LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016664.D
Acq On : 02 Oct 2021 09:56
Operator : CG/JU
Sample : M3829-15
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE120D2-20210917

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: BN016664.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	1331048	2445626	100.00%	52.381%
2	3.364	29	31	47	rVB	51416	139808	5.72%	2.994%
3	3.816	76	80	96	rVB	11505	46784	1.91%	1.002%
4	4.821	185	189	203	rVB	39873	90990	3.72%	1.949%
5	7.633	489	494	500	rVB2	54711	113689	4.65%	2.435%
6	7.864	515	519	526	rBV	17841	36113	1.48%	0.773%
7	8.784	601	605	610	rBV	25808	53467	2.19%	1.145%
8	10.191	713	716	726	rBV	40474	74121	3.03%	1.588%
9	10.407	729	733	736	rBV	106084	184818	7.56%	3.958%
10	12.003	918	931	942	rBV	51657	84475	3.45%	1.809%
11	12.886	1071	1074	1078	rBV	108913	174869	7.15%	3.745%
12	14.269	1180	1183	1186	rBV	138540	200740	8.21%	4.299%
13	17.017	1400	1403	1406	rBV	111158	166766	6.82%	3.572%
14	19.063	1688	1696	1726	rBV	143569	197353	8.07%	4.227%
15	19.673	1813	1819	1843	rBV	130487	169831	6.94%	3.637%
16	21.164	1993	1995	1998	rBV	59990	84190	3.44%	1.803%
