

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016610.D
 Acq On : 30 Sep 2021 21:34
 Operator : CG/JU
 Sample : M3782-07DL 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE132D3-20210914DL

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: BN016610.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	6	8	10	rBV	110999	118905	41.45%	6.401%
2	3.189	10	12	17	rVV	11916	43753	15.25%	2.355%
3	3.253	17	19	43	rVB	73165	286870	100.00%	15.442%
4	3.816	78	80	98	rVB	4439	19066	6.65%	1.026%
5	4.821	185	189	202	rVB	17673	44114	15.38%	2.375%
6	5.264	234	237	246	rVB	2764	8112	2.83%	0.437%
7	6.822	403	406	418	rVB2	2115	6560	2.29%	0.353%
8	7.264	451	454	461	rBV	3199	6986	2.44%	0.376%
9	7.642	490	495	500	rBV	49810	103177	35.97%	5.554%
10	7.864	515	519	527	rVB2	3547	7393	2.58%	0.398%
11	8.306	565	567	569	rVB2	5328	5335	1.86%	0.287%
12	8.785	602	605	610	rBV	9078	17854	6.22%	0.961%
13	10.191	713	716	729	rBV	15068	29935	10.44%	1.611%
14	10.407	730	733	737	rBV	105451	184817	64.43%	9.949%
15	12.007	920	932	943	rBV	18595	31013	10.81%	1.669%
16	12.899	1071	1075	1078	rBV	35418	63346	22.08%	3.410%
17	13.178	1094	1097	1104	rBV	2452	4528	1.58%	0.244%
18	14.269	1180	1183	1186	rBV	135867	196534	68.51%	10.579%
19	15.766	1299	1301	1308	rVB2	3866	6660	2.32%	0.359%
20	17.018	1400	1403	1407	rBV	88677	154203	53.75%	8.301%
21	19.068	1689	1697	1716	rBV	50704	72221	25.18%	3.888%
22	19.679	1813	1820	1842	rBV	48722	61993	21.61%	3.337%
23	21.026	1980	1982	1993	rVB	6047	9348	3.26%	0.503%
