LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE120D3-20210917

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: BN016663.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	11	rVB	45028	50310	23.03%	2.028%
2	3.364	29	31	45	rVB	5406	17472	8.00%	0.704%
3	3.816	76	80	97	rVB	12179	50277	23.01%	2.027%
4	4.821	185	189	203	rVB	40162	95472	43.70%	3.849%
5	5.263	234	237	245	rVB	6889	18140	8.30%	0.731%
6	6.646	383	387	397	rVB	5433	13204	6.04%	0.532%
7	6.821	403	406	419	rVB3	5818	20139	9.22%	0.812%
8	7.181	441	445	450	rVB2	2641	7517	3.44%	0.303%
9	7.264	450	454	460	rVB2	6816	15494	7.09%	0.625%
10	7.633	490	494	500	rVB	46794	99388	45.49%	4.007%
11	7.863	515	519	526	rBV	15256	30936	14.16%	1.247%
12	8.112	543	546	549	rBV	2626	5872	2.69%	0.237%
13	8.168	549	552	560	rVV	9977	28688	13.13%	1.157%
14	8.306	563	567	569	rVB	13233	17295	7.92%	0.697%
15	8.784	601	605	610	rBV	23826	48090	22.01%	1.939%
16	10.191	713	716	726	rBV	30743	57477	26.31%	2.317%
17	10.406	729	733	739	rVV	99924	173291	79.32%	6.986%
18	11.205	793	796	803	rBV2	3765	8793	4.02%	0.355%
19	12.002	919	931	943	rBV	48623	78192	35.79%	3.152%
20	12.885	1071	1074	1078	rBV	97236	162764	74.50%	6.562%
21	13.177	1094	1097	1104	rBV2	3323	6789	3.11%	0.274%
22	14.268	1180	1183	1186	rBV	127016	184000	84.22%	7.418%
23	15.766	1299	1301	1305	rVB2	12088	18678	8.55%	0.753%
24	16.835	1385	1388	1395	rVB	3607	5730	2.62%	0.231%
25	17.017	1400	1403	1406	rBV	99464	153220	70.13%	6.177%
26	17.954	1477	1480	1483	rBV	10017	16115	7.38%	0.650%
27	18.015	1483	1485	1503	rVB5	4294	6183	2.83%	0.249%
28	19.063	1688	1696	1720	rBV	141372	192444	88.09%	7.759%
29	19.246	1727	1733	1756	rBV	14265	22965	10.51%	0.926%
30	19.430	1765	1770	1774	rBV	2364	2944	1.35%	0.119%
31	19.678	1813	1820	1840	rBV	130178	167620	76.72%	6.758%
32	20.006	1884	1886	1890	rBV3	1859	4767	2.18%	0.192%
33	20.983	1975	1978	1980	rBV	3341	7202	3.30%	0.290%
34	21.025	1980	1982	1992	rVB	2926	5308	2.43%	0.214%
35	21.163	1992	1995	1999	rBV	162759	218469	100.00%	8.808%
36	21.227	1999	2001	2011	rVB	128894	189101	86.56%	7.624%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE120D3-20210917

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	22.321	2100	2104	2108	rBV2	3615	7235	3.31%	0.292%
38	22.841	2232	2239	2256	rVB	4912	7613	3.48%	0.307%
39	23.423	2400	2409	2415	rBV	7559	12687	5.81%	0.511%
40	23.481	2415	2426	2474	rVB	97603	198784	90.99%	8.014%
41	24.083	2593	2602	2619	rVB	7858	15514	7.10%	0.625%
42	24.853	2815	2827	2849	rBV	8311	19438	8.90%	0.784%
43	25.757	3073	3091	3111	rBV	2509	7337	3.36%	0.296%
44	26.821	3382	3402	3424	rBV	2123	7184	3.29%	0.290%
45	28.081	3749	3770	3791	rBV	1160	4236	1.94%	0.171%

Sum of corrected areas: 2480374

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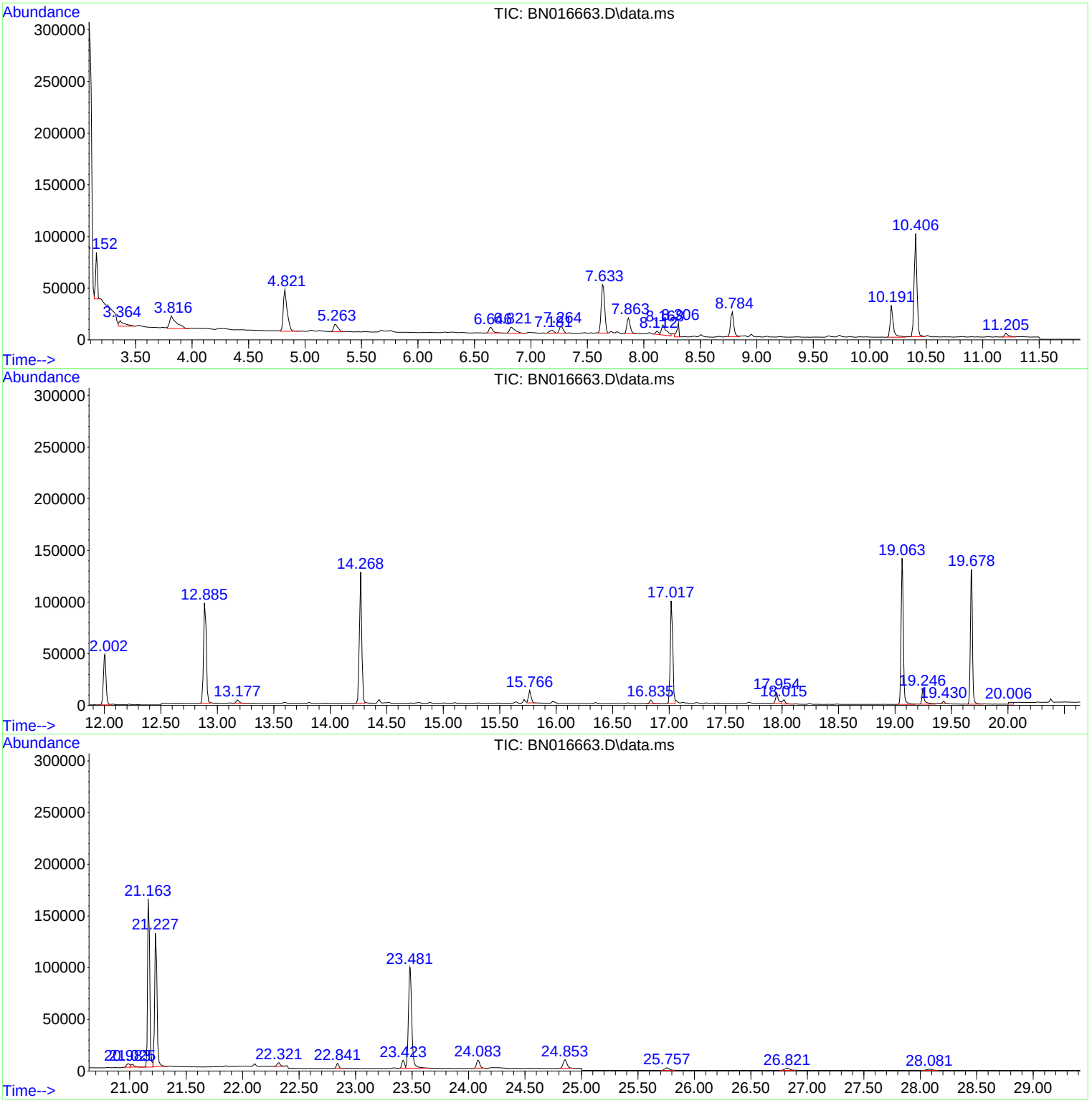
Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

