LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE105D1-20210917

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: BN016661.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	5	8	11	rBV	186370	270301	74.36%	8.323%
2	3.253	17	19	29	rVB	114611	363516	100.00%	11.193%
3	3.364	29	31	47	rVB	58121	165744	45.59%	5.104%
4	3.816	76	80	97	rVB	9123	38458	10.58%	1.184%
5	4.240	122	126	139	rVV	15191	52697	14.50%	1.623%
6	4.388	140	142	154	rVB	2711	9233	2.54%	0.284%
7	4.821	185	189	204	rVB	146442	336917	92.68%	10.374%
8	5.107	217	220	227	rVB2	4283	10829	2.98%	0.333%
9	5.264	234	237	245	rVB	5898	15660	4.31%	0.482%
10	6.296	345	349	354	rBV	16366	35789	9.85%	1.102%
11	6.361	354	356	369	rVB	3402	8248	2.27%	0.254%
12	6.637	383	386	398	rVB2	3823	9743	2.68%	0.300%
13	6.822	403	406	417	rVB3	4549	17436	4.80%	0.537%
14	7.080	431	434	440	rVB2	2174	4717	1.30%	0.145%
15	7.181	441	445	450	rVV2	2597	7104	1.95%	0.219%
16	7.264	450	454	460	rVB2	7347	16269	4.48%	0.501%
17	7.633	489	494	499	rBV2	50110	104532	28.76%	3.219%
18	7.864	515	519	526	rBV	14645	29634	8.15%	0.912%
19	8.113	543	546	549	rBV	2700	6040	1.66%	0.186%
20	8.168	549	552	560	rVV	9861	27910	7.68%	0.859%
21	8.306	563	567	569	rVB	12949	17398	4.79%	0.536%
22	8.784	601	605	610	rBV	22075	45322	12.47%	1.396%
23	9.089	626	629	634	rBV2	3967	7560	2.08%	0.233%
24	10.191	713	716	726	rBV	20972	41001	11.28%	1.263%
25	10.407	729	733	739	rBV	101385	178927	49.22%	5.510%
26	12.003	916	931	942	rBV	43812	72354	19.90%	2.228%
27	12.886	1071	1074	1078	rBV	92383	152377	41.92%	4.692%
28	14.269	1180	1183	1186	rBV	129561	188485	51.85%	5.804%
29	15.766	1299	1301	1305	rVB2	10878	17081	4.70%	0.526%
30	17.018	1400	1403	1406	rBV	103940	156959	43.18%	4.833%
31	18.016	1483	1485	1497	rVB5	2794	3994	1.10%	0.123%
32	19.063	1688	1696	1726	rBV	134149	187895	51.69%	5.786%
33	19.242	1727	1732	1749	rBV	2417	4049	1.11%	0.125%
34	19.679	1813	1820	1850	rBV	129151	162436	44.68%	5.002%
35	20.006	1885	1886	1890	rBV3	1824	4986	1.37%	0.154%
36	20.983	1974	1978	1992	rBV2	4054	16011	4.40%	0.493%

LSC Area Percent Report

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Instrument : BNA_N
ClientSampleId : RE105D1-20210917

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

37	21.164	1992	1995	1998	rBV	33691	43229	11.89%	1.331%
38	21.227	1998	2001	2011	rVB	127189	187531	51.59%	5.774%
39	22.841	2232	2239	2257	rVB	3061	4770	1.31%	0.147%
40	23.419	2400	2408	2414	rBV	4222	7060	1.94%	0.217%
41	23.481	2414	2426	2478	rVB	97014	194852	53.60%	6.000%
42	24.084	2593	2602	2620	rBV	4441	8854	2.44%	0.273%
43	24.850	2817	2826	2848	rVB2	4201	9856	2.71%	0.303%
44	25.754	3072	3090	3113	rBV	1269	3810	1.05%	0.117%