24	21.174	1993	1996	1998	rBV	9795	13324	4.64%	0.717%
25	21.238	1998	2002	2011	rBV2	113610	177081	61.73%	9.532%
26	22.311	2100	2103	2110	rBV	2185	5176	1.80%	0.279%
27	23.485	2414	2427	2459	rVV	91859	179392	62.53%	9.657%

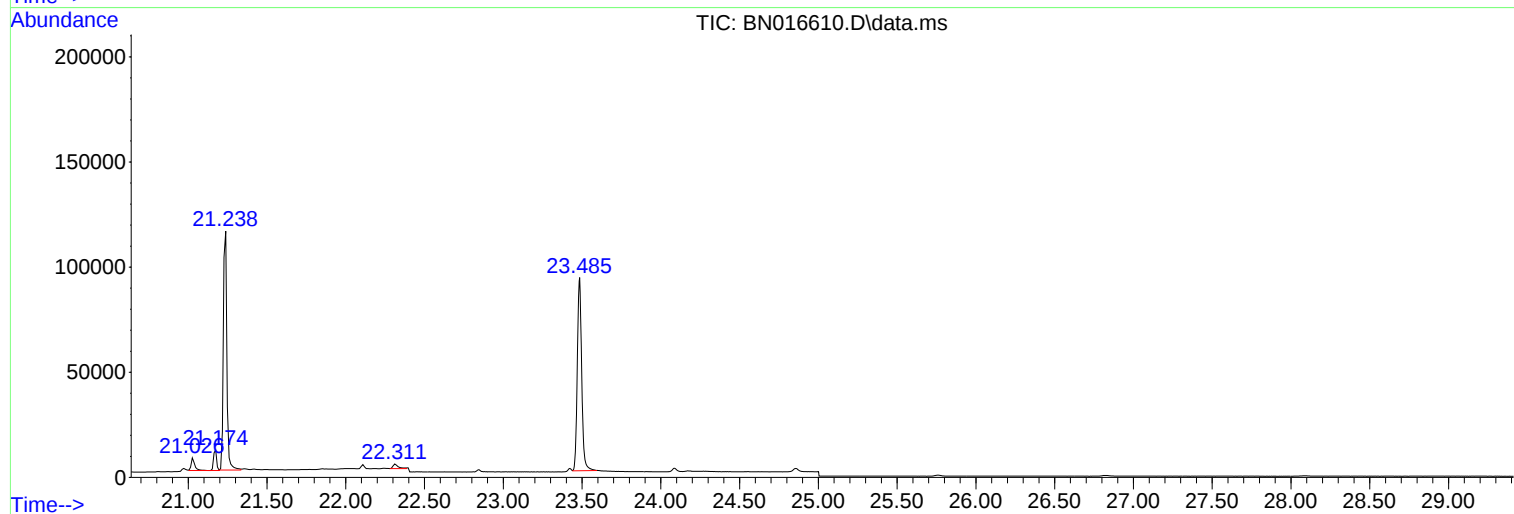
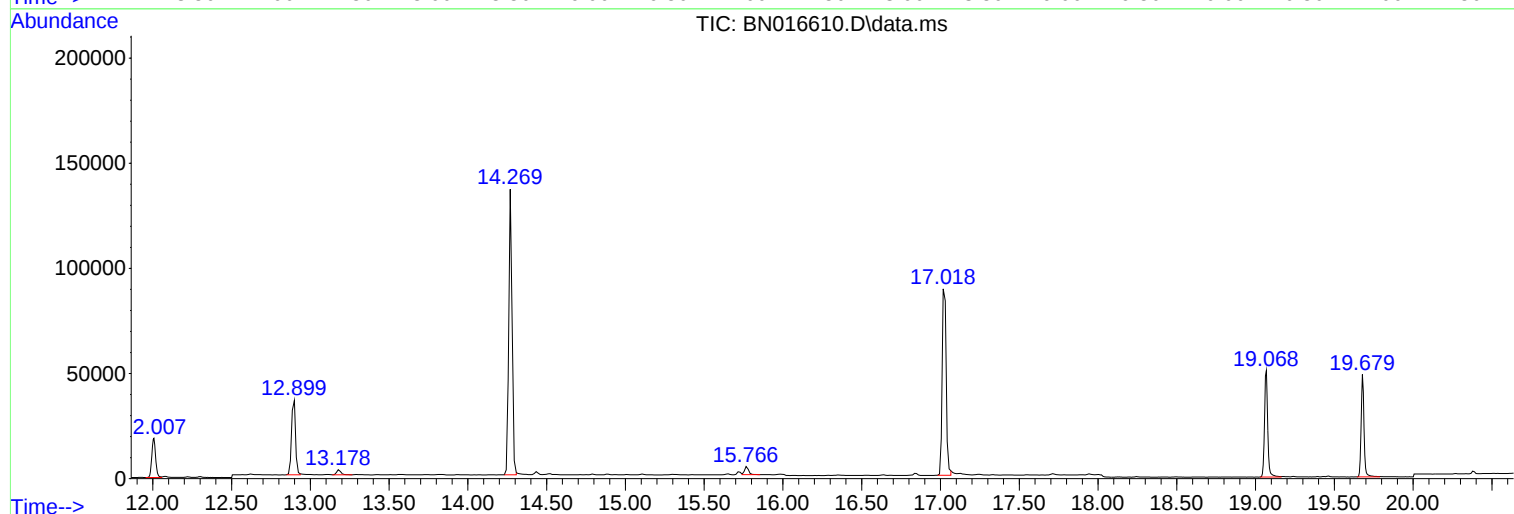
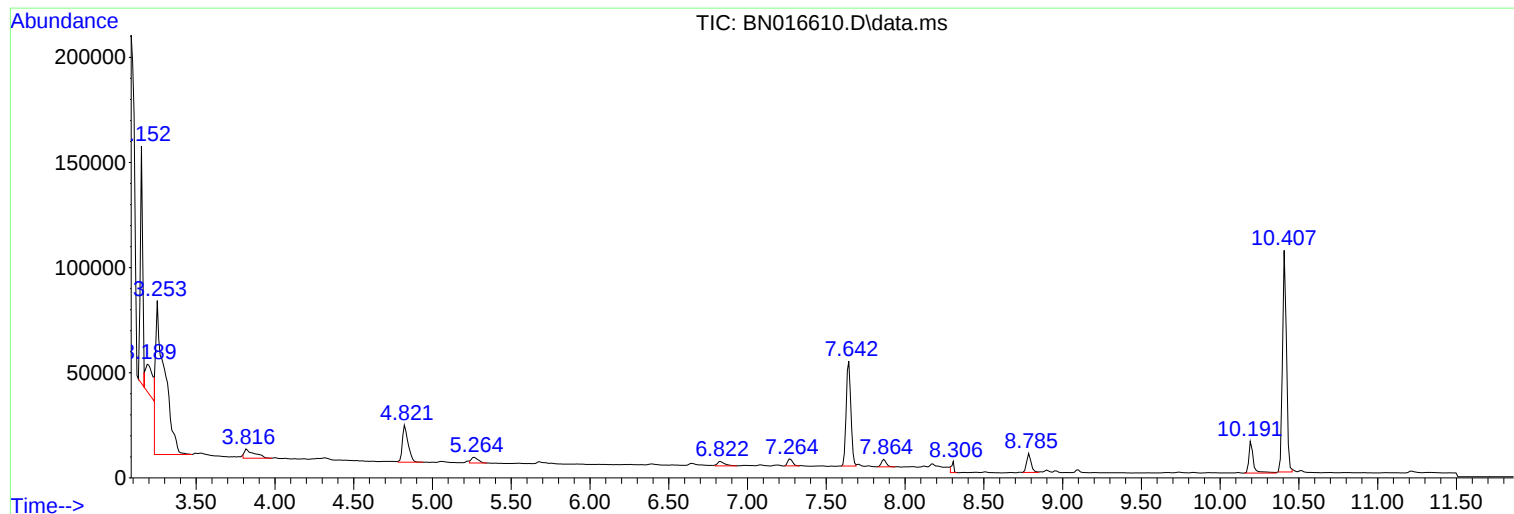
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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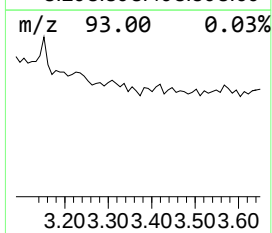
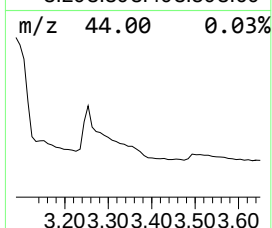
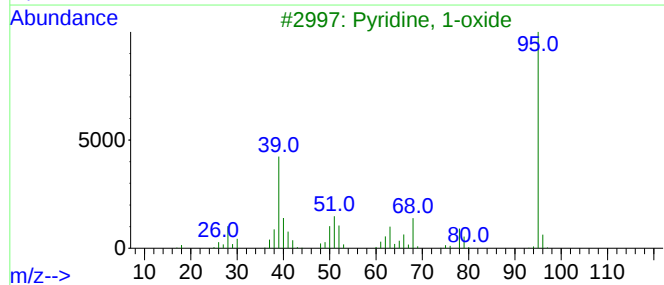
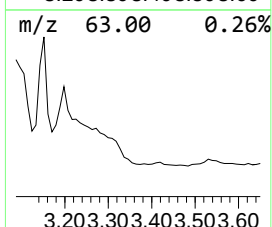
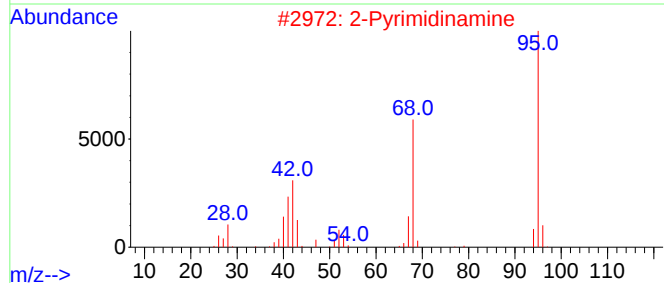
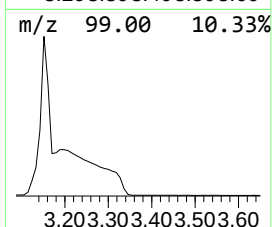
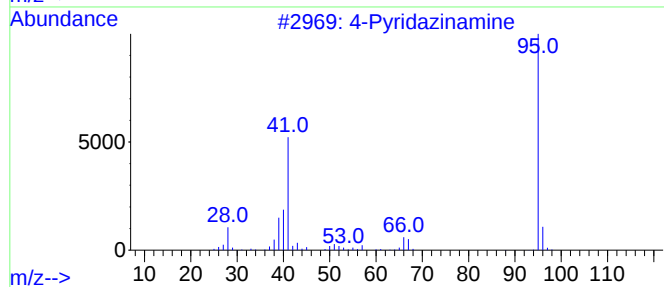