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\
Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
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ALS Vial : 31 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RE120D3-20210917

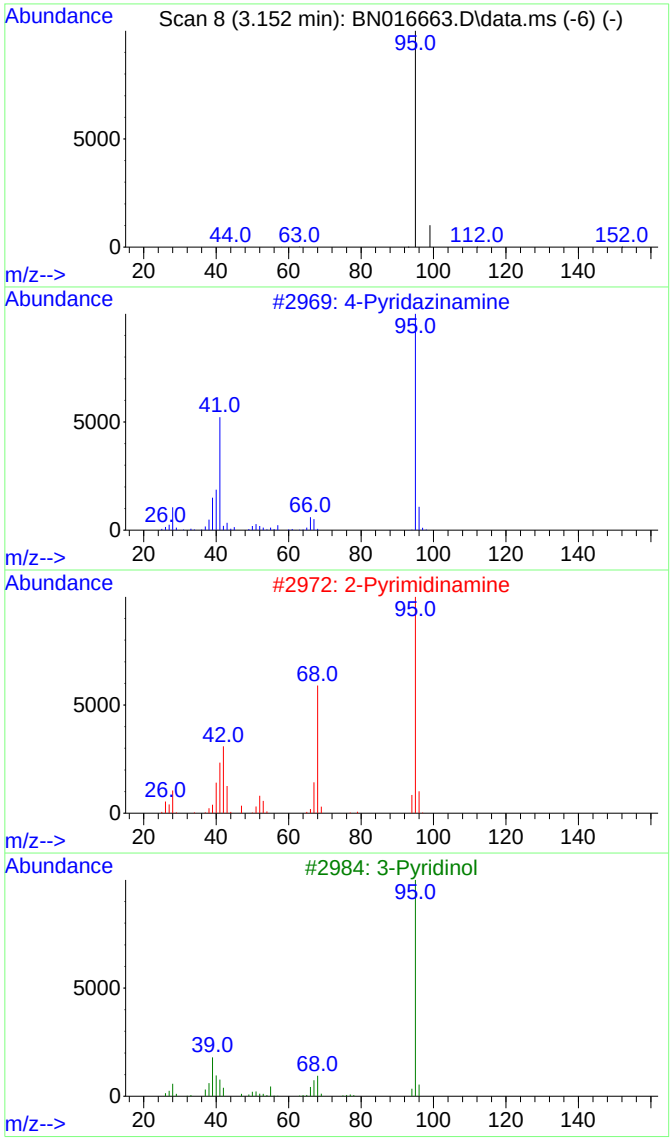
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

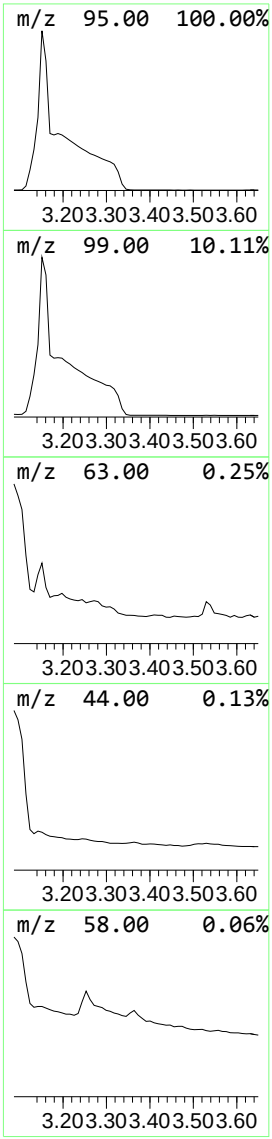
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Pyridazinamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.20 ng	50310	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	3-Pyridinol	95	C5H5NO	000109-00-2	2
4	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
5	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2





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Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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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

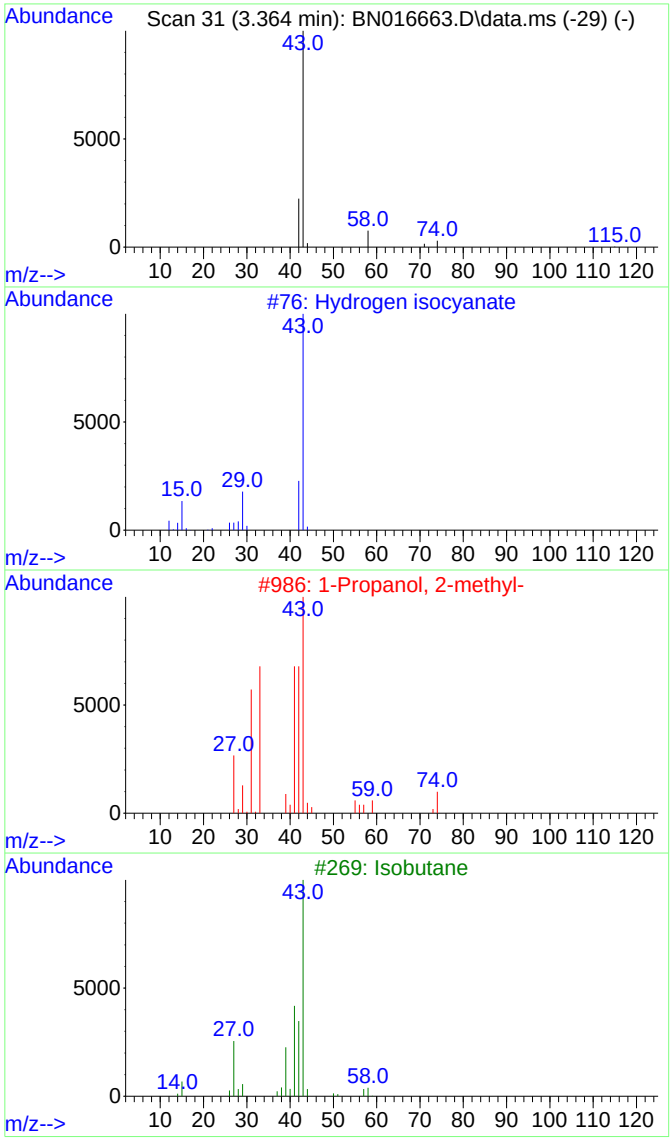
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