17	21.227	1998	2001	2011	rVB	121709	197201	8.06%	4.224%
18	23.484	2415	2427	2464	rVB	102841	208093	8.51%	4.457%

Sum of corrected areas: 4668934

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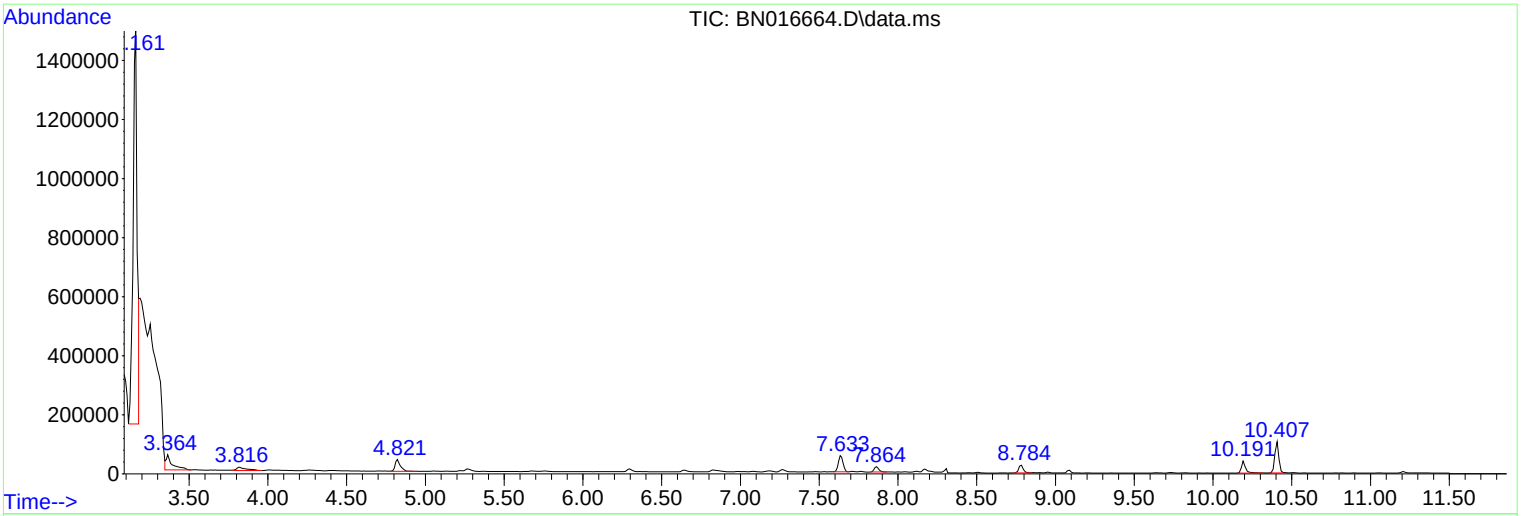
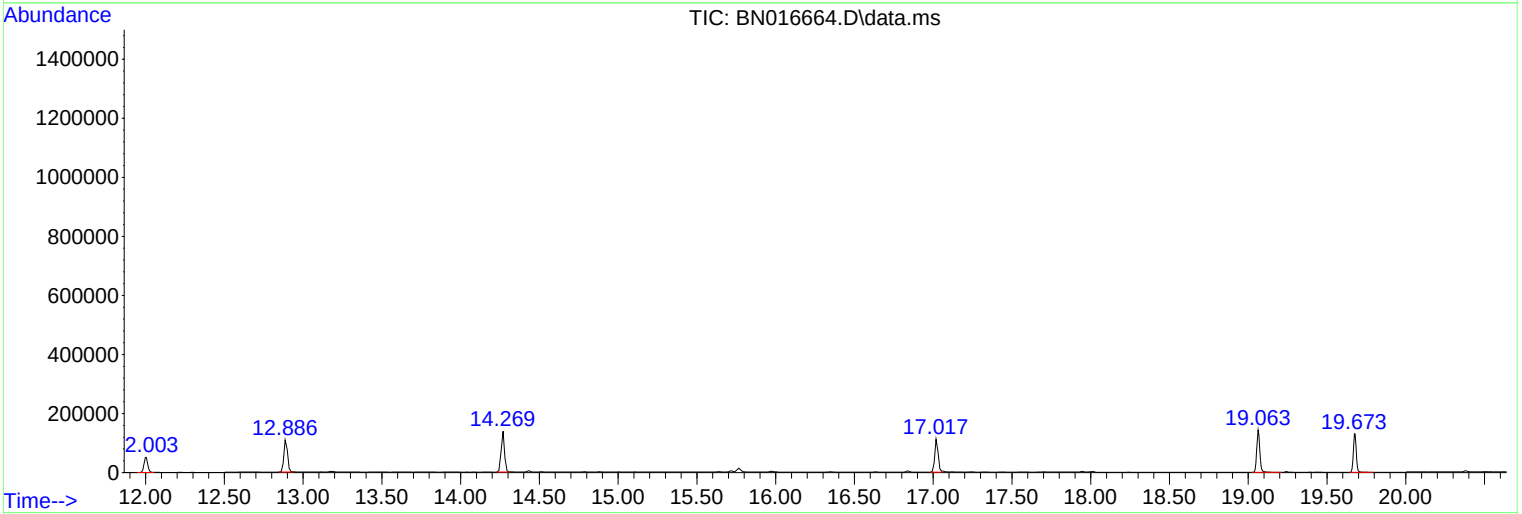
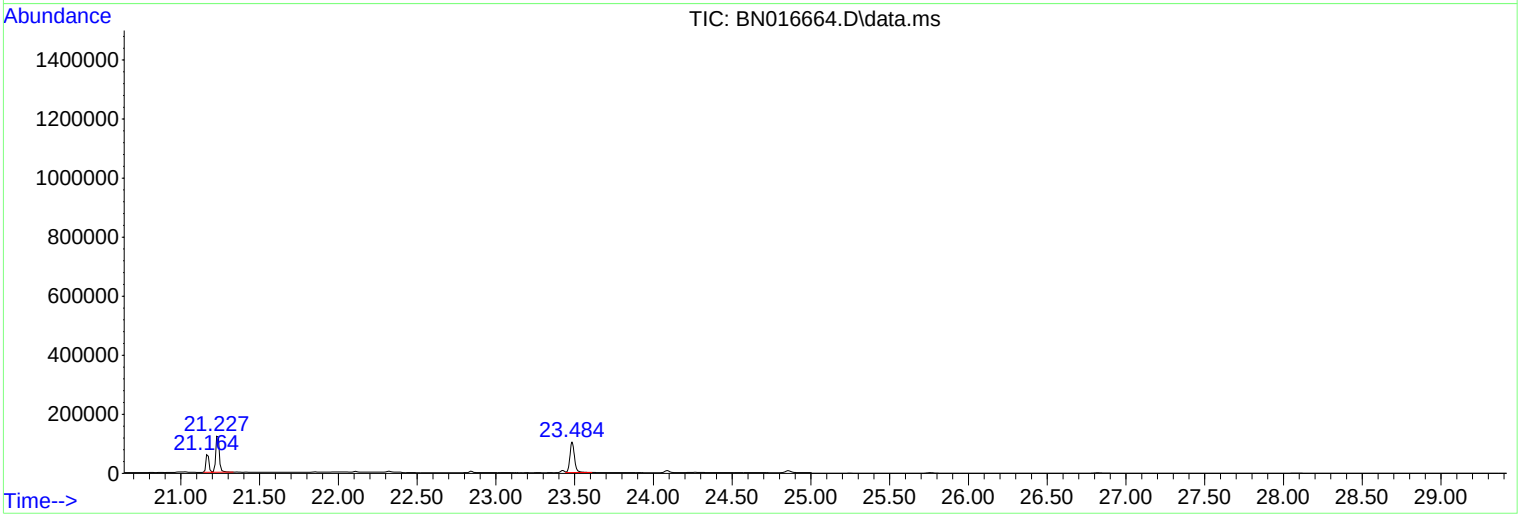
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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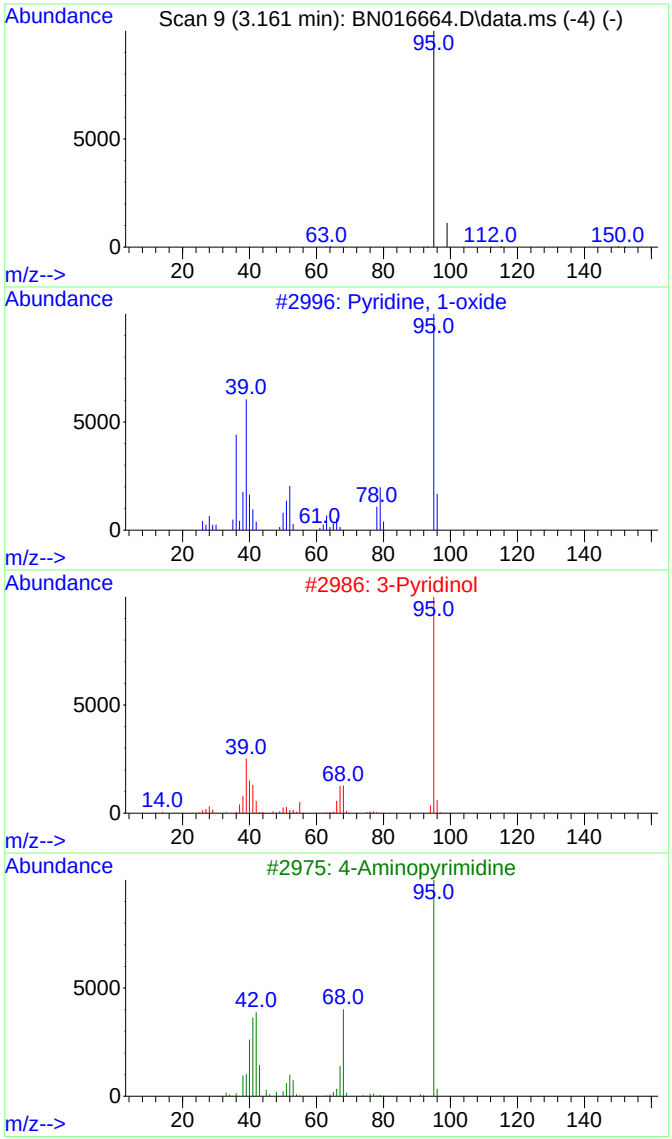
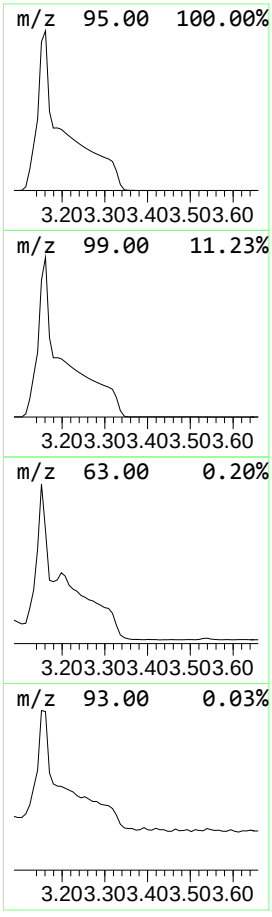