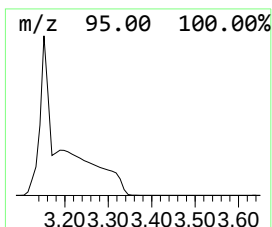
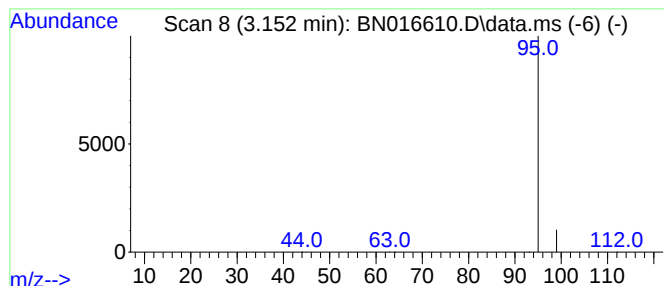
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Pyridazinamine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.46 ng	118905	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridazinamine	95	C4H5N3	020744-39-2	2
2			2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
3			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
4			3-Pyridinol	95	C5H5NO	000109-00-2	2
5			4-Pyridinol	95	C5H5NO	000626-64-2	2



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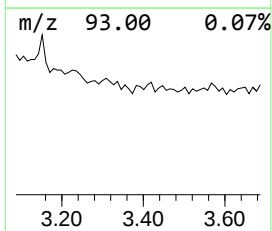
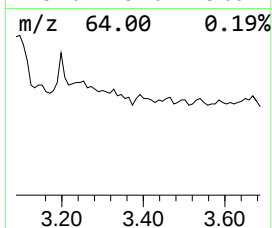
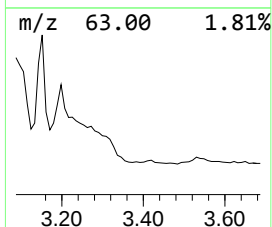
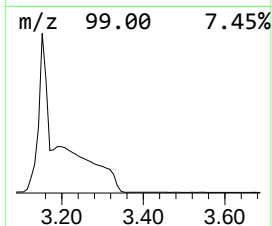