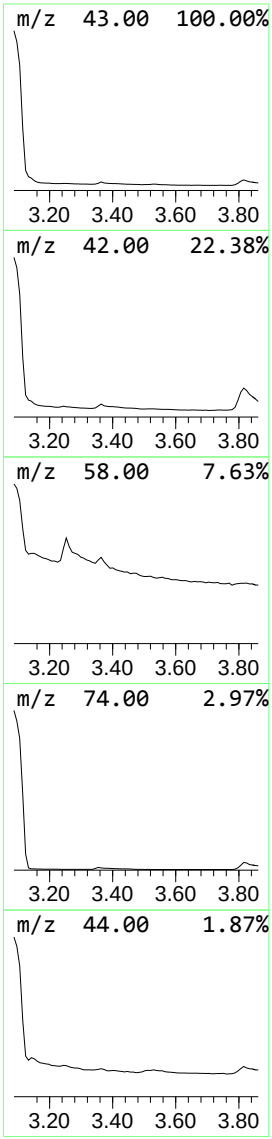
****

Peak Number 2 Hydrogen isocyanate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.07 ng	17472	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-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	Isobutane	58	C4H10	000075-28-5	3
4	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	2
5	Butane	58	C4H10	000106-97-8	2





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Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

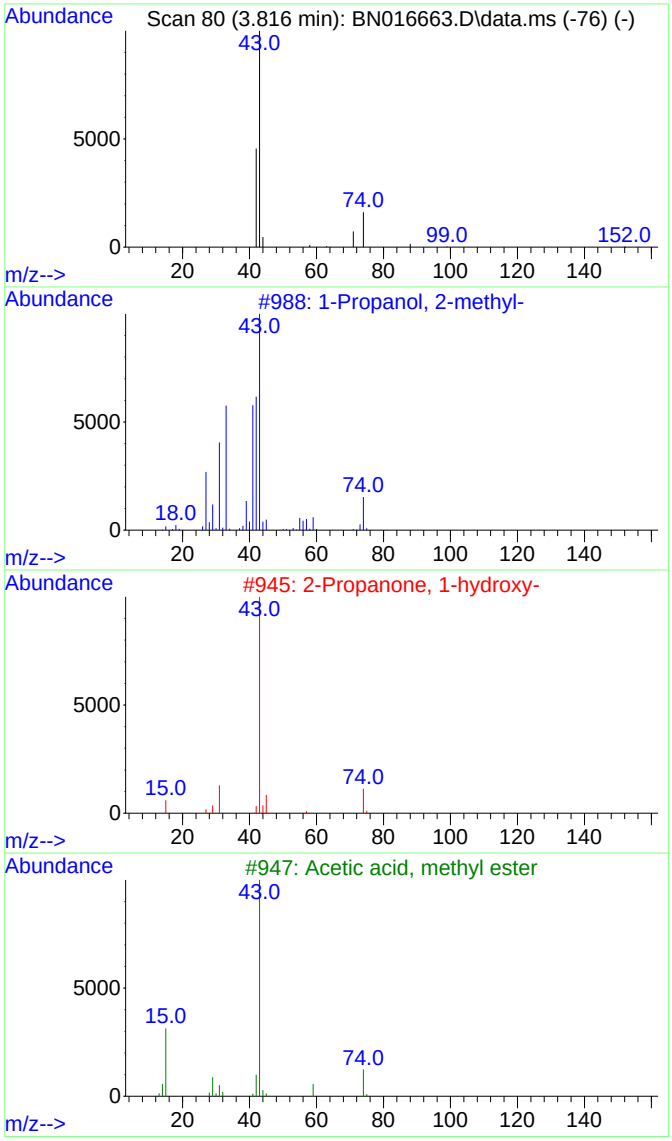
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

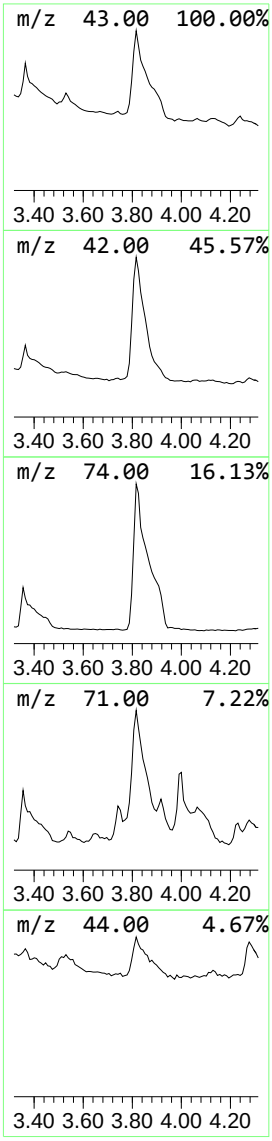
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.20 ng	50277	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	9
2	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

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

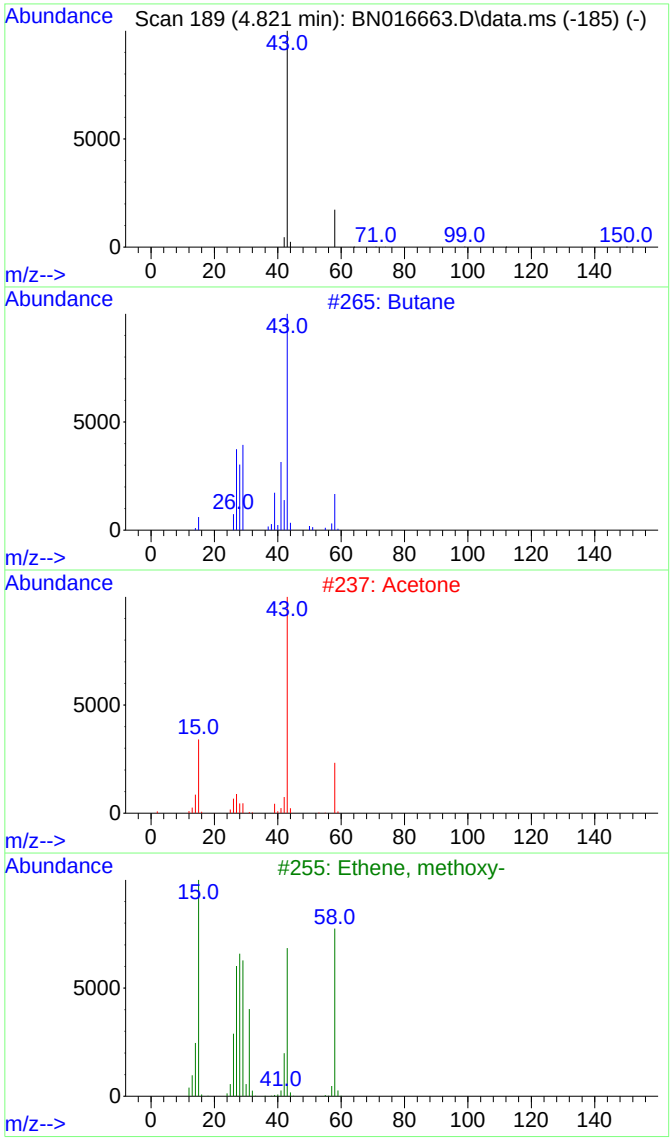
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