Sum of corrected areas: 3247574

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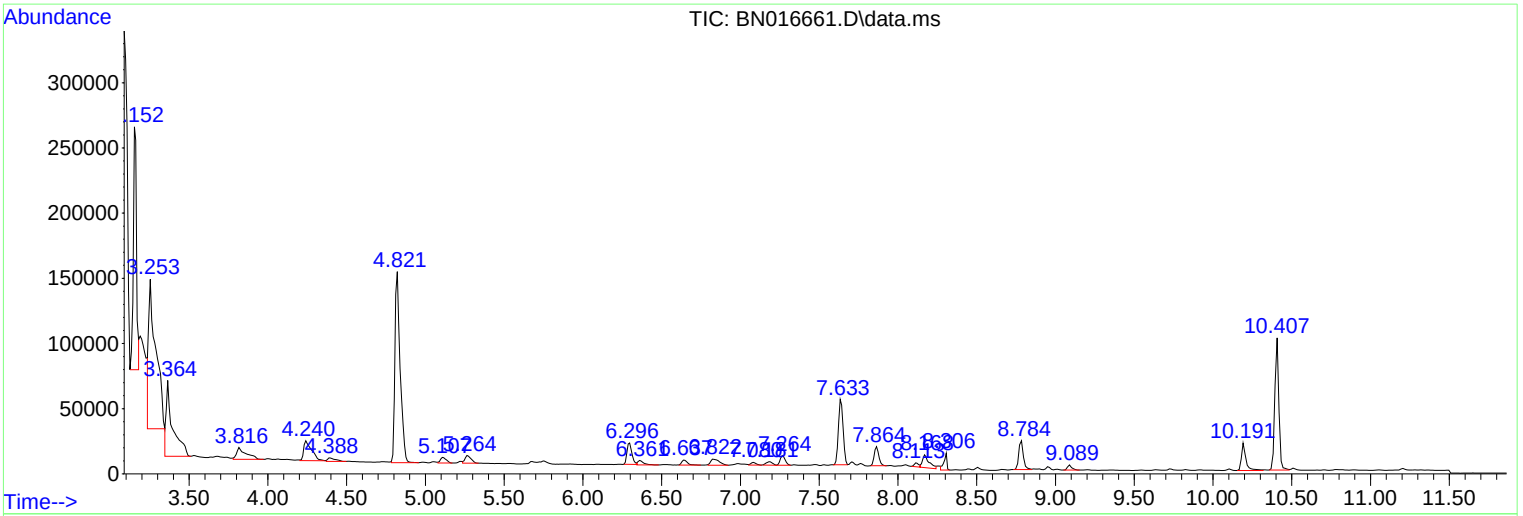
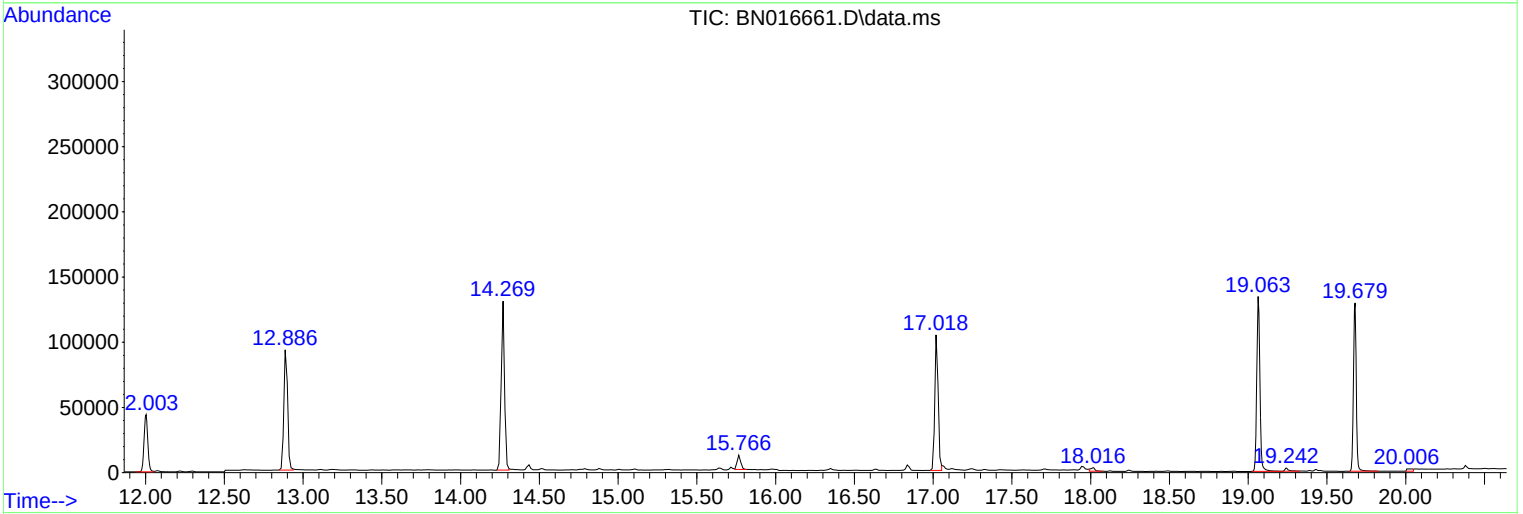
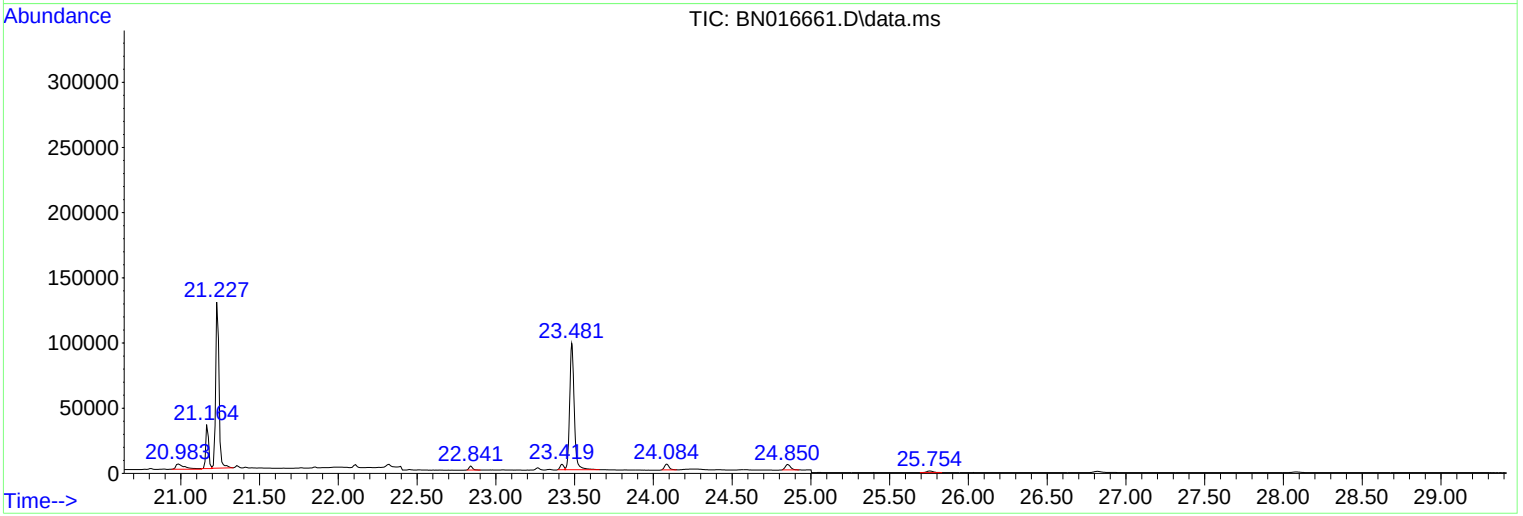
Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
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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

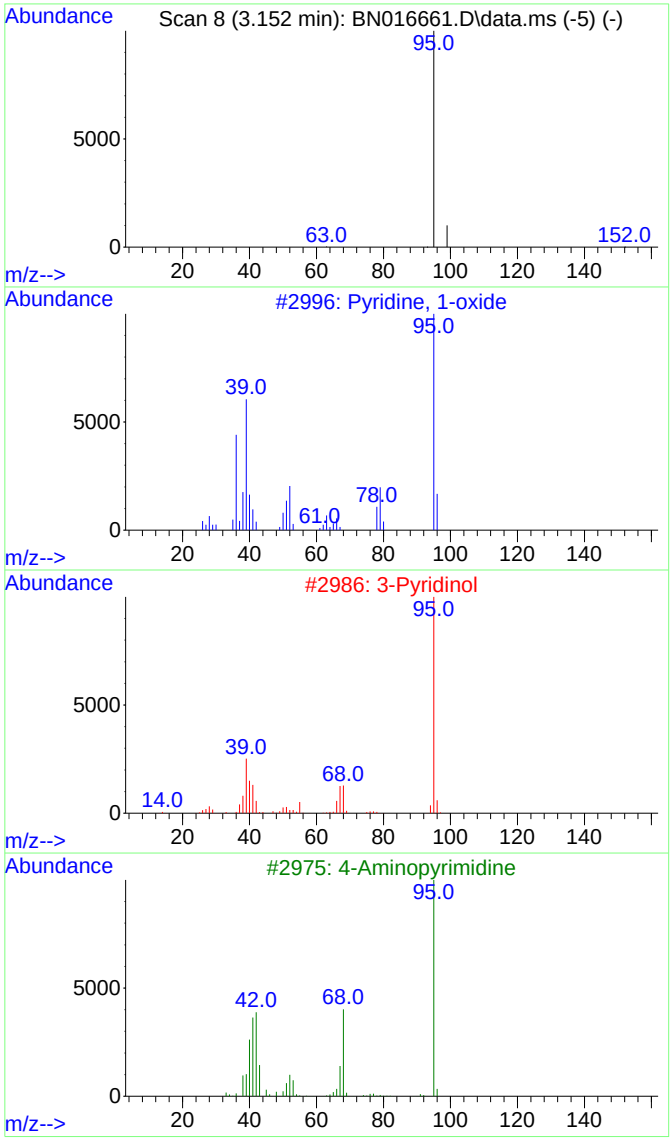
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