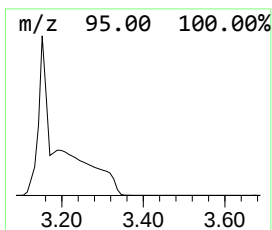
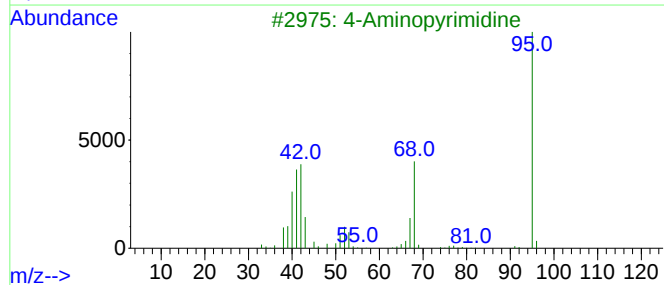
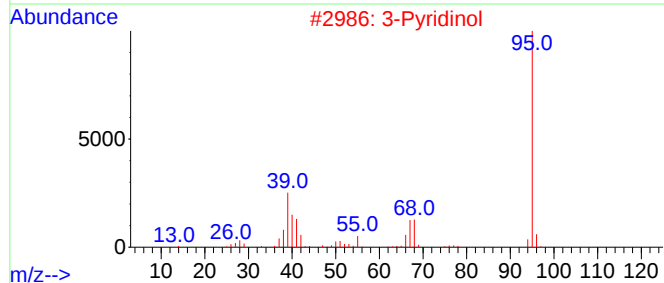
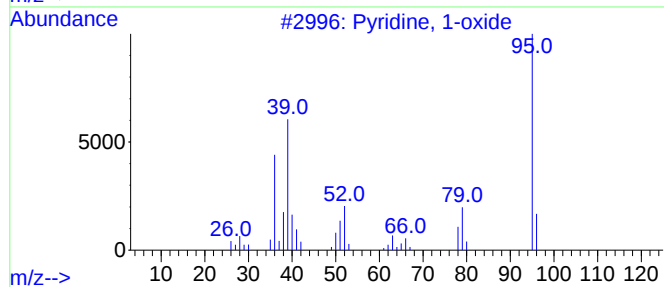
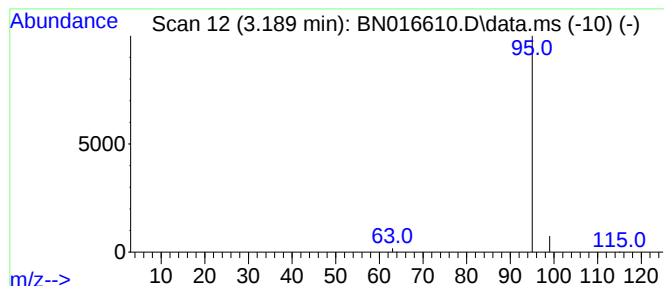
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Pyridine, 1-oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	0.17 ng	43753	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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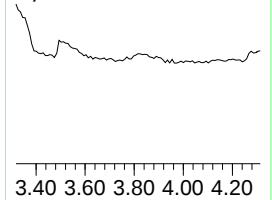
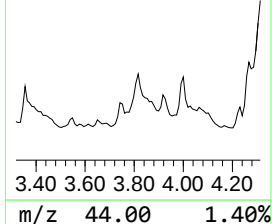
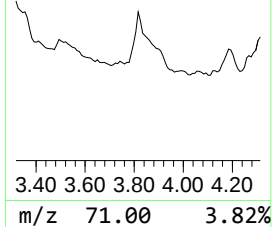
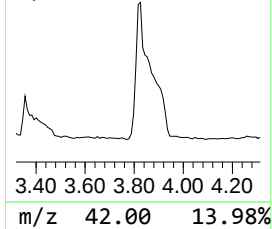
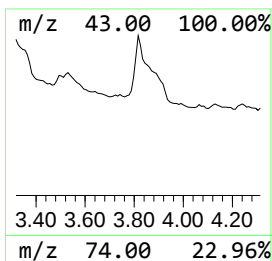
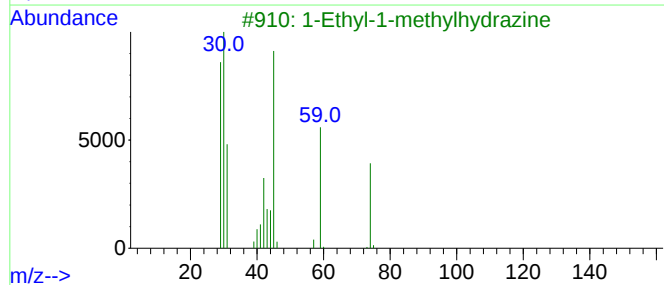
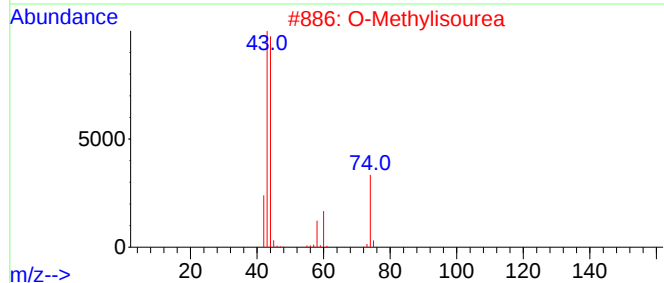