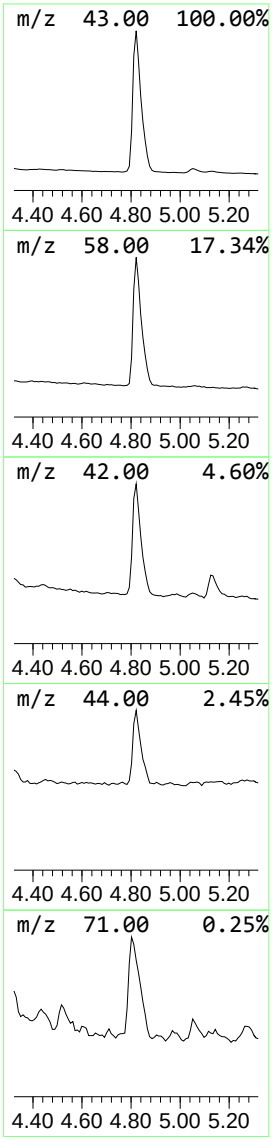
****

Peak Number 4 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.38 ng	95472	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

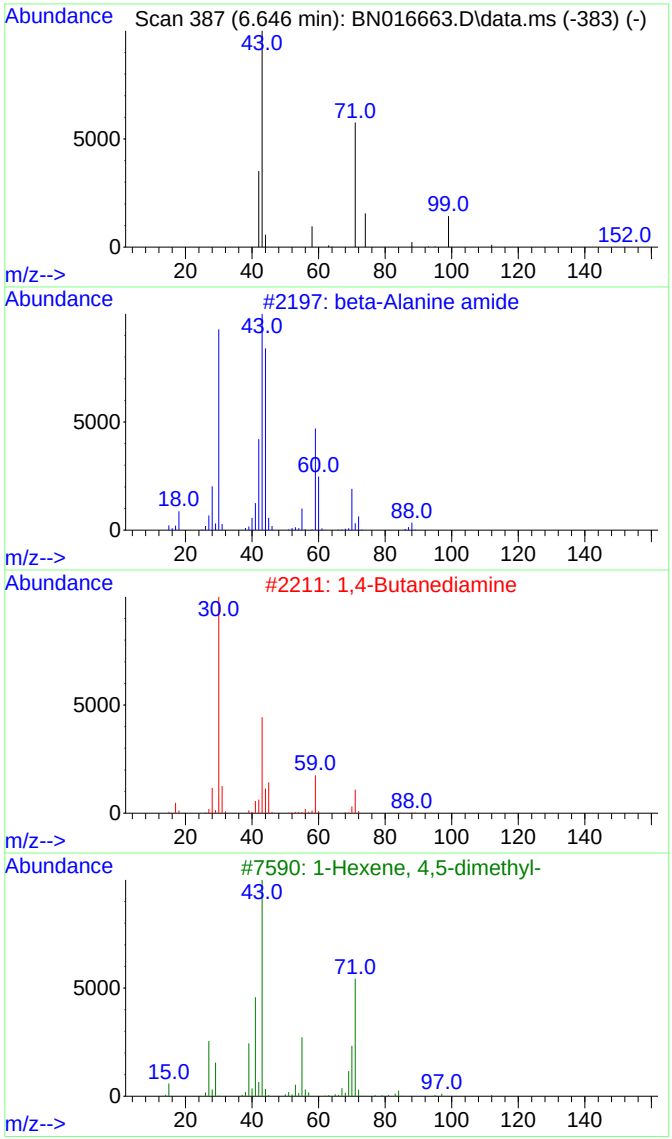
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

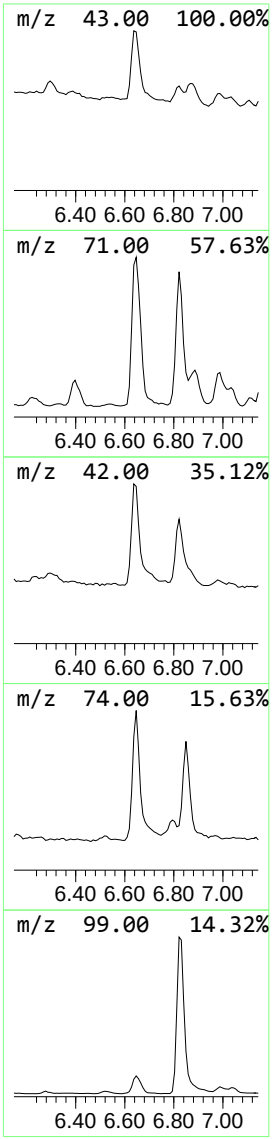
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 beta-Alanine amide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.05 ng	13204	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	beta-Alanine amide	88	C3H8N2O	004726-85-6	5
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	5
3	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	5
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4





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Instrument : BNA_N
ClientSampleId : RE120D3-20210917