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	8.60 ng	2445630	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)aminoacrylontrile	95	C4H5N3	167320-31-2	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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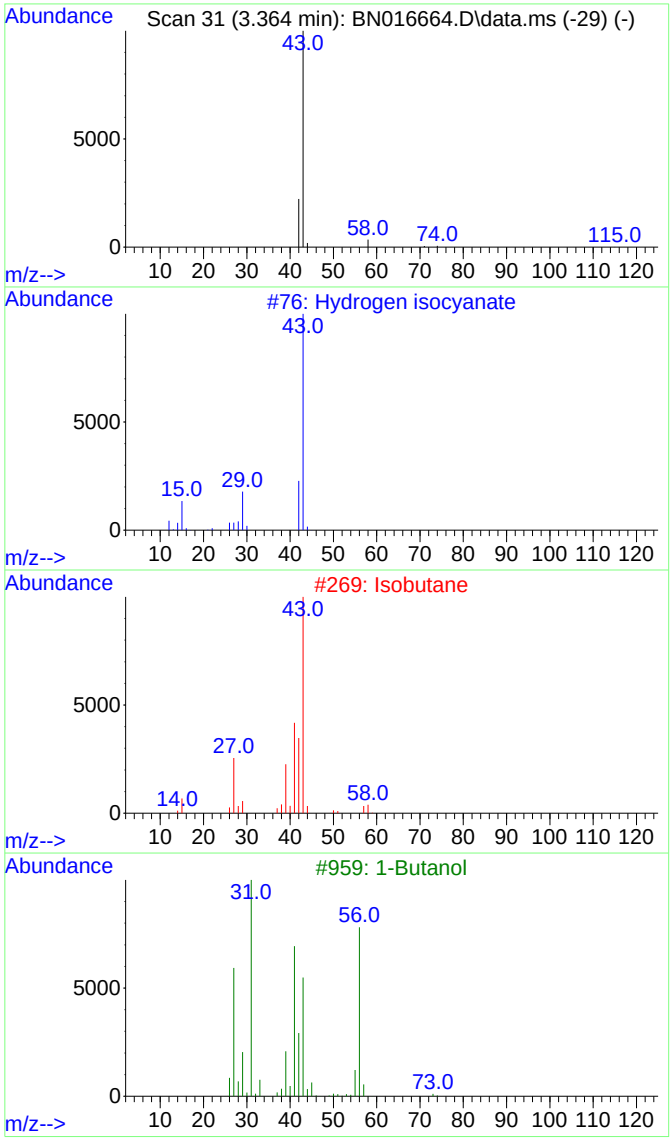
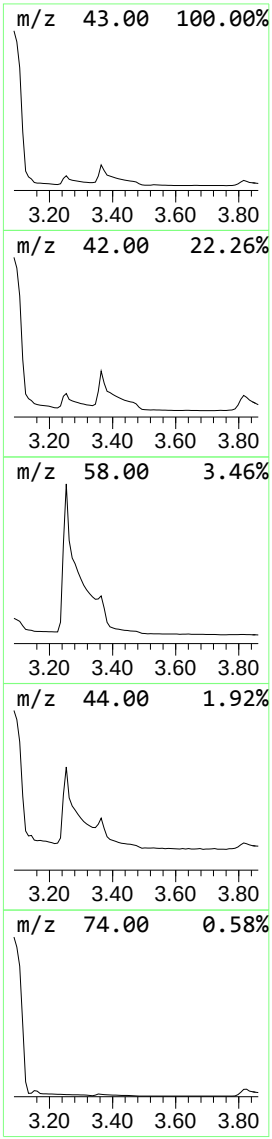
Peak Number 2 Hydrogen isocyanate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.49 ng	139808	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	4
2	Isobutane	58	C4H10	000075-28-5	4
3	1-Butanol	74	C4H10O	000071-36-3	2