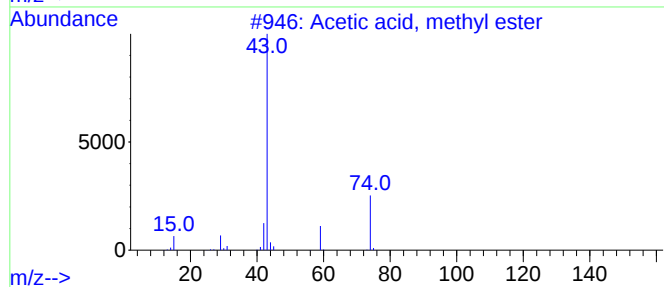
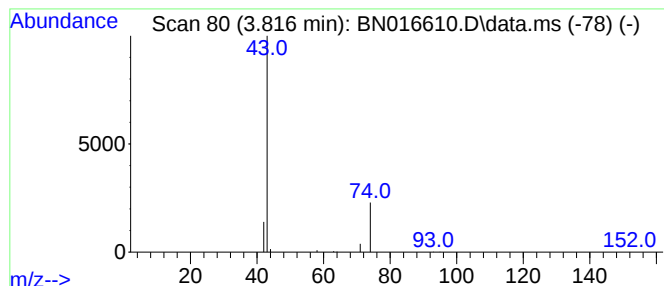
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.07 ng	19066	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			O-Methylisourea	74	C2H6N2O	002440-60-0	4
3			1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3
4			Urea, methyl-	74	C2H6N2O	000598-50-5	3
5			Methoxyacetoneitrile	71	C3H5NO	001738-36-9	3



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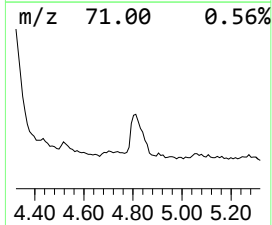
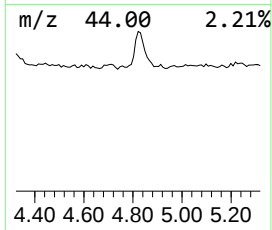
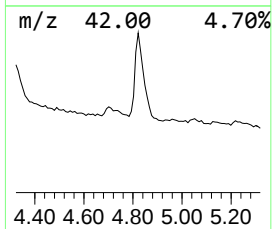
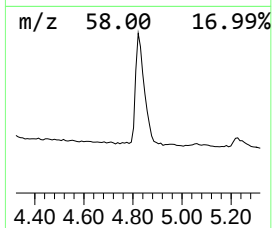
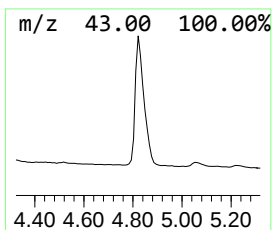
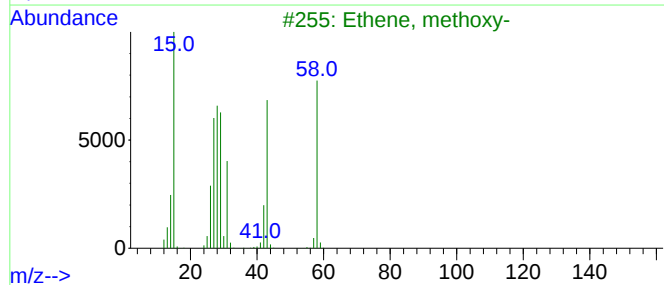
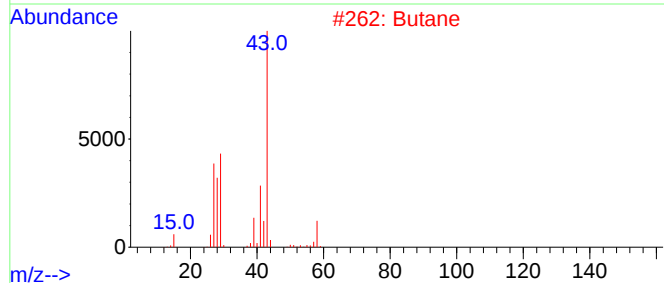
