

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016624.D
 Acq On : 01 Oct 2021 07:11
 Operator : CG/JU
 Sample : M3833-10
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE103D3-20210920

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: BN016624.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	11	rBV	875348	1482765	100.00%	45.429%
2	3.502	43	46	62	rVB	3938	18026	1.22%	0.552%
3	3.816	76	80	97	rVB	9719	41295	2.78%	1.265%
4	4.821	185	189	201	rVB	29572	69759	4.70%	2.137%
5	5.263	234	237	245	rVB	6314	16709	1.13%	0.512%
6	6.849	403	409	418	rVB2	8663	24475	1.65%	0.750%
7	7.642	490	495	499	rBV	42206	89041	6.01%	2.728%
8	8.784	601	605	611	rBV	23093	46242	3.12%	1.417%
9	10.191	713	716	724	rBV	33005	54966	3.71%	1.684%
10	10.407	729	733	736	rBV	92987	161441	10.89%	4.946%
11	12.003	920	931	943	rBV2	40062	64777	4.37%	1.985%
12	12.886	1071	1074	1078	rBV	81306	138745	9.36%	4.251%
13	14.269	1180	1183	1190	rBV	122416	181062	12.21%	5.547%
14	17.018	1400	1403	1406	rBV	94570	143347	9.67%	4.392%
15	19.063	1688	1696	1721	rBV	123913	168503	11.36%	5.163%
16	19.678	1813	1820	1842	rBV	110306	147348	9.94%	4.514%
17	21.164	1993	1995	1998	rBV	38839	52589	3.55%	1.611%
18	21.227	1998	2001	2011	rVB	113798	168378	11.36%	5.159%
19	22.109	2081	2084	2089	rBV2	12976	17721	1.20%	0.543%
20	23.481	2414	2426	2467	rVB	90310	176704	11.92%	5.414%

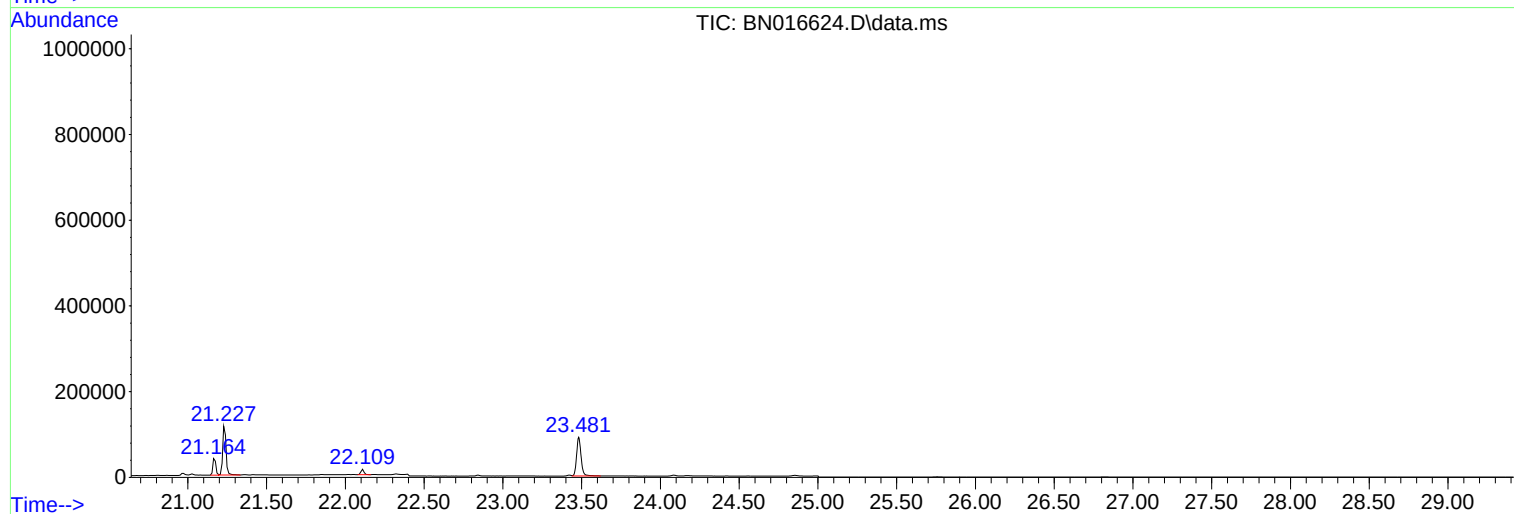
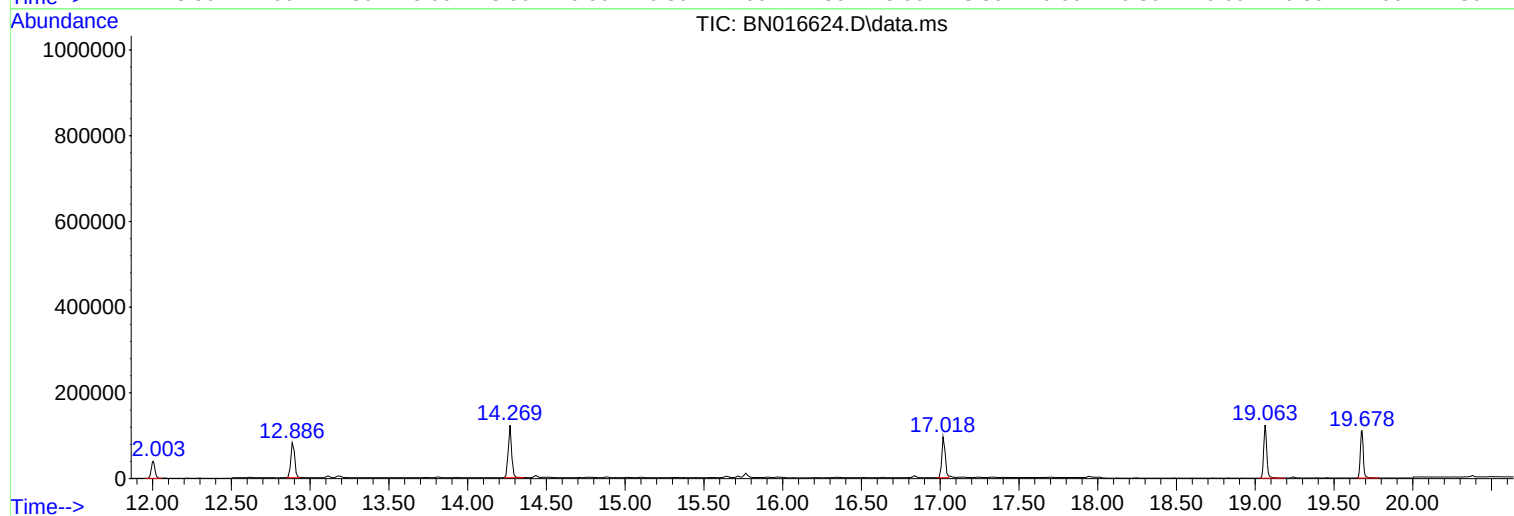
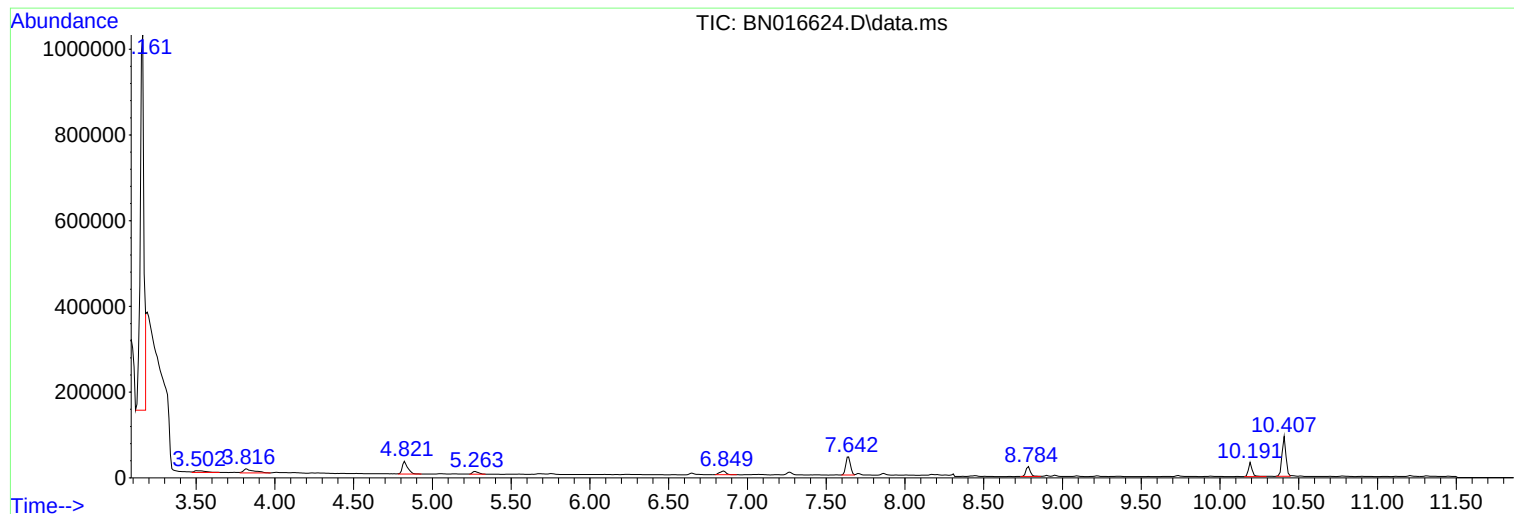
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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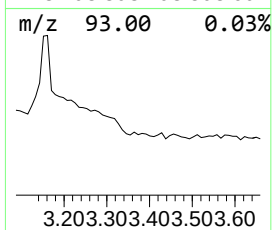
