

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016641.D
 Acq On : 01 Oct 2021 18:21
 Operator : CG/JU
 Sample : M3833-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE103D1-20210920

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: BN016641.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	4	10	12	rBV	1480672	2863417	100.00%	57.991%
2	3.825	77	81	98	rVB	14473	54079	1.89%	1.095%
3	4.821	185	189	202	rVB	61737	136181	4.76%	2.758%
4	6.849	403	409	418	rVB2	9878	29250	1.02%	0.592%
5	7.642	490	495	500	rBV	55015	110541	3.86%	2.239%
6	8.784	602	605	610	rBV	30454	55971	1.95%	1.134%
7	10.191	713	716	721	rBV	26762	46769	1.63%	0.947%
8	10.407	730	733	737	rBV	108312	187664	6.55%	3.801%
9	12.007	916	932	942	rBV	47869	78981	2.76%	1.600%
10	12.899	1071	1075	1078	rBV	94872	169139	5.91%	3.425%
11	14.269	1180	1183	1187	rBV	140160	210722	7.36%	4.268%
12	17.030	1400	1404	1406	rBV	95150	172968	6.04%	3.503%
13	19.068	1689	1697	1713	rBV	144434	197234	6.89%	3.994%
14	19.679	1814	1820	1838	rVB	142176	172854	6.04%	3.501%
15	21.164	1993	1995	1998	rBV	31631	45275	1.58%	0.917%
16	21.227	1998	2001	2011	rVB	126916	198110	6.92%	4.012%
17	23.481	2415	2426	2458	rVB	108275	208546	7.28%	4.224%

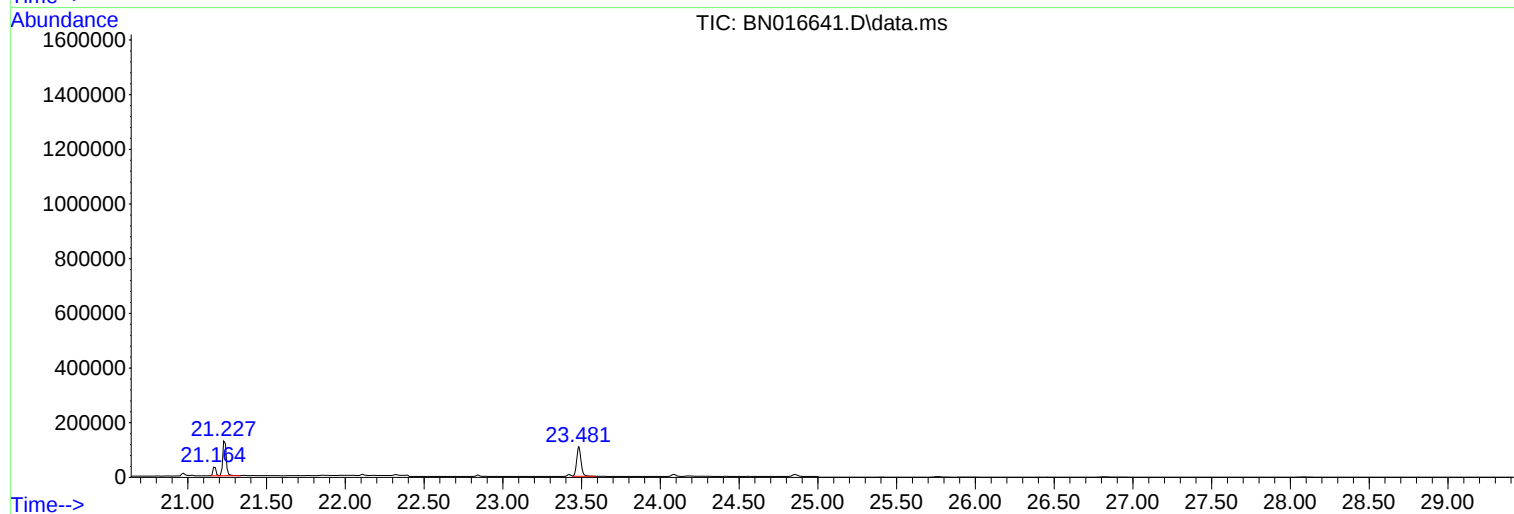
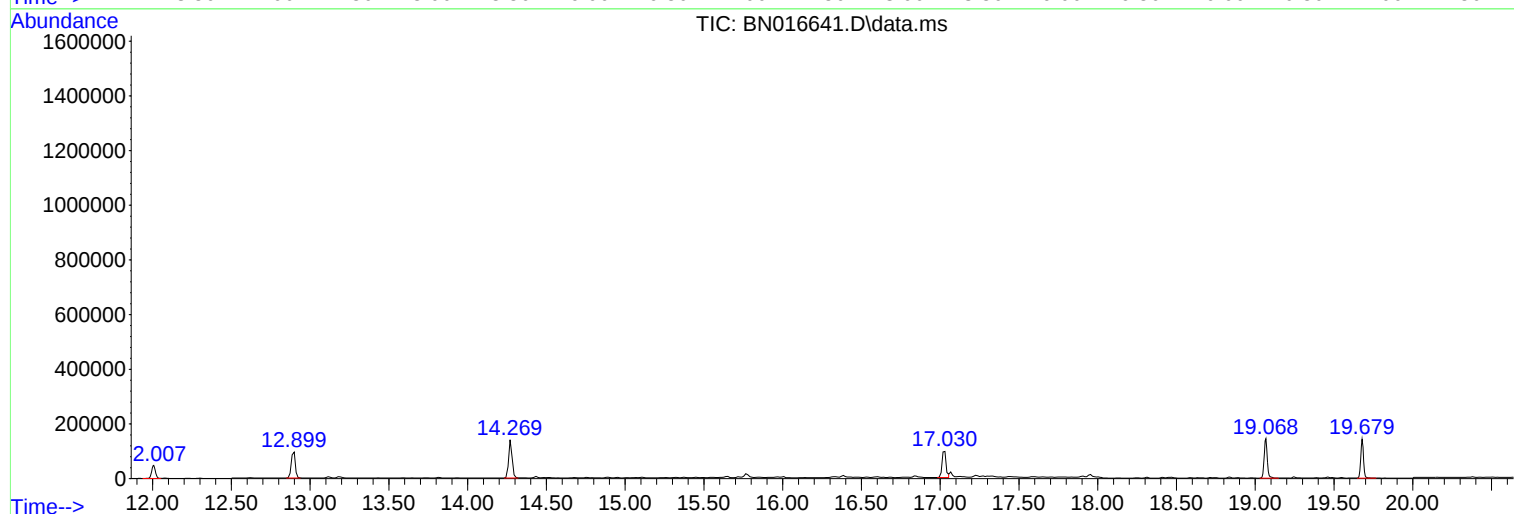
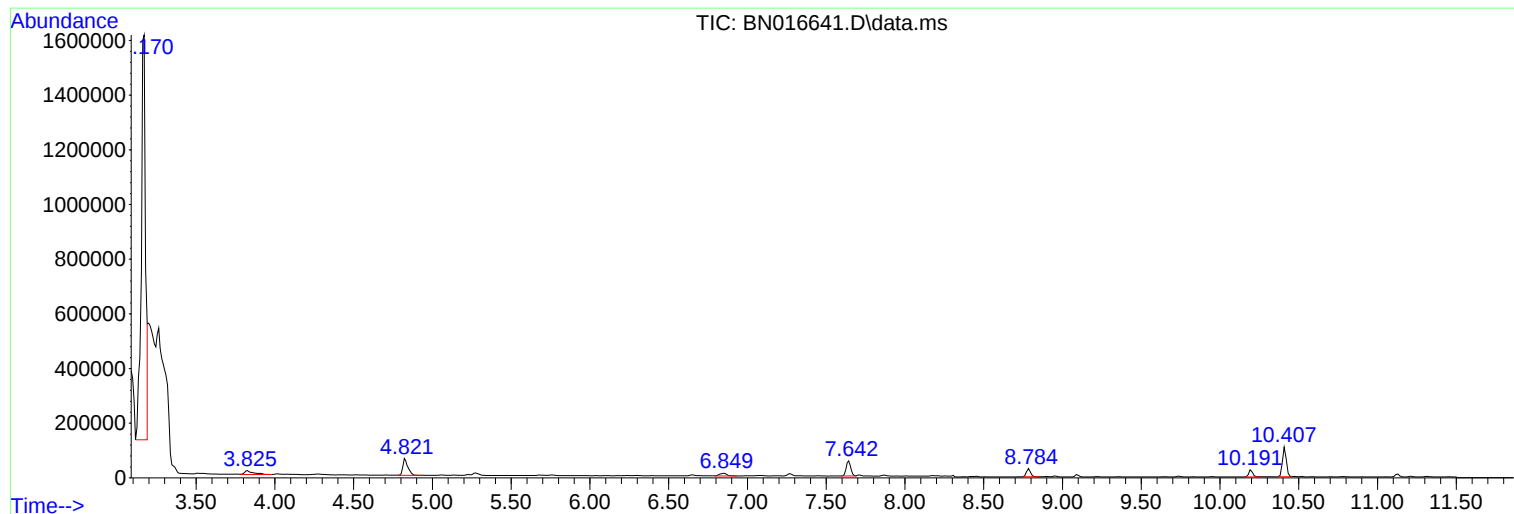