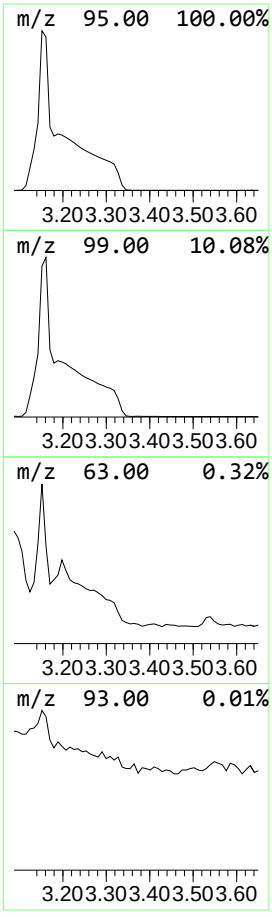
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	1.03 ng	270301	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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Data File : BN016661.D
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Sample : M3829-09
Misc :
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Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

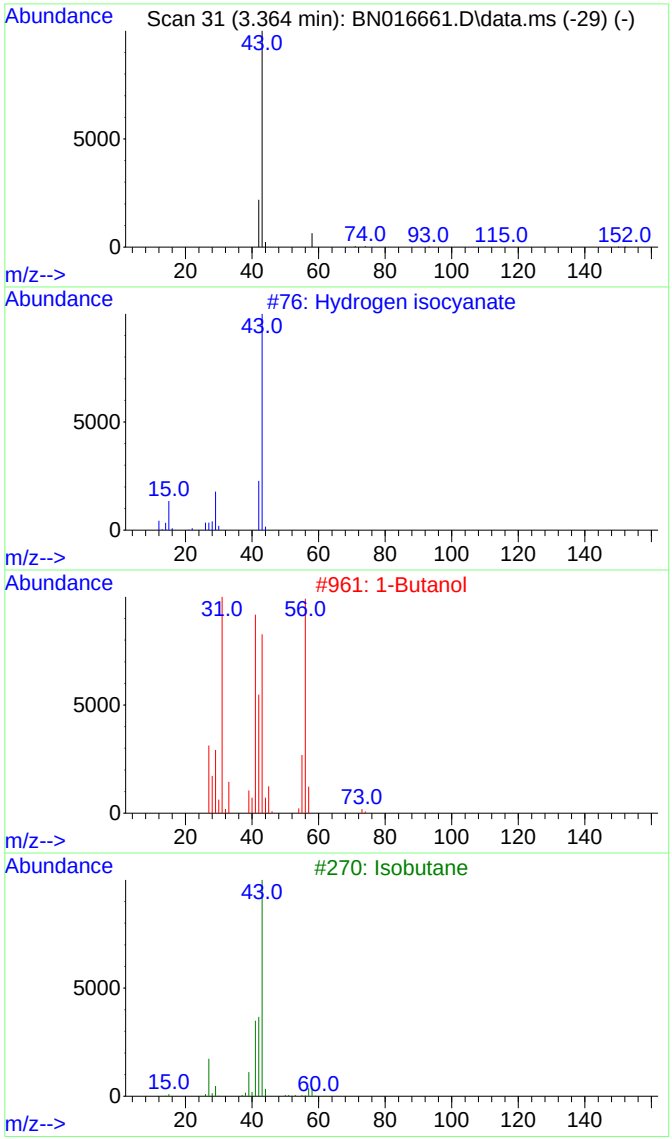
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

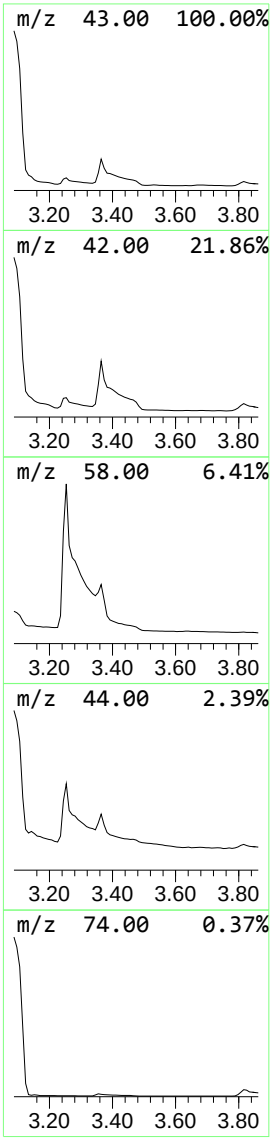
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.63 ng	165744	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	1-Butanol	74	C4H10O	000071-36-3	3
3	Isobutane	58	C4H10	000075-28-5	3
4	Hydrogen azide	43	HN3	007782-79-8	2
5	Butane	58	C4H10	000106-97-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

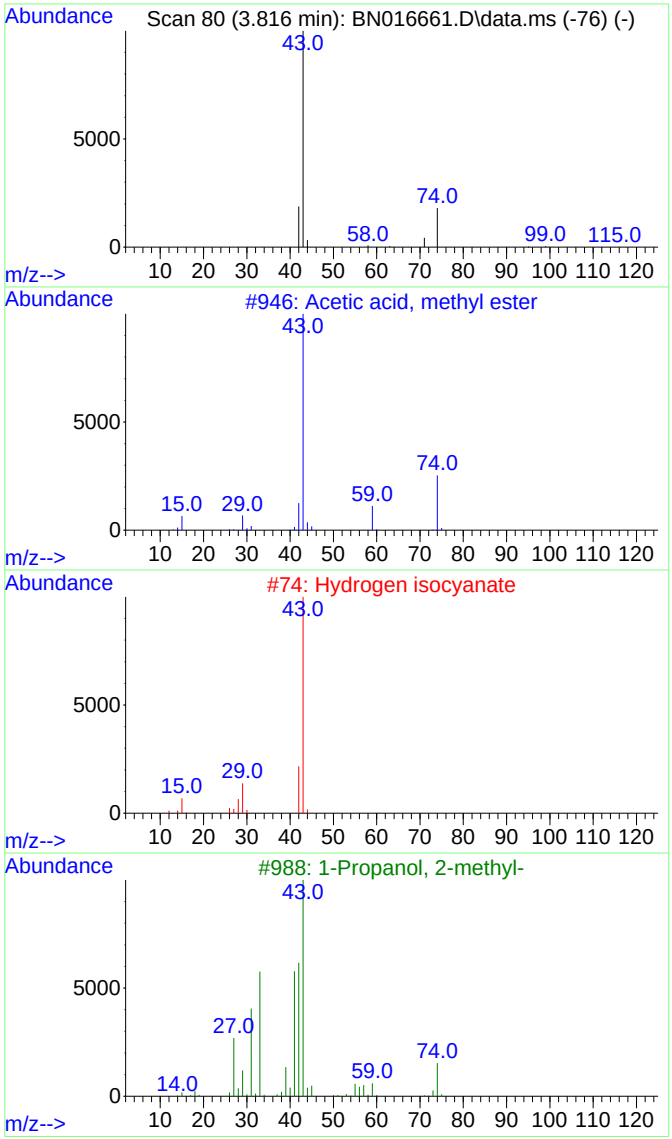
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