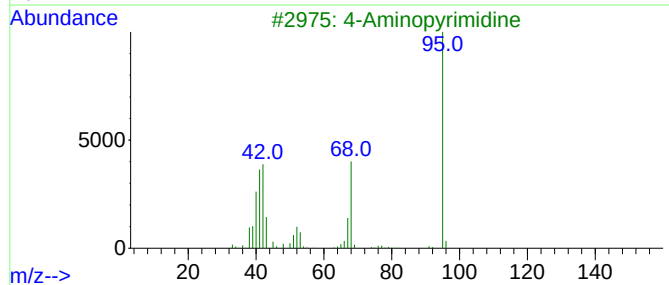
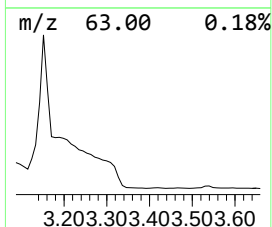
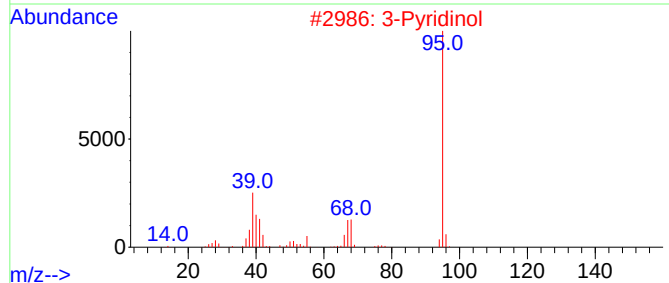
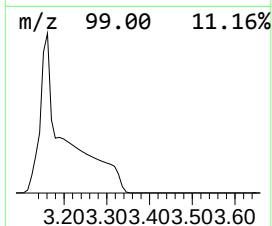
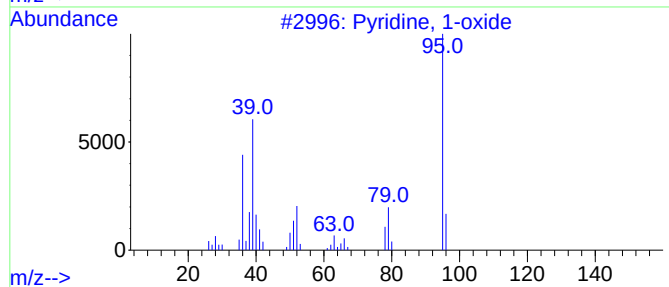
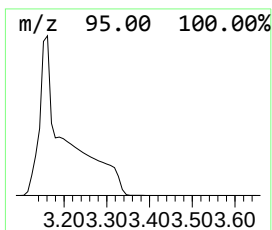
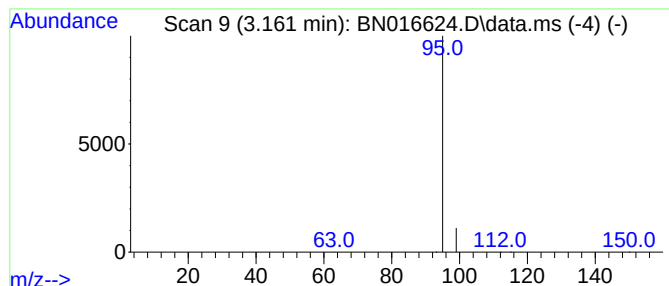
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Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	6.66 ng	1482770	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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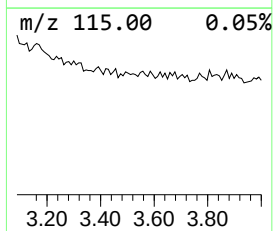
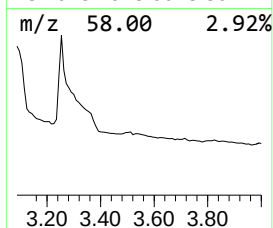
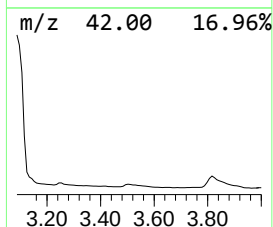
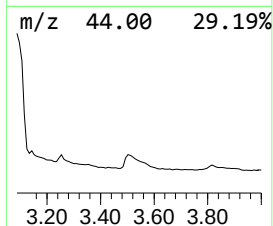
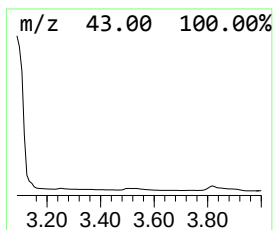
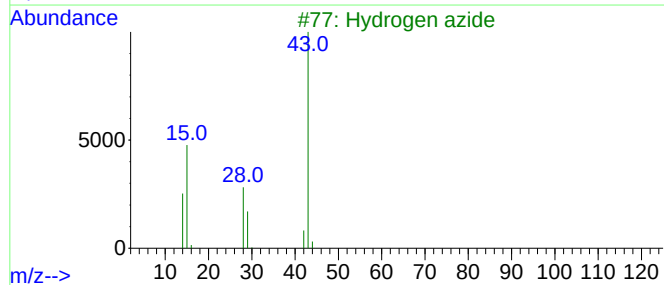