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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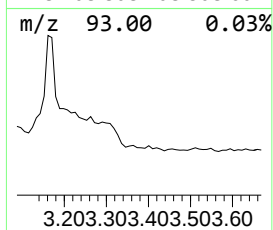
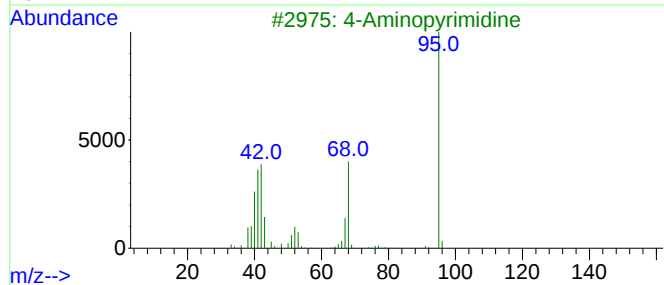
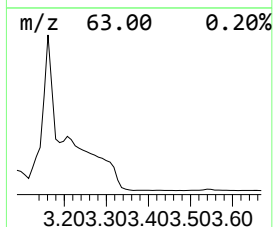
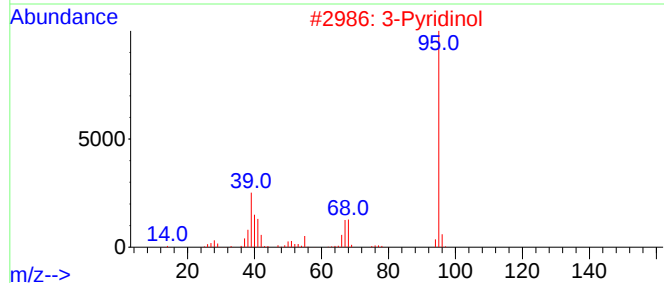
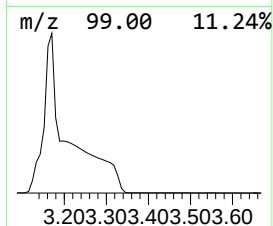
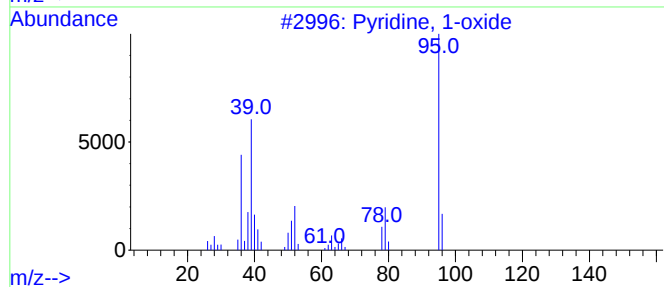
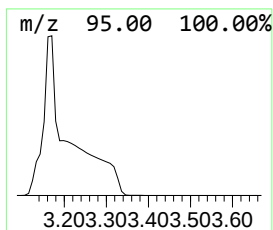
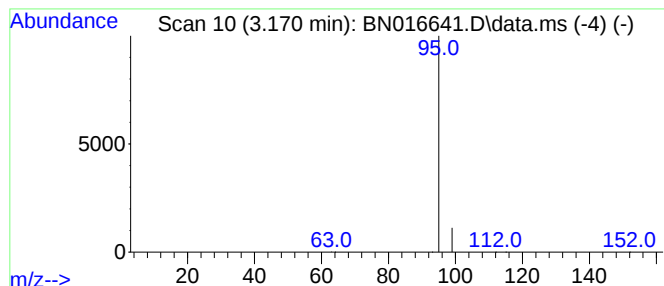
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	10.36 ng	2863420	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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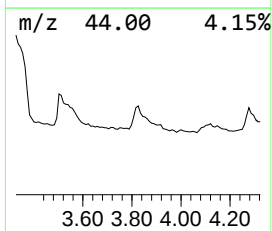
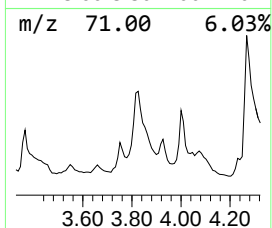
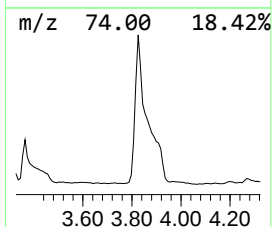