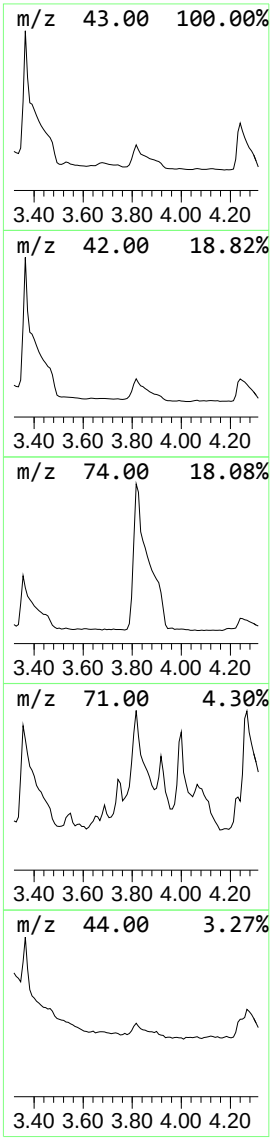
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.15 ng	38458	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	9
2	Hydrogen isocyanate	43	CHNO	000075-13-8	4
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	O-Methylisourea	74	C2H6N2O	002440-60-0	4





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Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

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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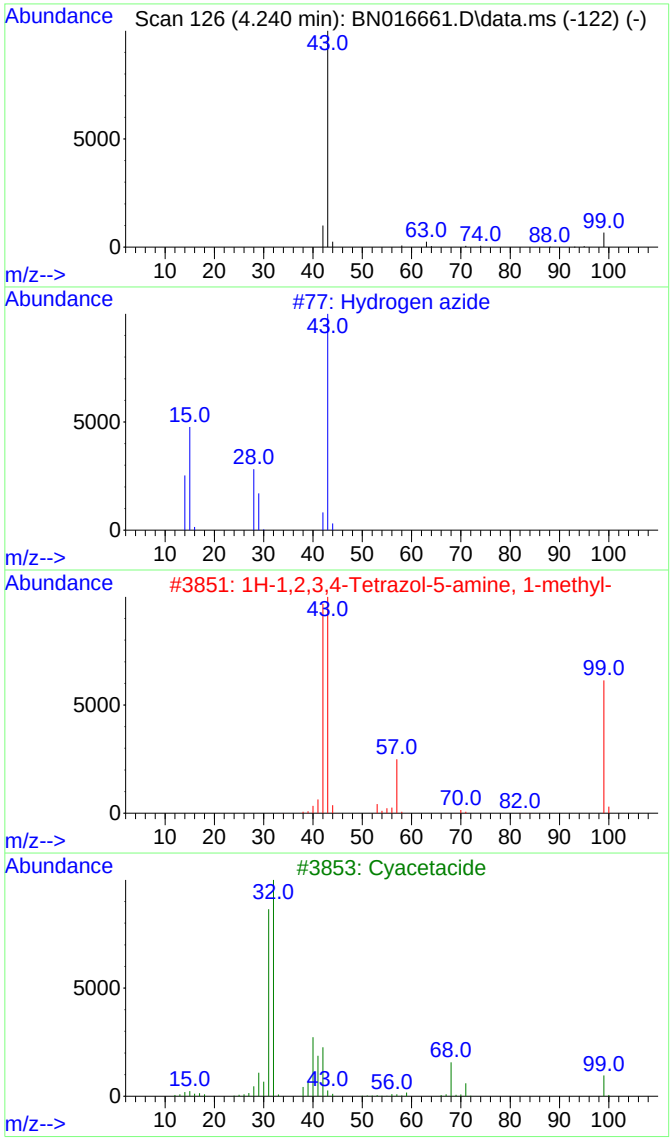
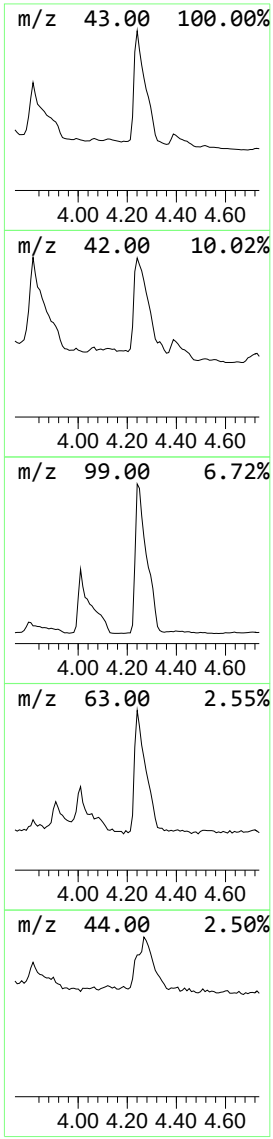
Peak Number 4 Hydrogen azide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	0.20 ng	52697	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen azide	43	HN3	007782-79-8	4
2	1H-1,2,3,4-Tetrazol-5-amine, 1-m...	99	C2H5N5	005422-44-6	3
3	Cyacetacide	99	C3H5N3O	000140-87-4	3
4	Hydrogen isocyanate	43	CHNO	000075-13-8	2
5	4-Methyl-pent-3-enylamine	99	C6H13N	013296-28-1	2





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Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

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
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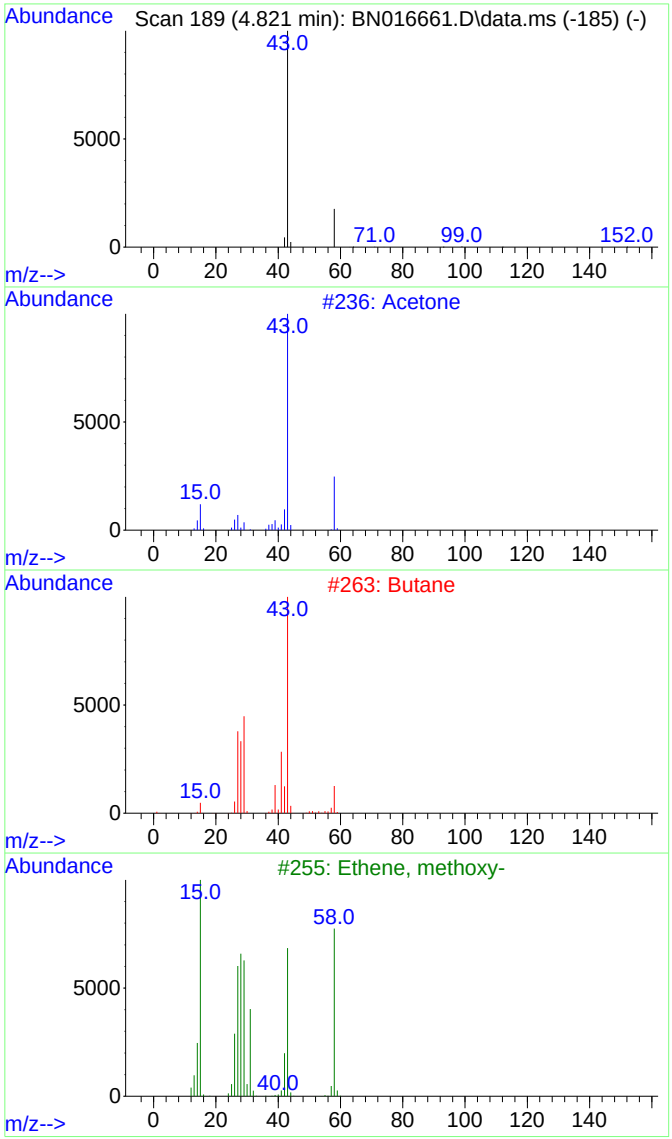
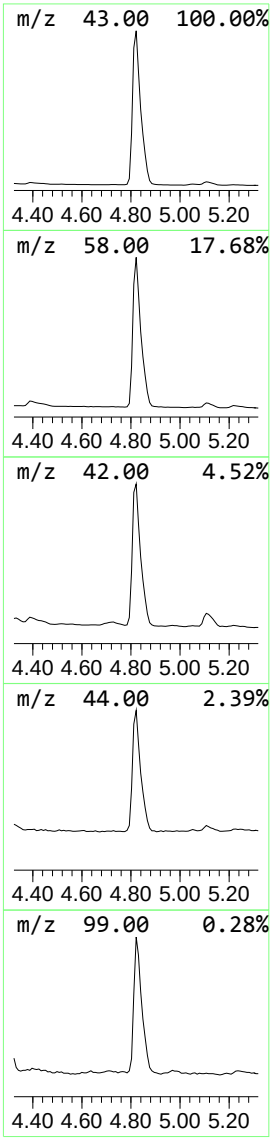
****