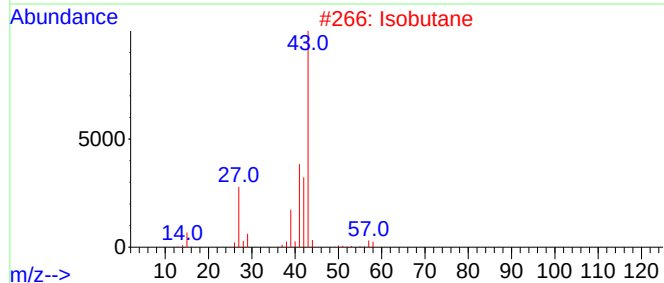
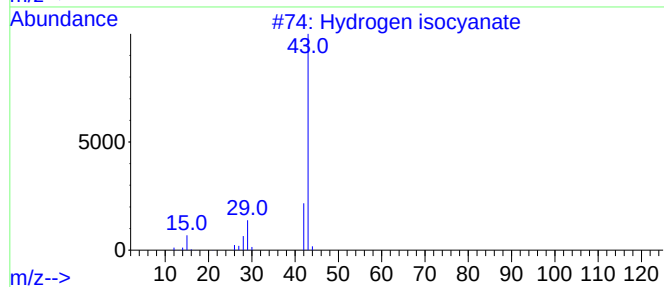
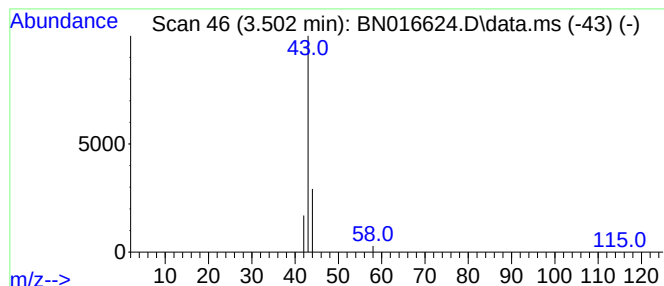
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hydrogen isocyanate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.502	0.08 ng	18026	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	3
2	Isobutane	58	C4H10	000075-28-5	3
3	Hydrogen azide	43	HN3	007782-79-8	3
4	Acetaldehyde	44	C2H4O	000075-07-0	2
5	Ethylene oxide	44	C2H4O	000075-21-8	2



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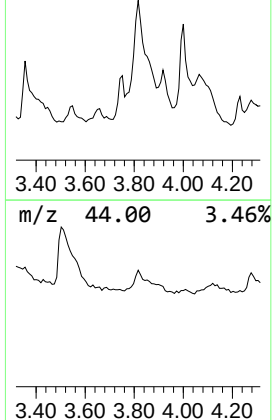
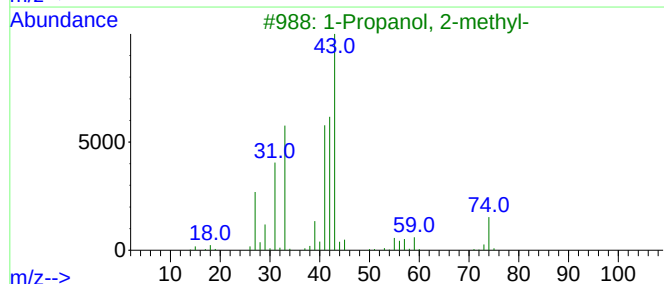
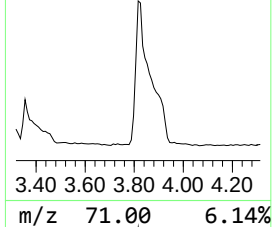
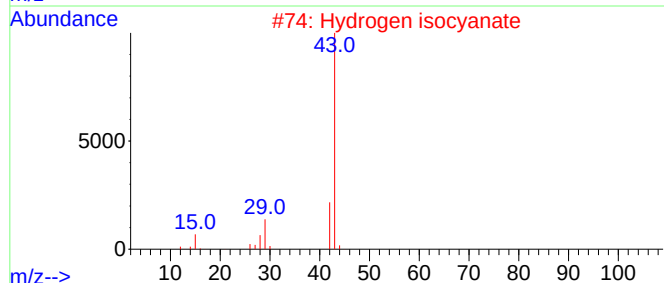
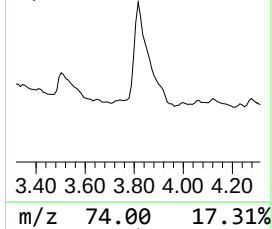
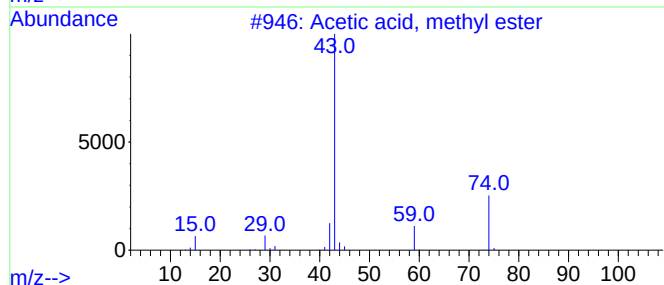
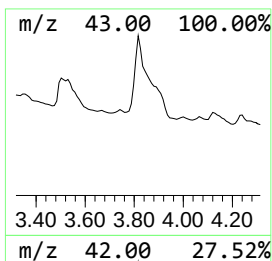