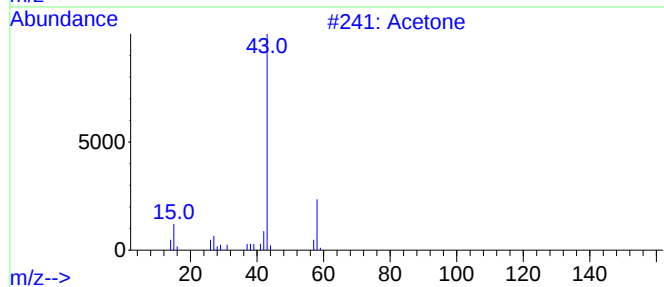
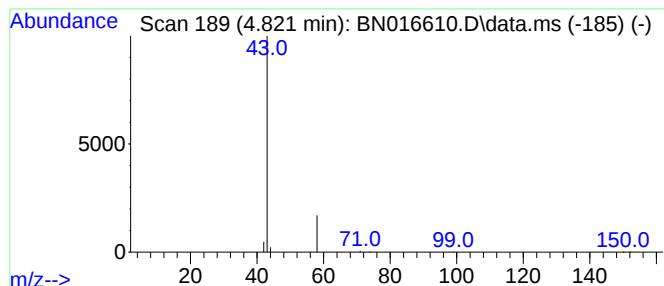
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Acetone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.17 ng	44114	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetone	58	C3H6O	000067-64-1	4
2			Butane	58	C4H10	000106-97-8	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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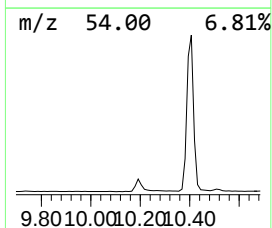
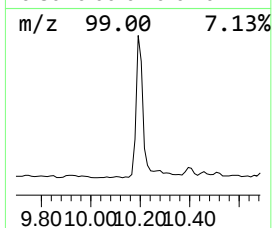
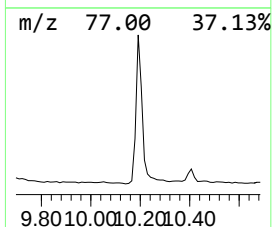
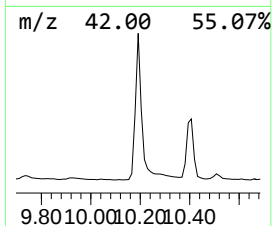
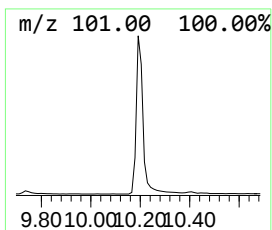
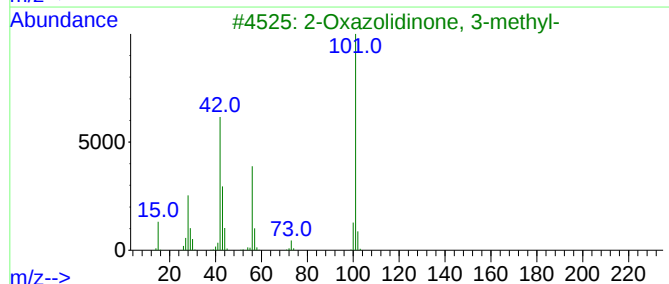
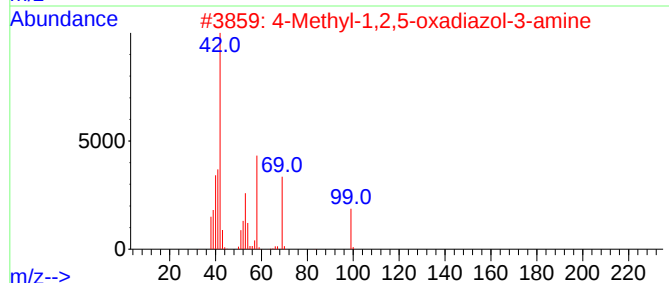
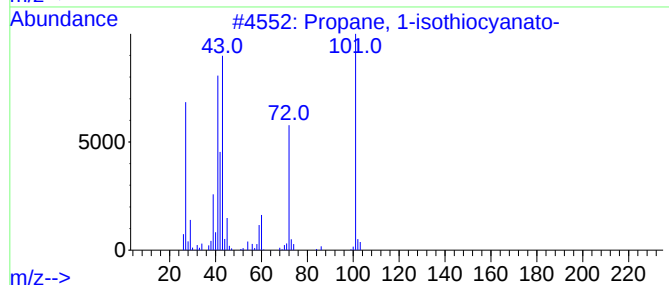