Peak Number 5 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	1.29 ng	336917	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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Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
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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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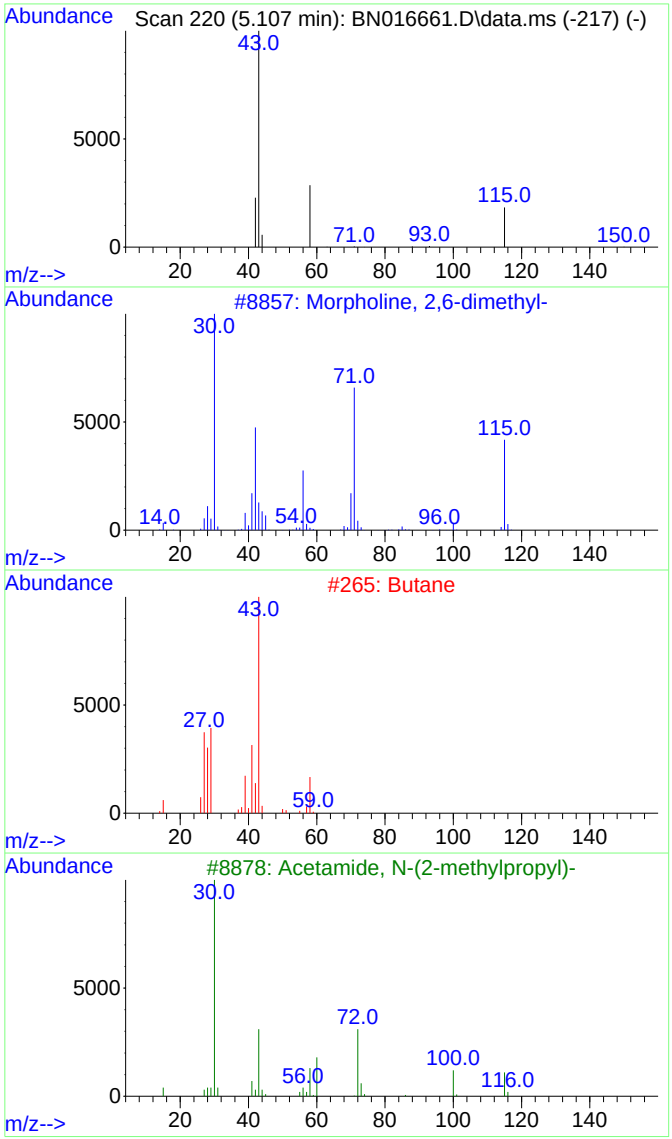
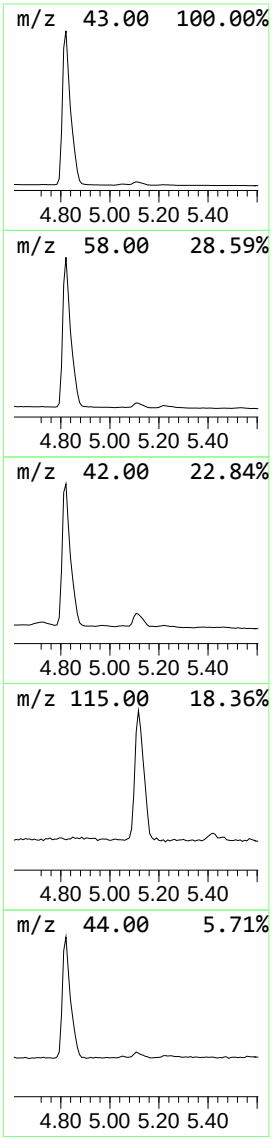
Peak Number 6 Morpholine, 2,6-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.107	0.04 ng	10829	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	5
2	Butane	58	C4H10	000106-97-8	4
3	Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	4
4	Cyclopropanesulfonamide, acetate	163	C5H9NO3S	1010507-55-0	4
5	Acetone	58	C3H6O	000067-64-1	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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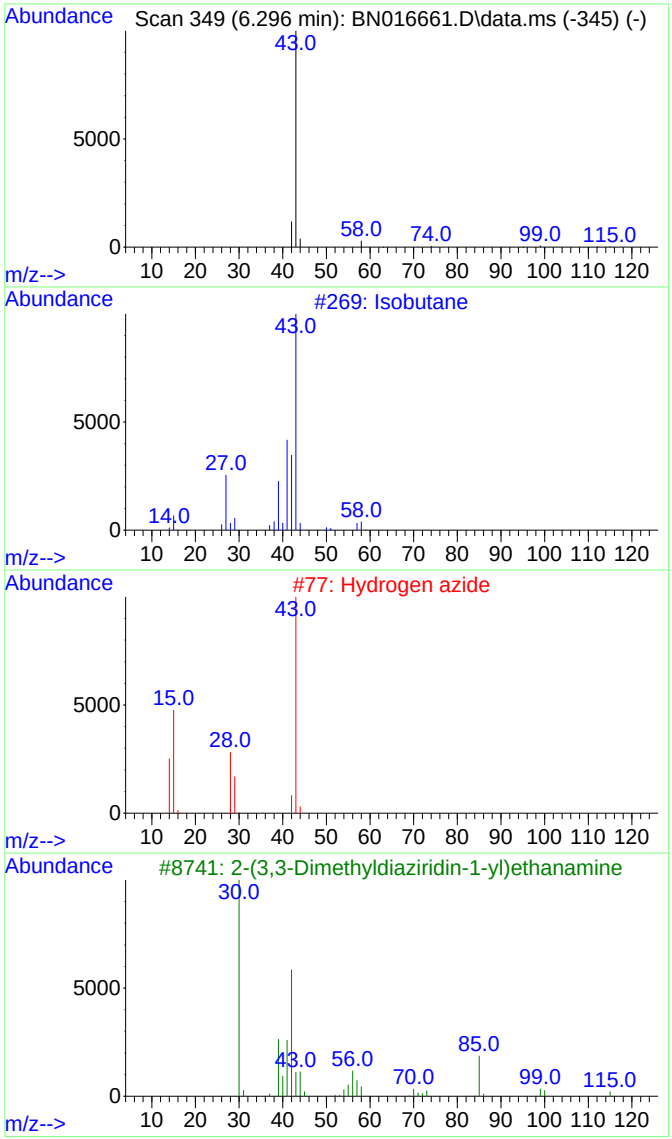
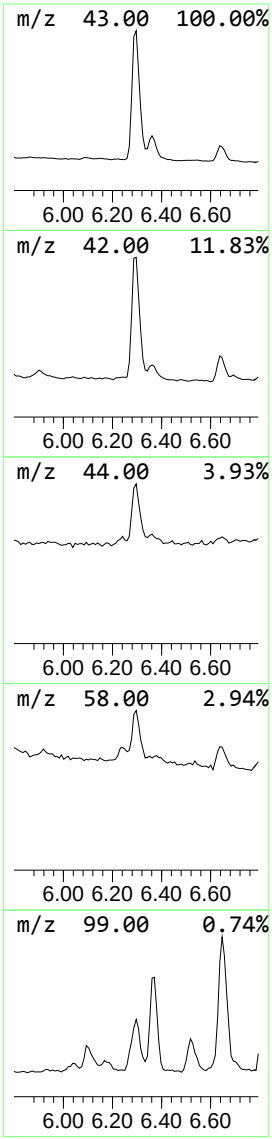
Peak Number 7 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.14 ng	35789	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	4
2	Hydrogen azide	43	HN3	007782-79-8	4
3	2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	2
4	2,3-Octanedione	142	C8H14O2	000585-25-1	2
5	1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-66-3	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