4	Methane, diazo-	42	CH2N2	000334-88-3	2
5	Diazirine	42	CH2N2	1000305-84-1	2





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Sample : M3829-15
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE120D2-20210917

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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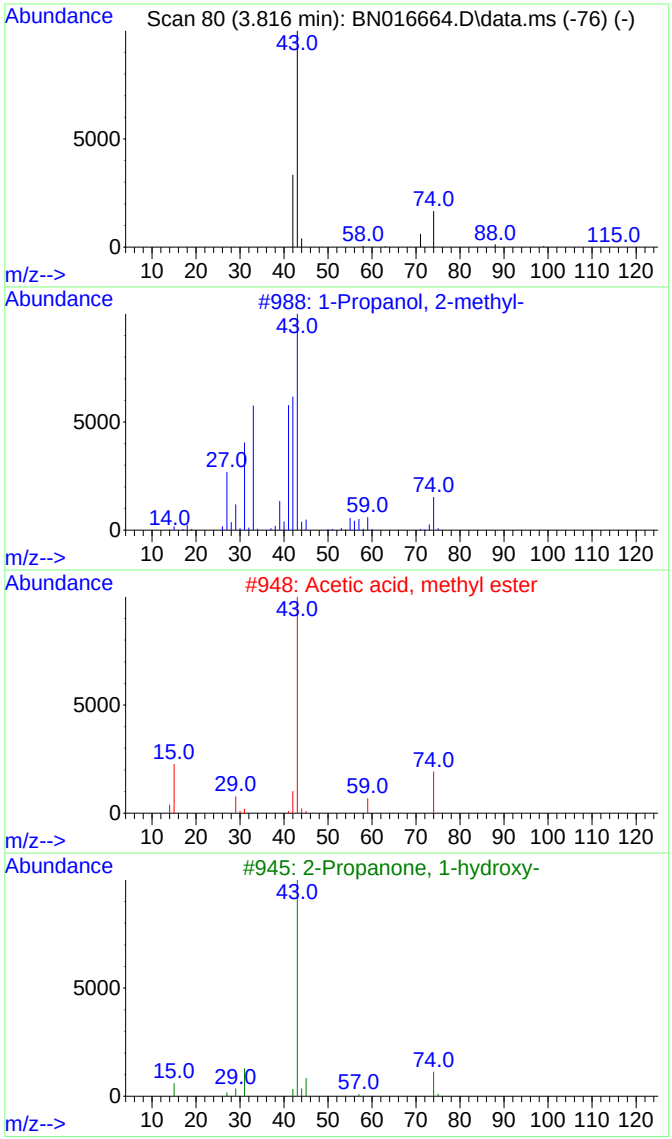
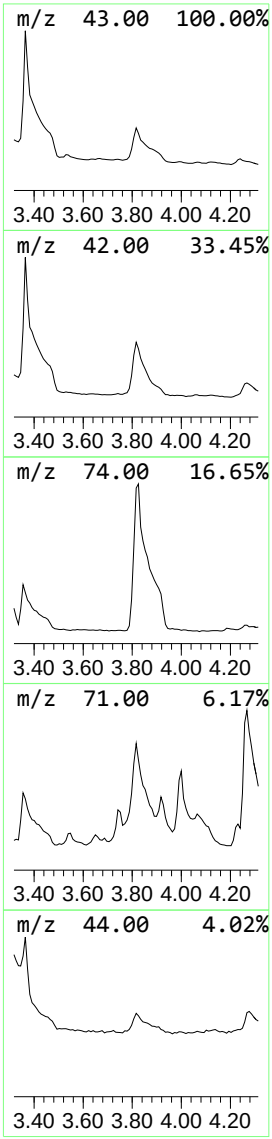
Peak Number 3 1-Propanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.16 ng	46784	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	