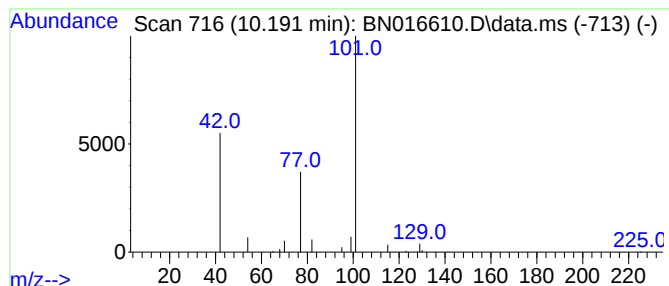
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Propane, 1-isothiocyanato- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.06 ng	29935	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
2			4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
3			2-Oxazolidinone, 3-methyl-	101	C4H7N02	019836-78-3	5
4			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
5			Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Pyridazinamine	3.152	0.5	ng	118905	1	7.642	103177	0.4
Pyridine, 1-oxide	3.189	0.2	ng	43753	1	7.642	103177	0.4
Acetic acid, me...	3.816	0.1	ng	19066	1	7.642	103177	0.4
Acetone	4.821	0.2	ng	44114	1	7.642	103177	0.4
Propane, 1-isot...	10.191	0.1	ng	29935	2	10.407	184817	0.4