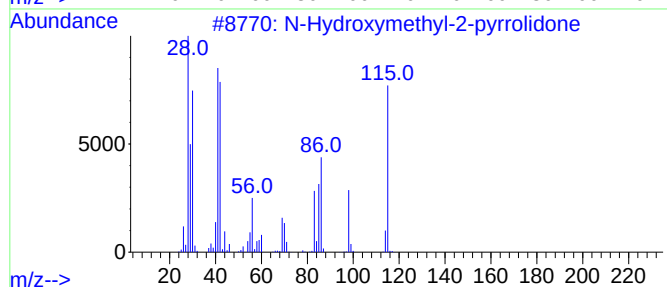
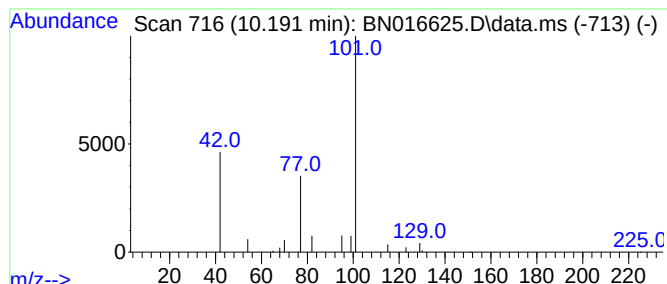
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Peak Number 4 N-Hydroxymethyl-2-pyrrolidone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.12 ng	53004	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			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
5			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	7.7	ng	1923350	1	7.642	100177	0.4
1-Propanol, 2-m...	3.816	0.2	ng	53546	1	7.642	100177	0.4
Butane	4.821	0.6	ng	139945	1	7.642	100177	0.4
N-Hydroxymethyl...	10.191	0.1	ng	53004	2	10.407	175184	0.4