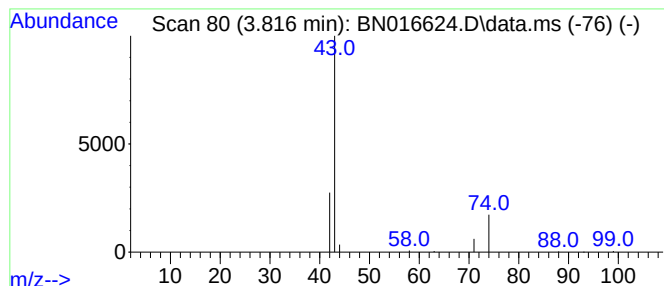
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Peak Number 3 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.19 ng	41295	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			Hydrogen isocyanate	43	CHNO	000075-13-8	4
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4			Formic acid, propyl ester	88	C4H8O2	000110-74-7	3
5			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3



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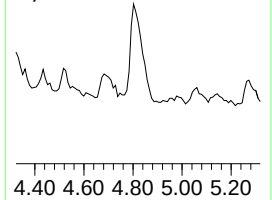
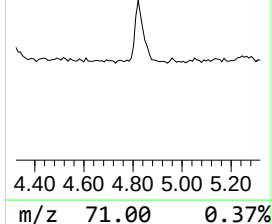
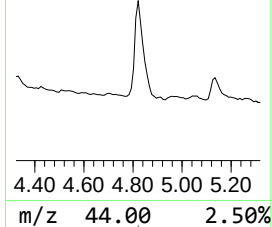
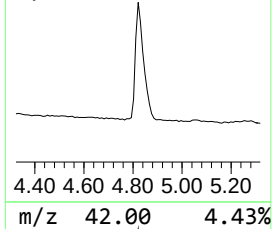
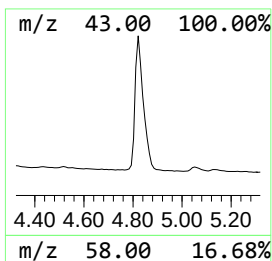
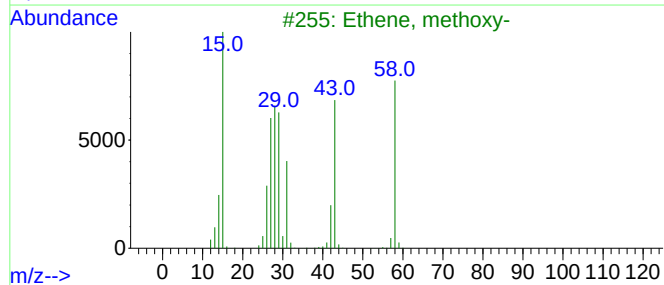
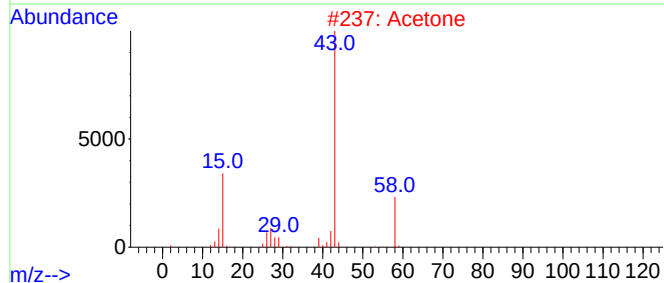