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

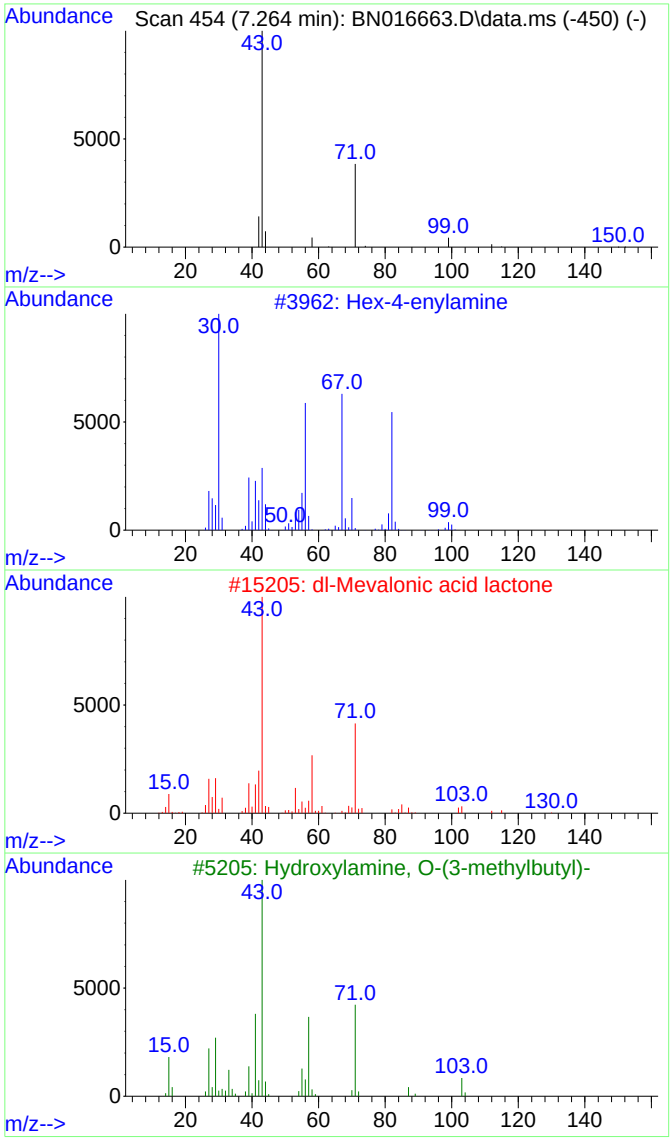
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

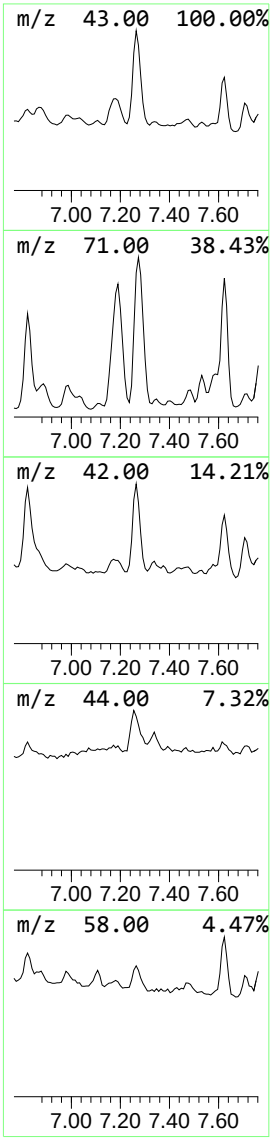
****

Peak Number 6 Hex-4-enylamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	15494	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hex-4-enylamine	99	C6H13N	055108-01-5	4
2	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
3	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	4
4	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
5	Isobutane	58	C4H10	000075-28-5	4





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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

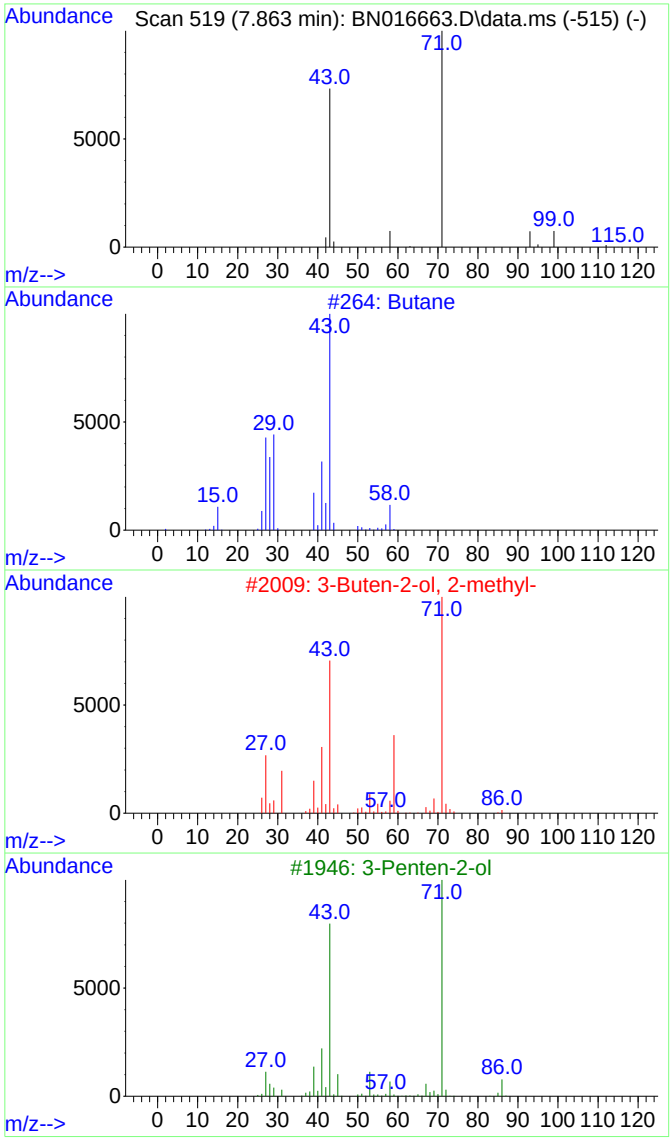
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