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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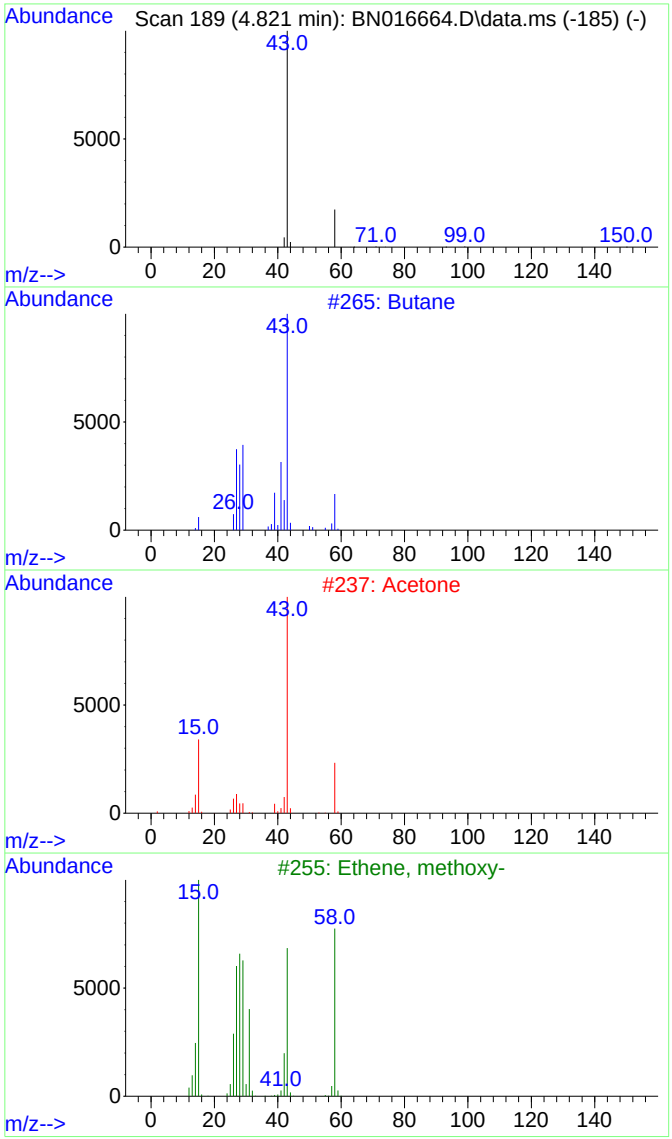
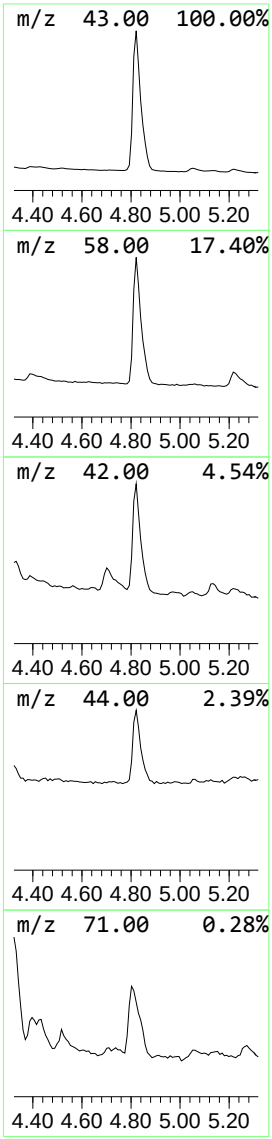
Peak Number 4 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.32 ng	90990	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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TIC Library : C:\Database\NIST20.L
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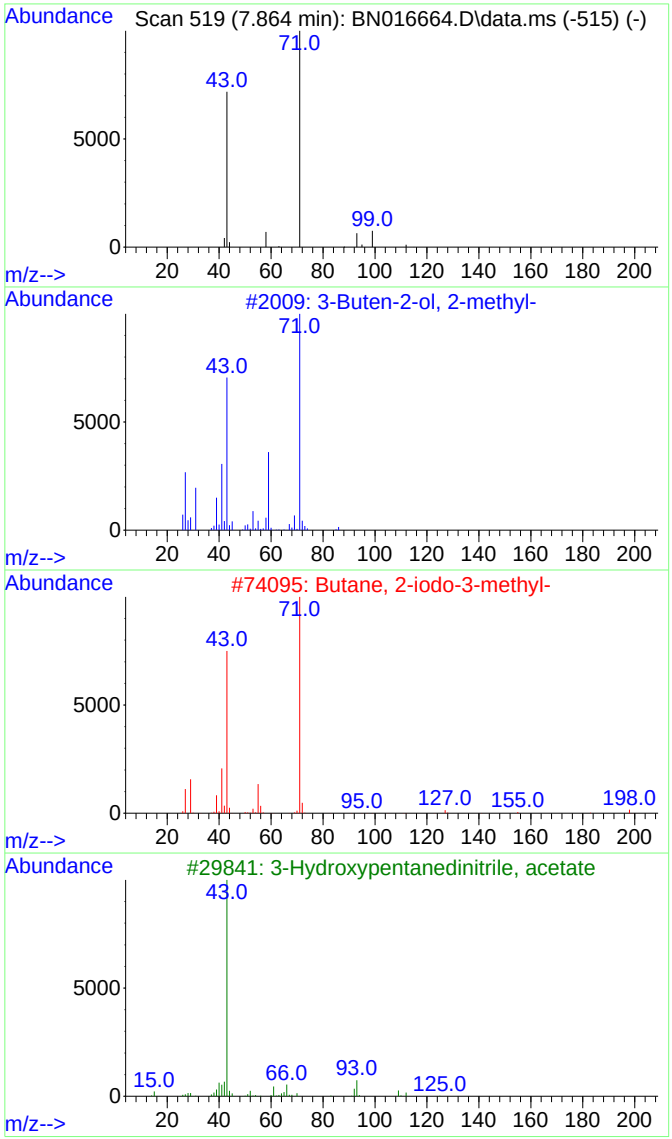
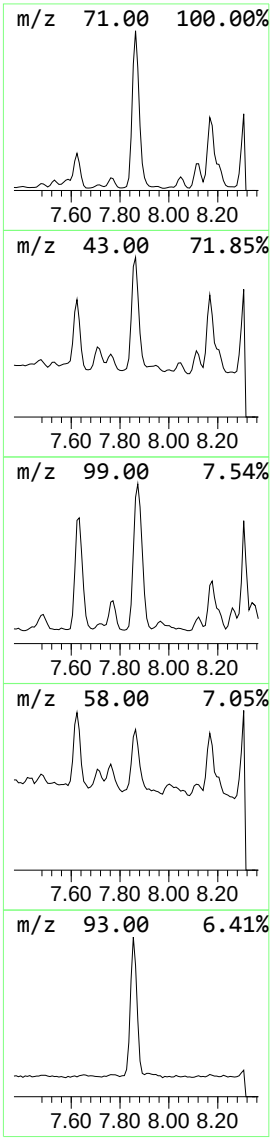