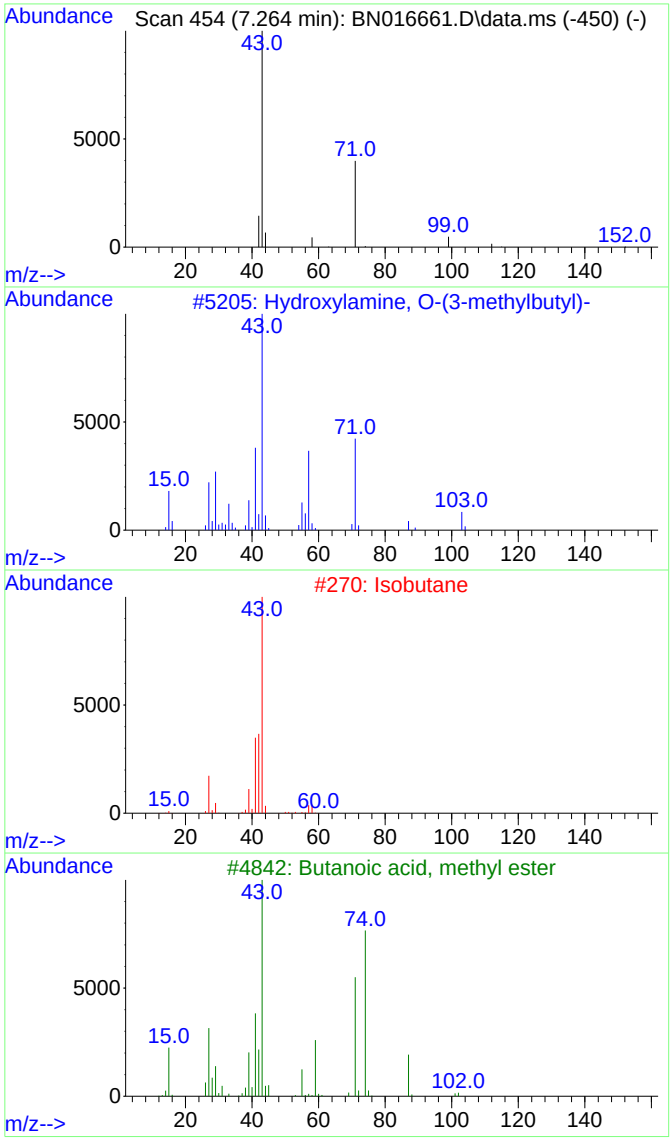
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

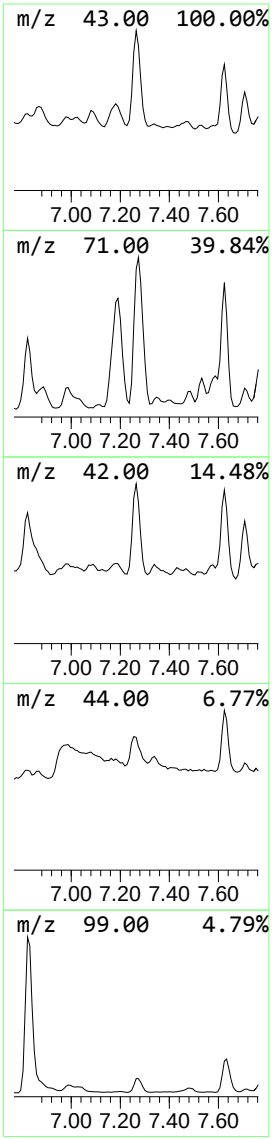
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hydroxylamine, O-(3-methylb... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	16269	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	4
2	Isobutane	58	C4H10	000075-28-5	4
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
4	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
5	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4





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Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

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

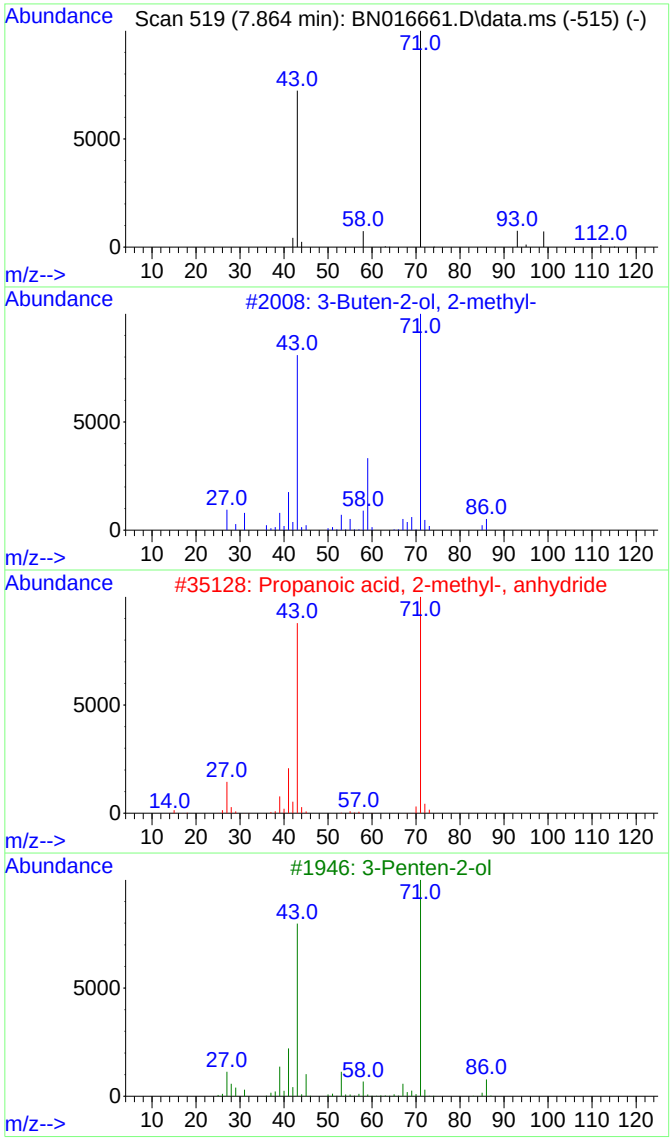
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