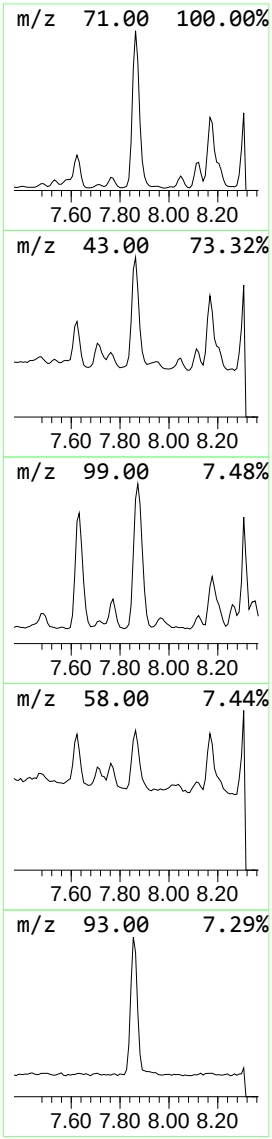
****

Peak Number 7 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	0.12 ng	30936	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
3	3-Penten-2-ol	86	C5H10O	001569-50-2	4
4	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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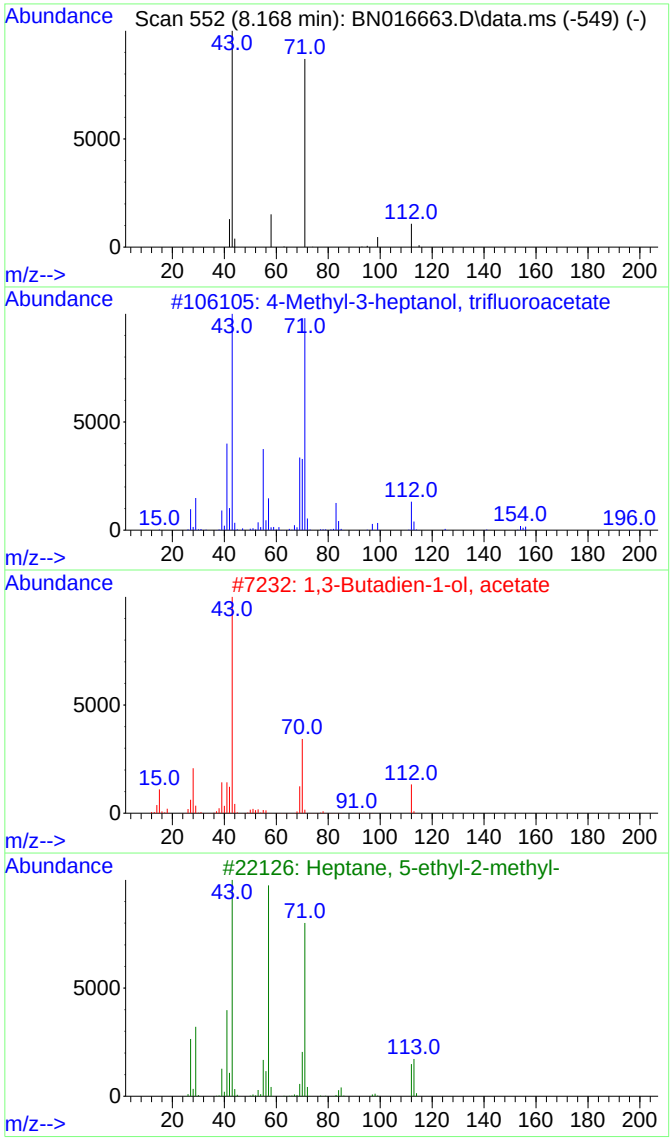
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

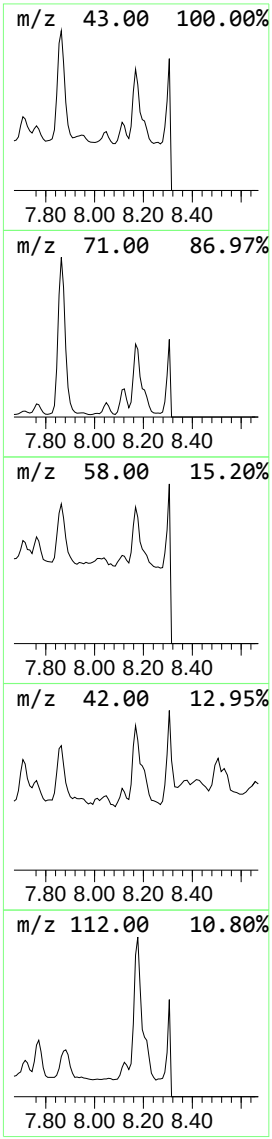
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Methyl-3-heptanol, triflu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.12 ng	28688	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	40
2	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3	Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	9
4	Decane, 4-methyl-	156	C11H24	002847-72-5	9
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016663.D
Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Integration Parameters: LSCINT.P

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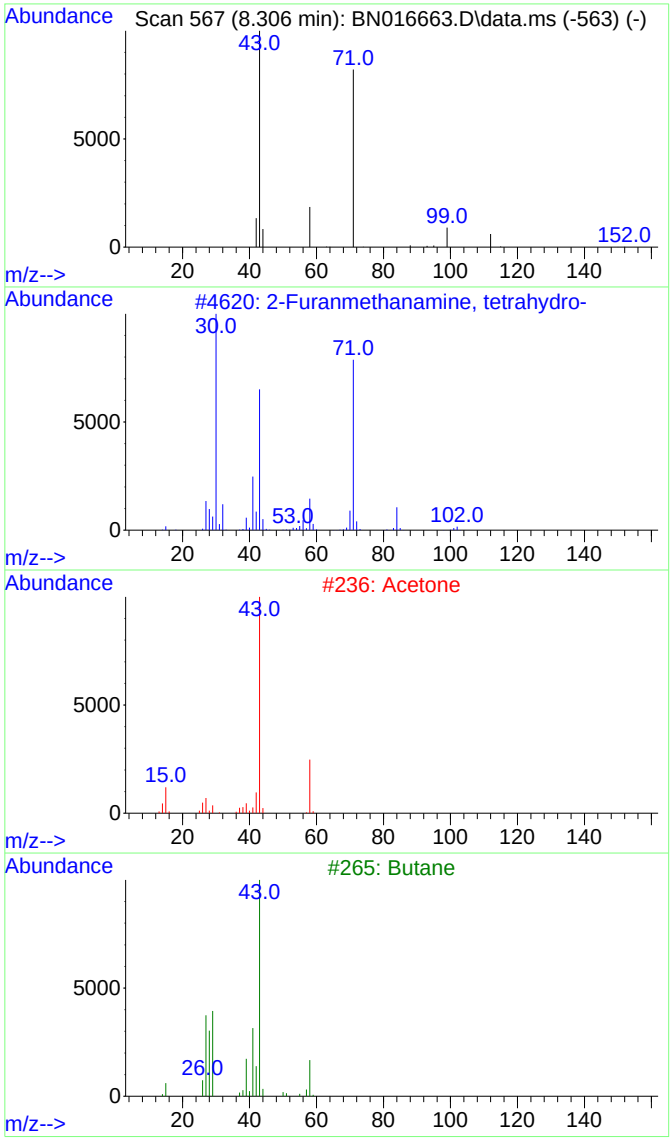
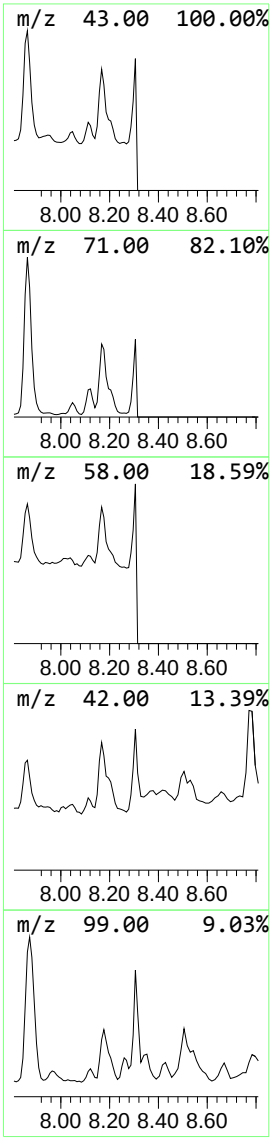
Peak Number 9 2-Furanmethanamine, tetrahy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.07 ng	17295	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9
2	Acetone	58	C3H6O	000067-64-1	5
3	Butane	58	C4H10	000106-97-8	5
4	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
5	Hexamethylenimine	99	C6H13N	000111-49-9	4