****
Peak Number 5 3-Buten-2-ol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.13 ng	36113	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
2	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
3	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
4	3-Penten-2-ol	86	C5H10O	001569-50-2	4
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4





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TIC Library : C:\Database\NIST20.L
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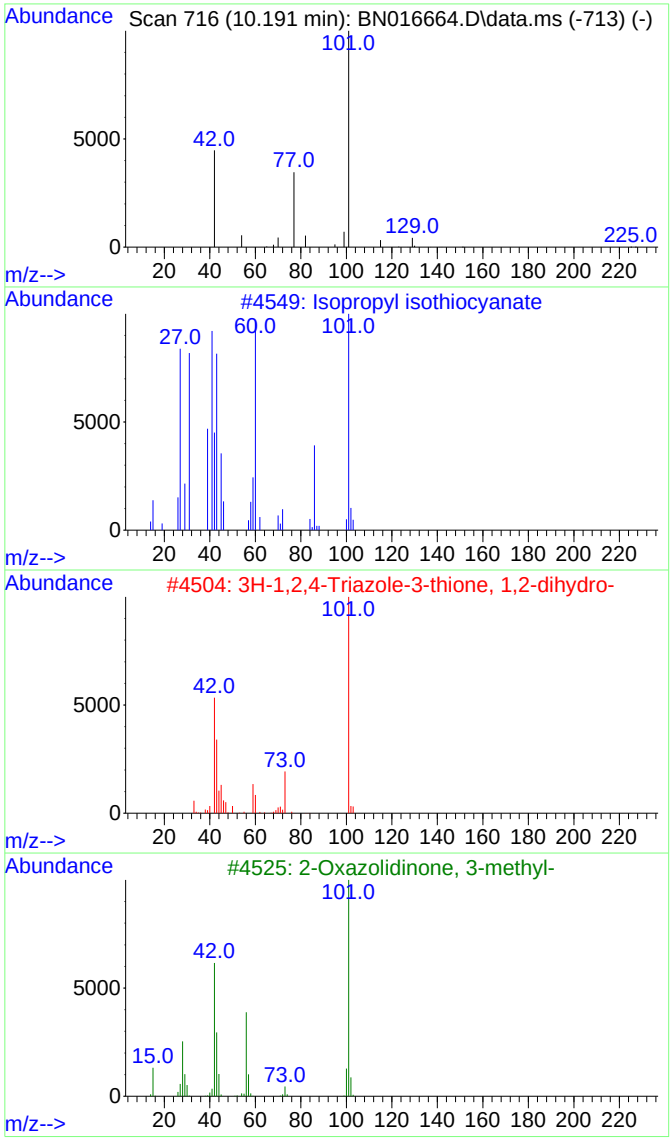