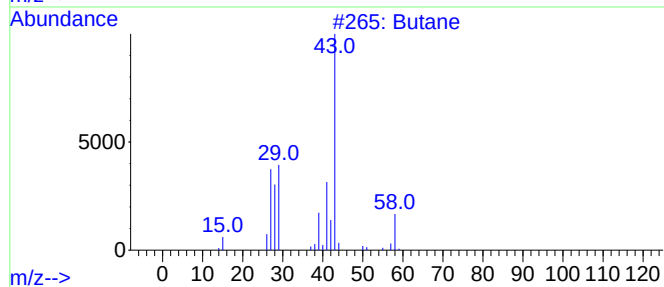
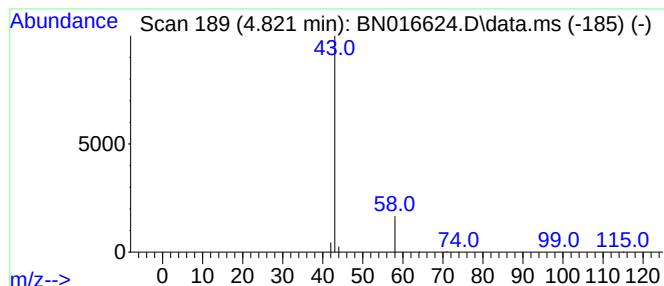
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Peak Number 4 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.31 ng	69759	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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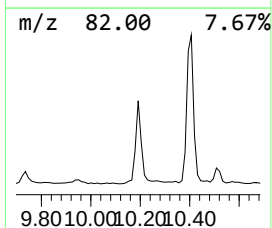
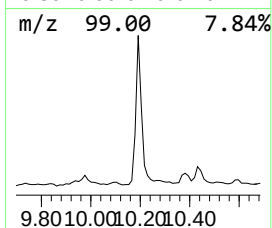
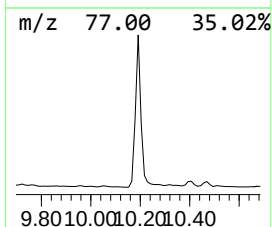
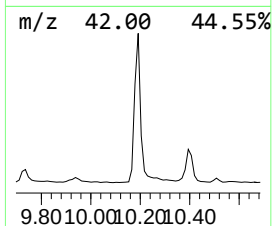
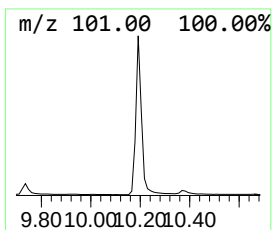
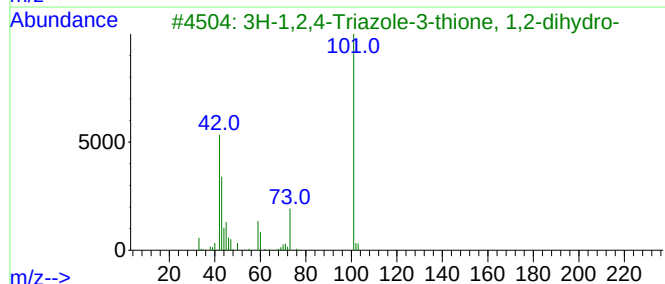
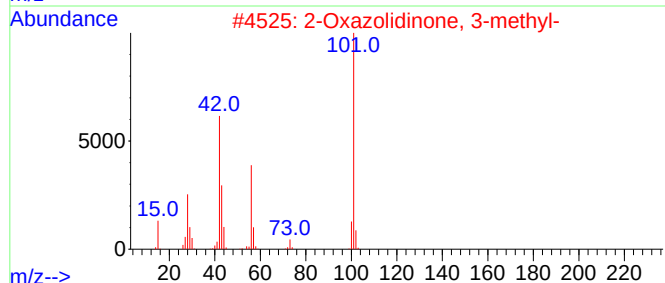
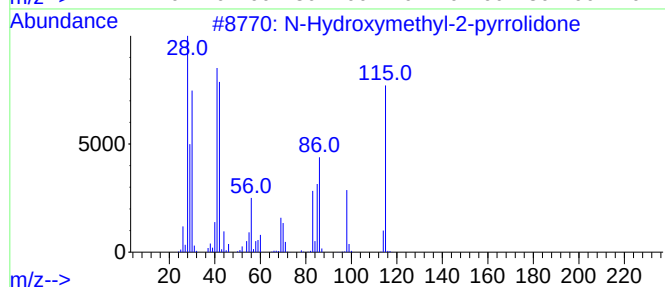
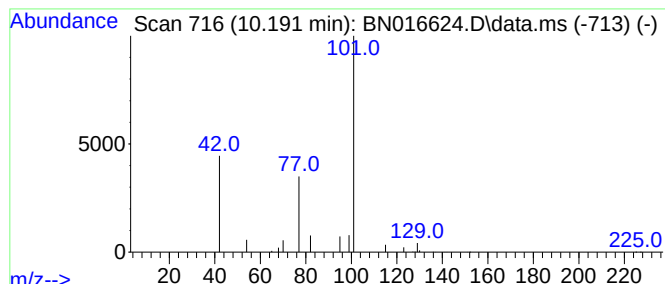
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Peak Number 5 N-Hydroxymethyl-2-pyrrolidone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.14 