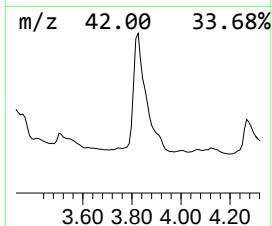
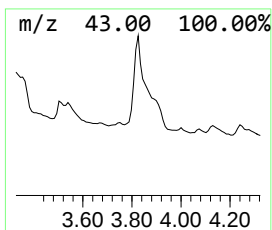
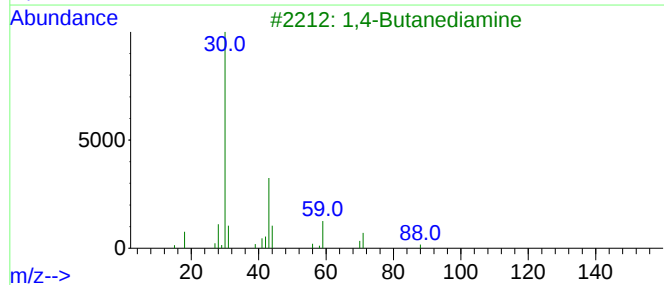
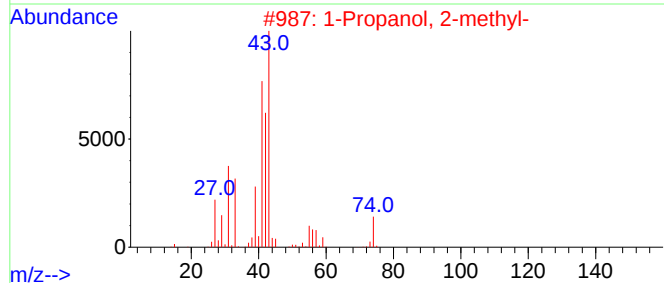
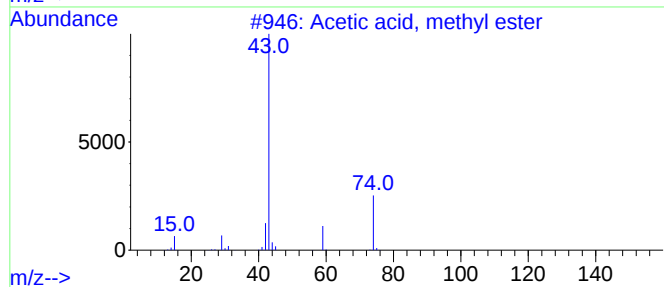
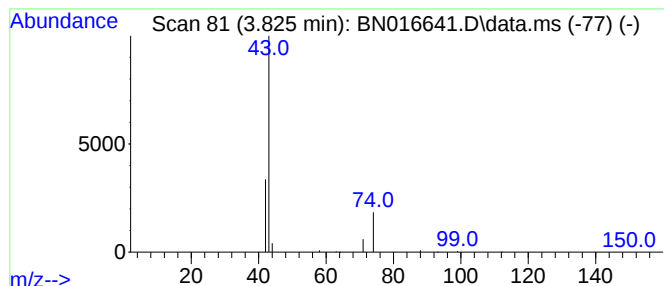
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Peak Number 2 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.20 ng	54079	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	5
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3



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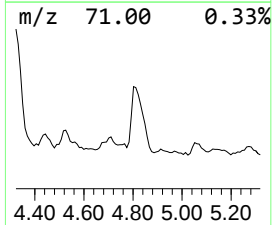
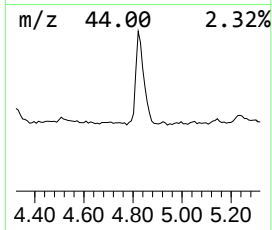
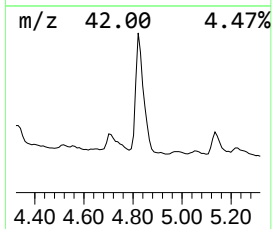