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Acq On : 02 Oct 2021 09:21
Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE120D3-20210917

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

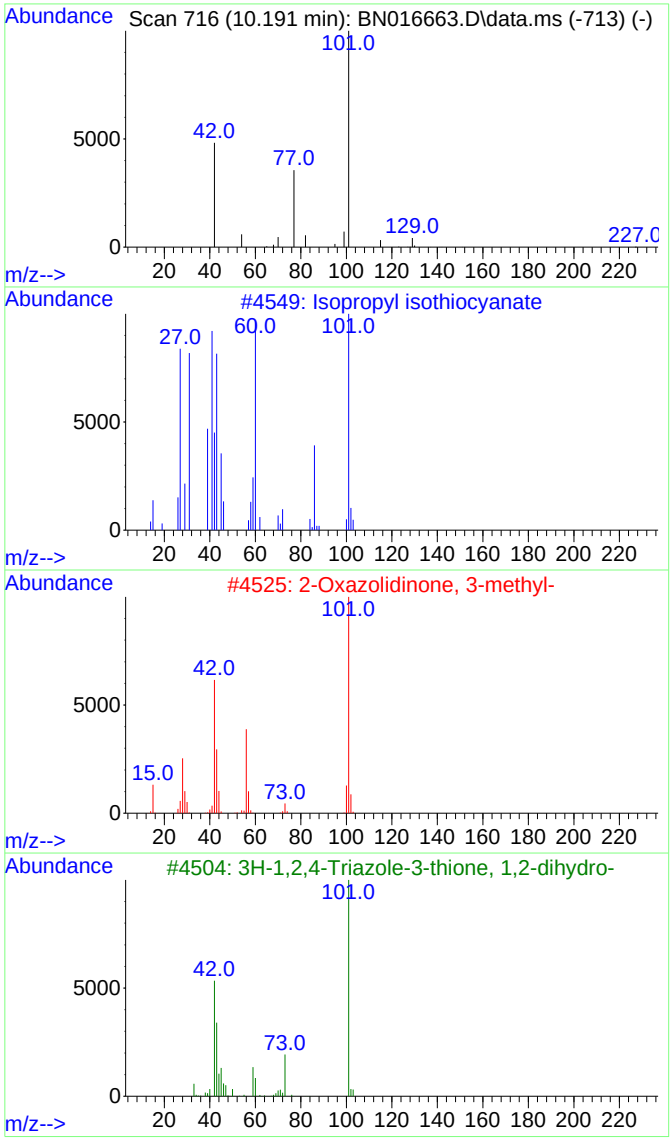
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

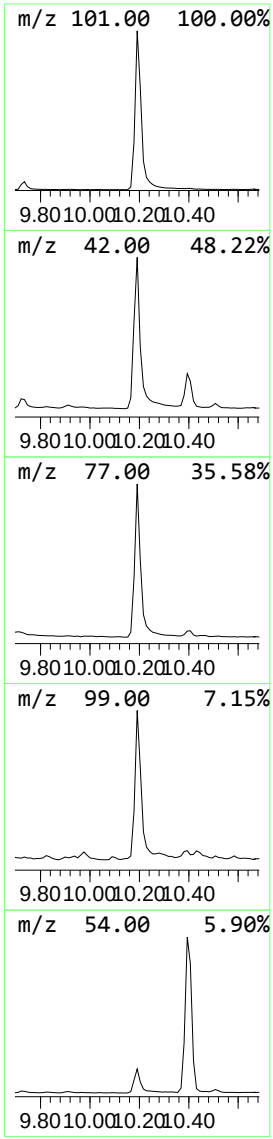
****

Peak Number 10 Isopropyl isothiocyanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.13 ng	57477	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
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	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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Data File : BN016663.D
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Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

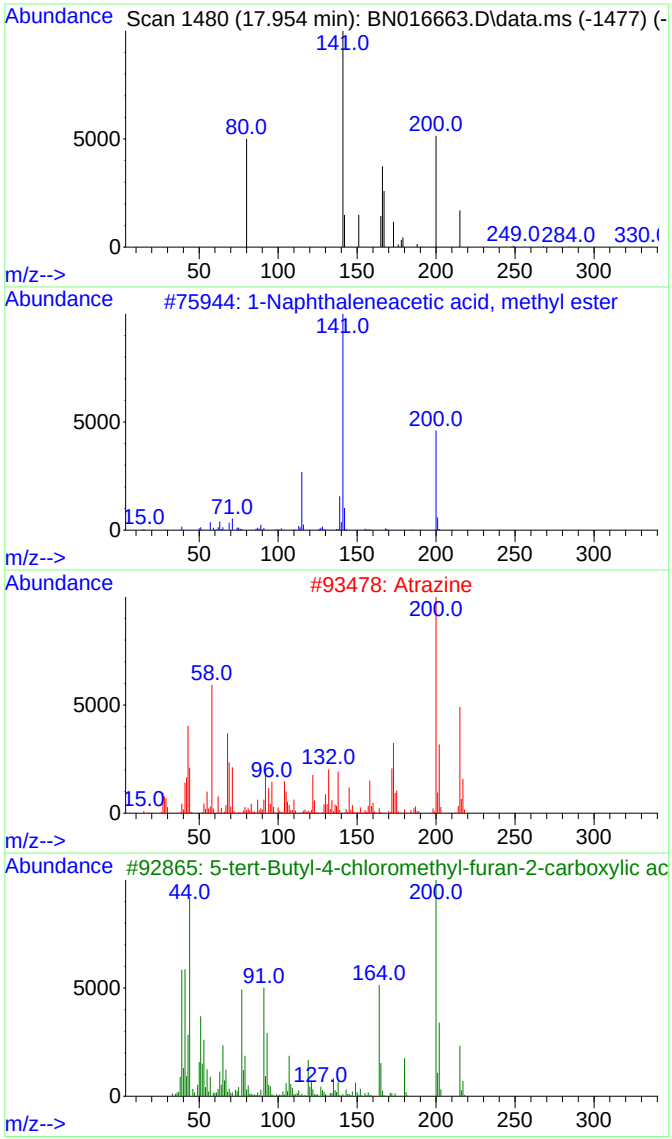
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