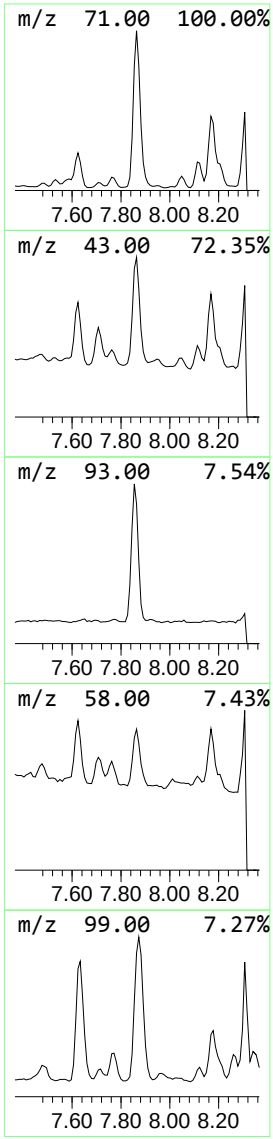
****

Peak Number 9 3-Buten-2-ol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.11 ng	29634	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	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
3	3-Penten-2-ol	86	C5H10O	001569-50-2	4
4	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
5	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4





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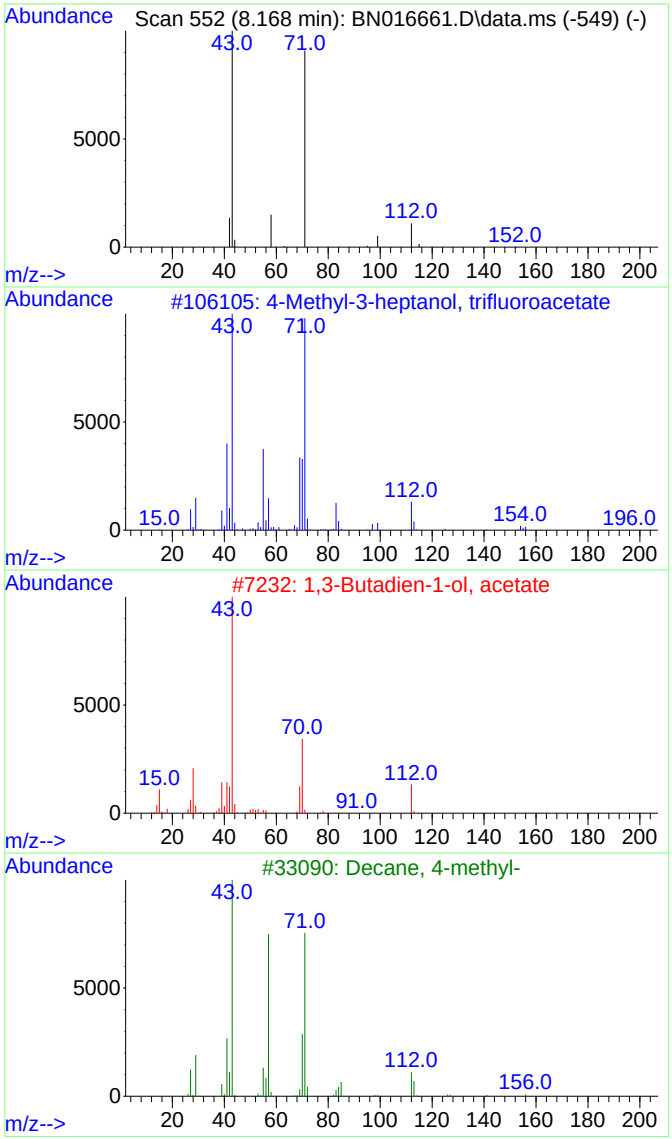
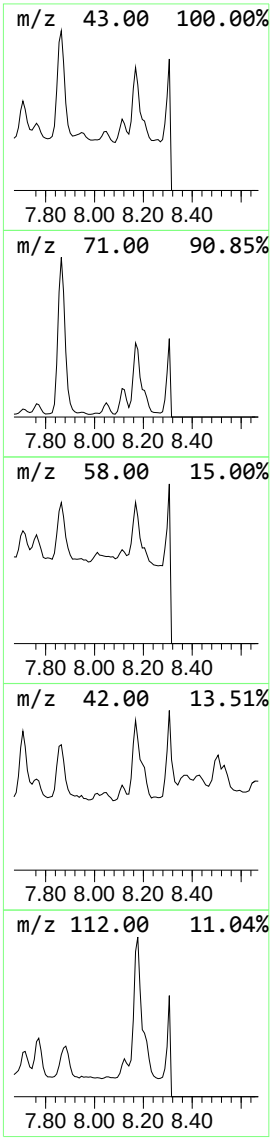
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 4-Methyl-3-heptanol, triflu... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.11 ng	27910	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	43
2	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3	Decane, 4-methyl-	156	C11H24	002847-72-5	9
4	Octane, 3-ethyl-	142	C10H22	005881-17-4	9
5	5-Hepten-2-one	112	C7H12O	006714-00-7	7





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Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

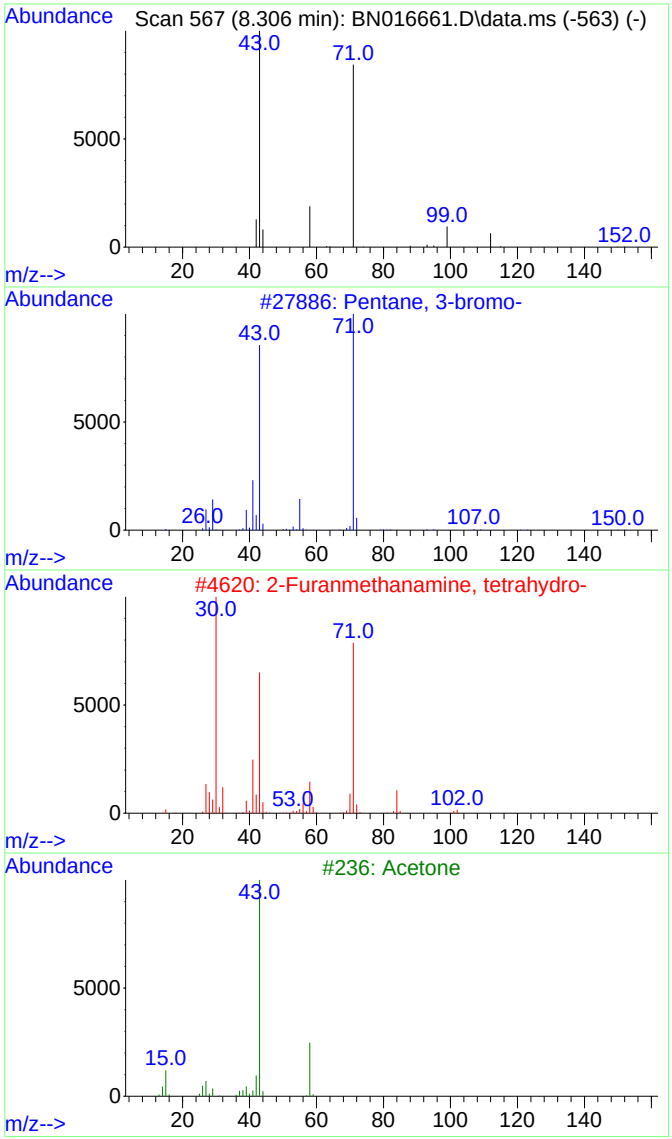
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