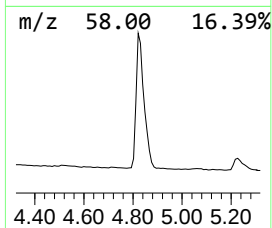
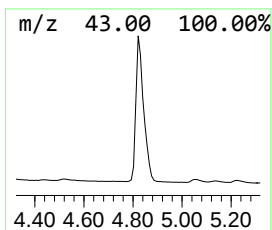
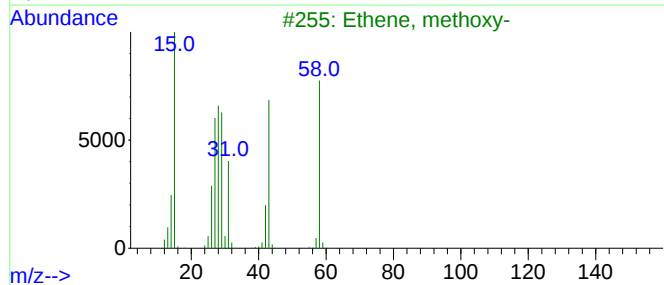
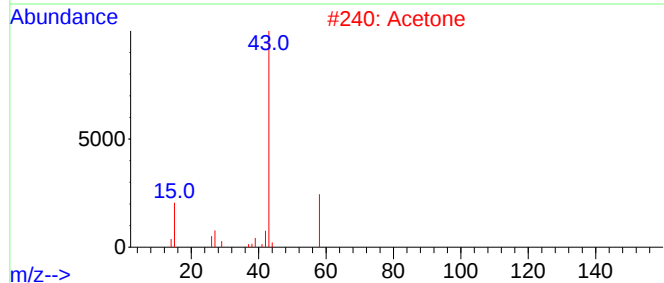
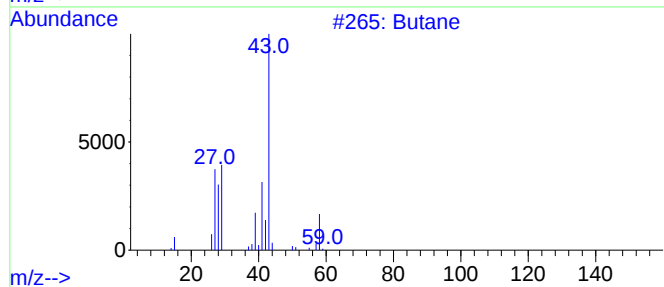
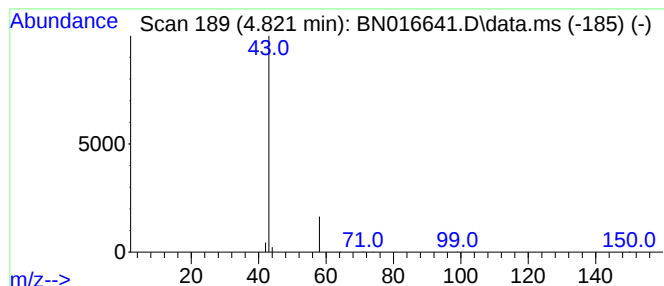
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Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.49 ng	136181	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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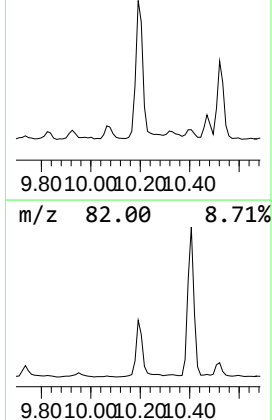
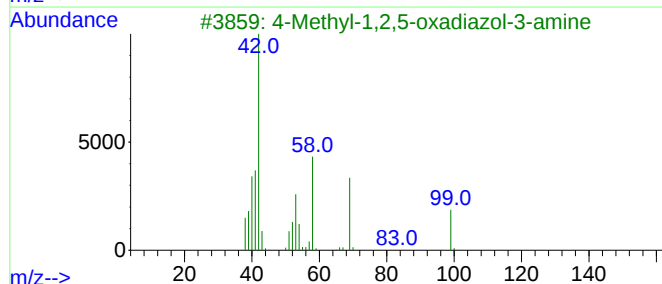
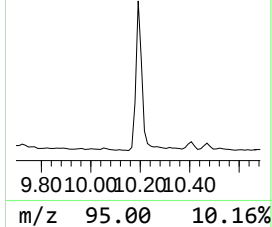
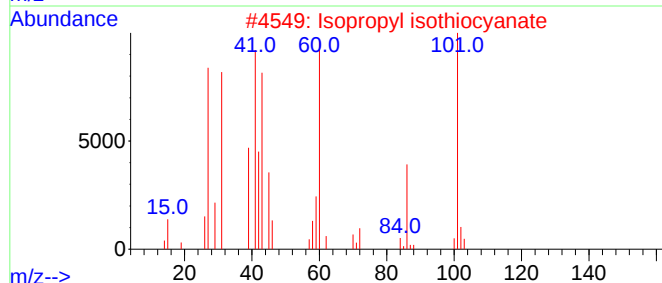
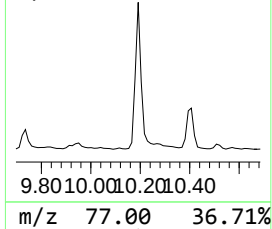
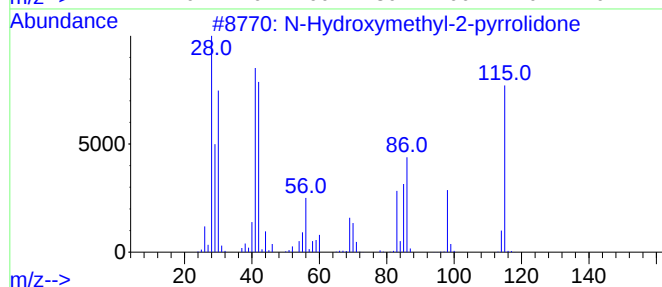