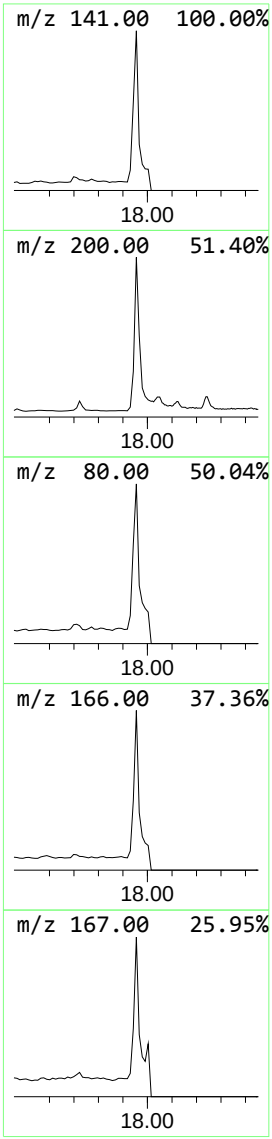
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1-Naphthaleneacetic acid, m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.954	0.04 ng	16115	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthaleneacetic acid, methyl...	200	C13H12O2	002876-78-0	9
2	Atrazine	215	C8H14ClN5	001912-24-9	9
3	5-tert-Butyl-4-chloromethyl-fura...	215	C10H14ClNO2	1000301-38-6	9
4	4-Chloro-2-methylphenol, O-metho...	200	C9H9ClO3	022979-64-2	9
5	1-Naphthalenepropionic acid	200	C13H12O2	003243-42-3	9





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Data File : BN016663.D
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Operator : CG/JU
Sample : M3829-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE120D3-20210917

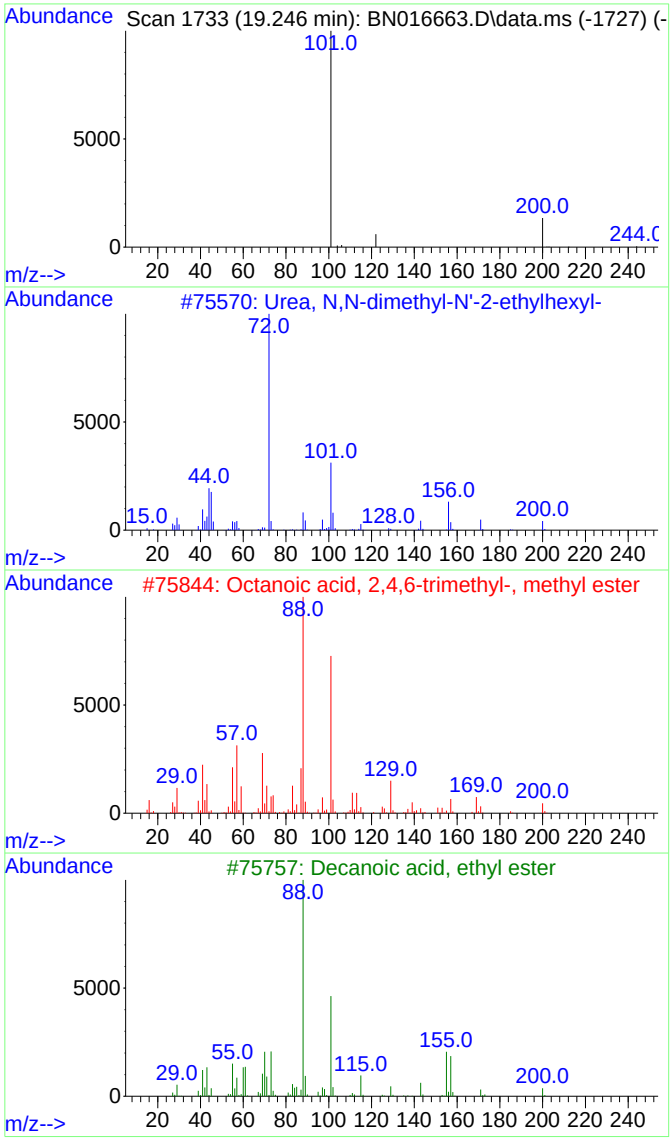
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

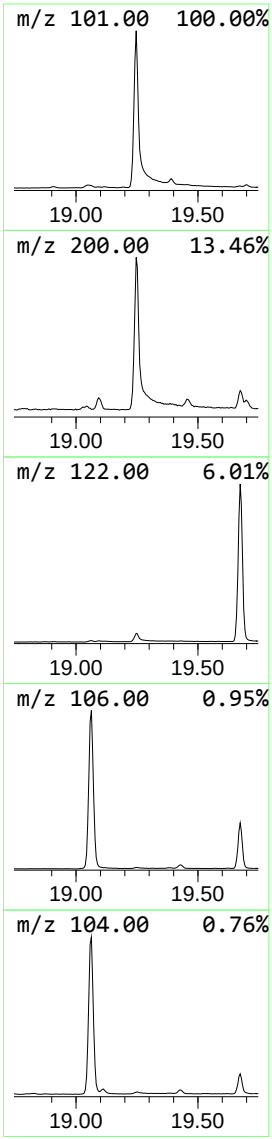
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Urea, N,N-dimethyl-N'-2-eth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.246	0.05 ng	22965	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urea, N,N-dimethyl-N'-2-ethylhexyl-	200	C11H24N2O	1010419-88-4	4
2	Octanoic acid, 2,4,6-trimethyl-,...	200	C12H24O2	054984-07-5	4
3	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	4
4	Nonanoic acid, 4,6-dimethyl-, me...	200	C12H24O2	055955-66-3	3
5	5-Hydroxy-4-methoxy-3-(1-methoxy...	244	C11H16O6	1000505-80-0	3





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016663.D
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ClientSampleId : RE120D3-20210917

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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
4-Pyridazinamine	3.152	0.2	ng	50310	1	7.642	99388	0.4
Hydrogen isocya...	3.364	0.1	ng	17472	1	7.642	99388	0.4
1-Propanol, 2-m...	3.816	0.2	ng	50277	1	7.642	99388	0.4
Butane	4.821	0.4	ng	95472	1	7.642	99388	0.4
beta-Alanine amide	6.646	0.1	ng	13204	1	7.642	99388	0.4
Hex-4-enylamine	7.264	0.1	ng	15494	1	7.642	99388	0.4
Butane	7.863	0.1	ng	30936	1	7.642	99388	0.4
4-Methyl-3-hept...	8.168	0.1	ng	28688	1	7.642	99388	0.4
2-Furanmethanam...	8.306	0.1	ng	17295	1	7.642	99388	0.4
Isopropyl isoth...	10.191	0.1	ng	57477	2	10.406	173291	0.4
1-Naphthaleneac...	17.954	0.0	ng	16115	4	17.017	153220	0.4
Urea, N,N-dimet...	19.246	0.0	ng	22965	5	21.227	189101	0.4