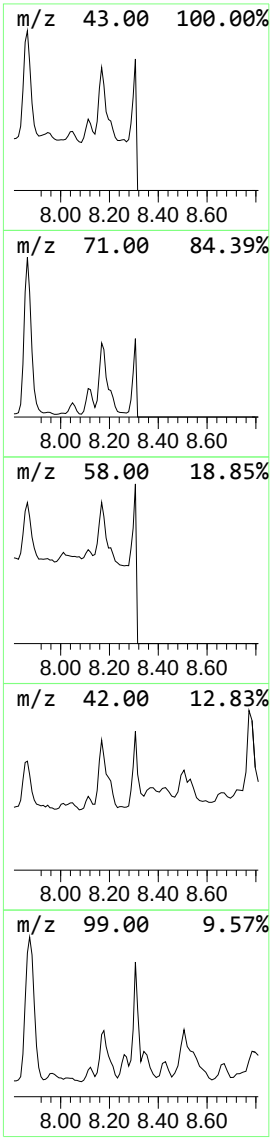
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Pentane, 3-bromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.07 ng	17398	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	9
2	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9
3	Acetone	58	C3H6O	000067-64-1	5
4	Butane	58	C4H10	000106-97-8	5
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4





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BNA_N
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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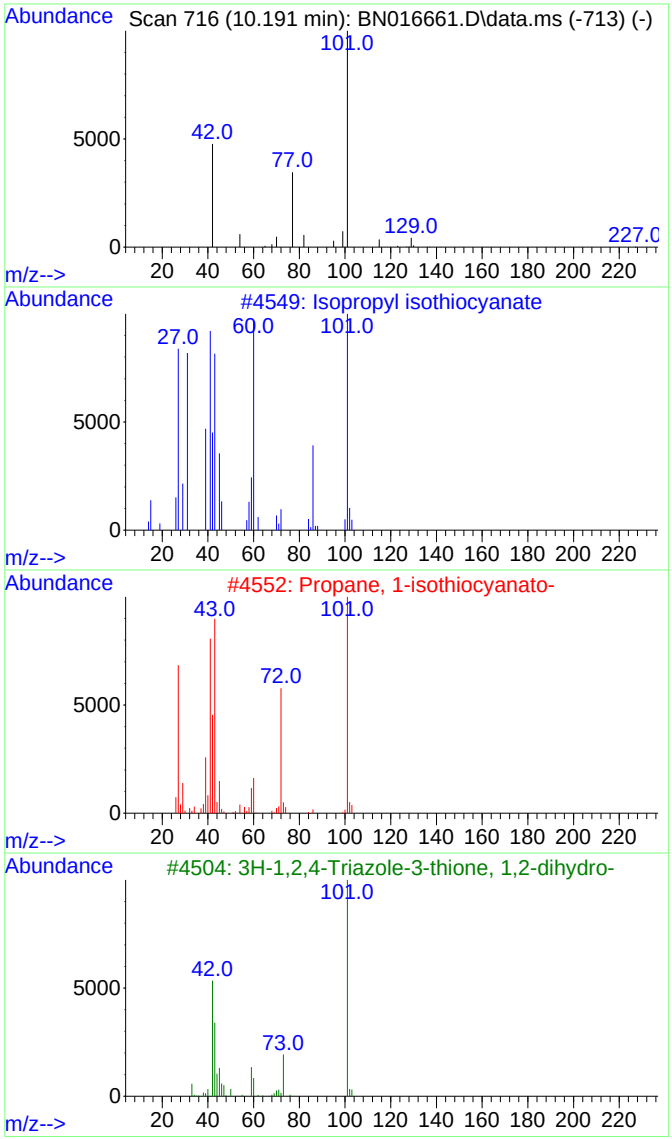
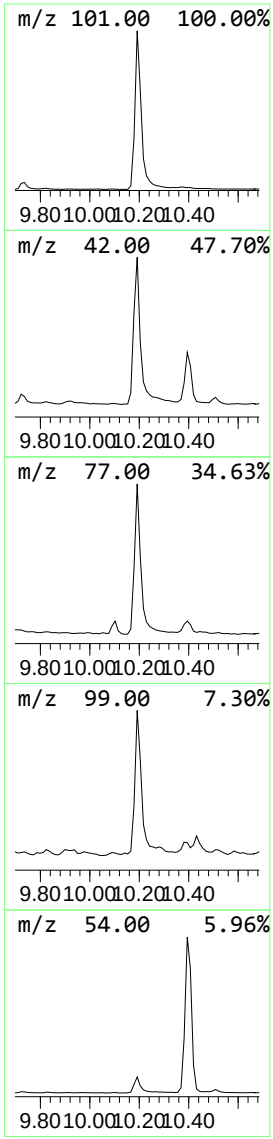
Peak Number 12 Isopropyl isothiocyanate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.09 ng	41001	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
2	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





Tentatively Identified Compound (LSC) summary

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Data File : BN016661.D
Acq On : 02 Oct 2021 08:09
Operator : CG/JU
Sample : M3829-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE105D1-20210917

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyridine, 1-oxide	3.152	1.0	ng	270301	1	7.642	104532	0.4
Hydrogen isocya...	3.364	0.6	ng	165744	1	7.642	104532	0.4
Acetic acid, me...	3.816	0.1	ng	38458	1	7.642	104532	0.4
Hydrogen azide	4.240	0.2	ng	52697	1	7.642	104532	0.4
Acetone	4.821	1.3	ng	336917	1	7.642	104532	0.4
Morpholine, 2,6...	5.107	0.0	ng	10829	1	7.642	104532	0.4
Isobutane	6.296	0.1	ng	35789	1	7.642	104532	0.4
Hydroxylamine, ...	7.264	0.1	ng	16269	1	7.642	104532	0.4
3-Buten-2-ol, 2...	7.864	0.1	ng	29634	1	7.642	104532	0.4
4-Methyl-3-hept...	8.168	0.1	ng	27910	1	7.642	104532	0.4
Pentane, 3-bromo-	8.306	0.1	ng	17398	1	7.642	104532	0.4
Isopropyl isoth...	10.191	0.1	ng	41001	2	10.407	178927	0.4