ng	54966	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			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5



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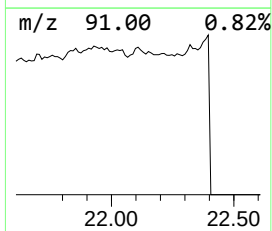
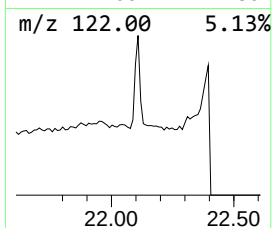
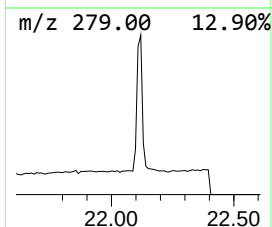
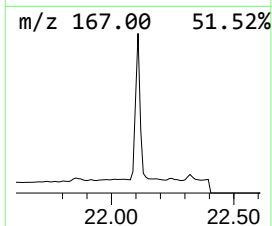
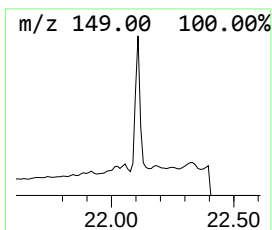
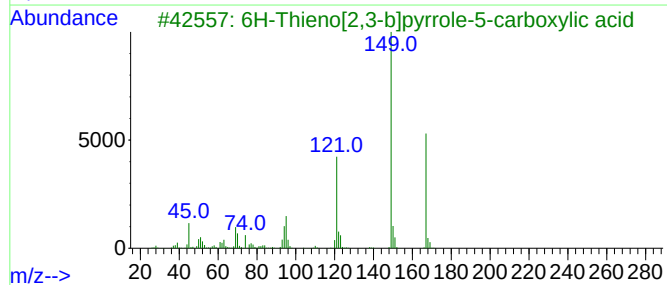
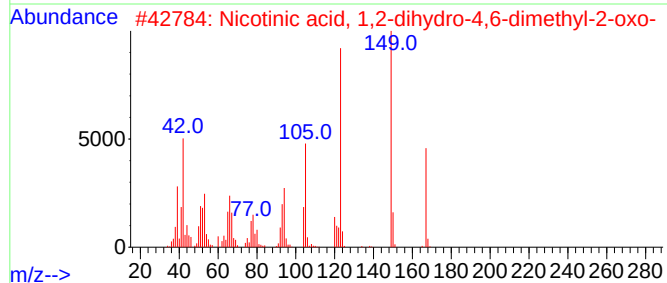
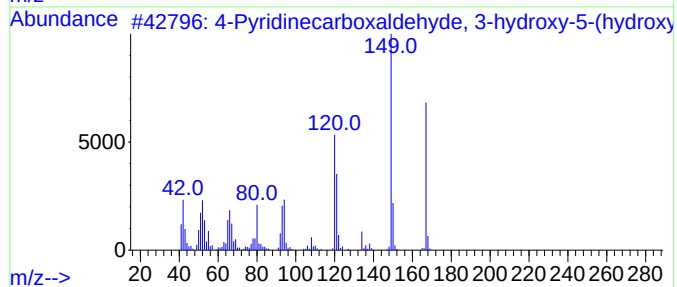
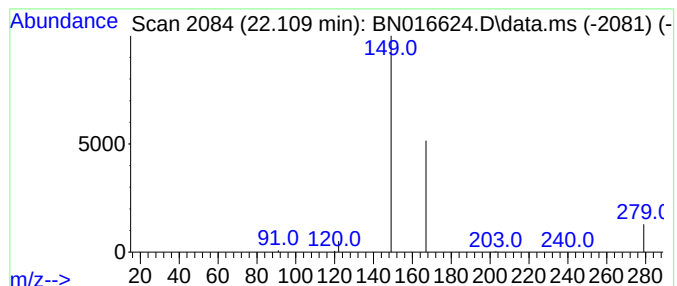
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Peak Number 6 4-Pyridinecarboxaldehyde, 3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.109	0.04 ng	17721	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	9
2			Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5
3			6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5NO2S	051856-25-8	5
4			4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	5
5			2-Amino-6-methoxybenzoic acid	167	C8H9NO3	1000496-75-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016624.D
Acq On : 01 Oct 2021 07:11
Operator : CG/JU
Sample : M3833-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE103D3-20210920

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	6.7	ng	1482770	1	7.642	89041	0.4
Hydrogen isocya...	3.502	0.1	ng	18026	1	7.642	89041	0.4
Acetic acid, me...	3.816	0.2	ng	41295	1	7.642	89041	0.4
Butane	4.821	0.3	ng	69759	1	7.642	89041	0.4
N-Hydroxymethyl...	10.191	0.1	ng	54966	2	10.407	161441	0.4
4-Pyridinecarbo...	22.109	0.0	ng	17721	5	21.227	168378	0.4