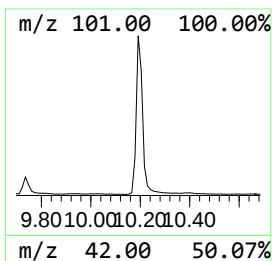
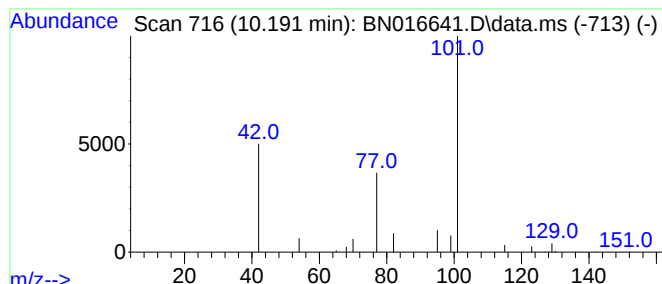
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Peak Number 4 N-Hydroxymethyl-2-pyrrolidone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.10 ng	46769	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			4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
4			Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
5			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.170	10.4	ng	2863420	1	7.642	110541	0.4
Acetic acid, me...	3.825	0.2	ng	54079	1	7.642	110541	0.4
Butane	4.821	0.5	ng	136181	1	7.642	110541	0.4
N-Hydroxymethyl...	10.191	0.1	ng	46769	2	10.407	187664	0.4