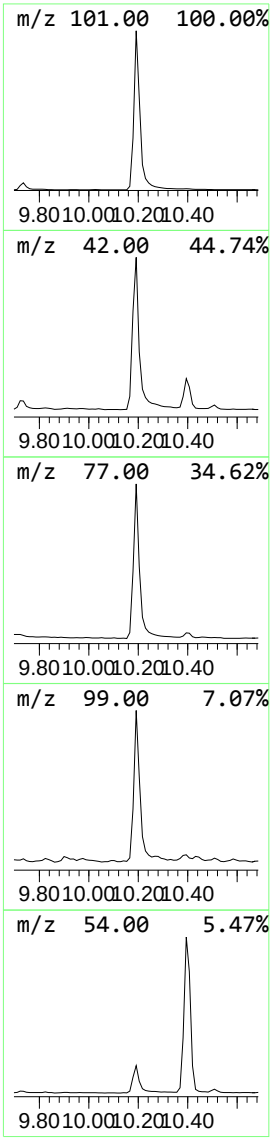
Peak Number 6 Isopropyl isothiocyanate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.16 ng	74121	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
2	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	8.6	ng	2445630	1	7.642	113689	0.4
Hydrogen isocya...	3.364	0.5	ng	139808	1	7.642	113689	0.4
1-Propanol, 2-m...	3.816	0.2	ng	46784	1	7.642	113689	0.4
Butane	4.821	0.3	ng	90990	1	7.642	113689	0.4
3-Buten-2-ol, 2...	7.864	0.1	ng	36113	1	7.642	113689	0.4
Isopropyl isoth...	10.191	0.2	ng	74121	2	10.406	184818	0.4