LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW179D1-20210916

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: BN016655.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	216544	298148	51.60%	8.940%
2	3.189	11	12	29	rVB	98327	577818	100.00%	17.326%
3	3.364	29	31	47	rVB	46679	150389	26.03%	4.509%
4	3.816	76	80	97	rVB	10594	44194	7.65%	1.325%
5	4.397	140	143	153	rVB2	4176	14512	2.51%	0.435%
6	4.821	185	189	203	rVB	31894	75425	13.05%	2.262%
7	5.273	234	238	244	rBV	5415	14098	2.44%	0.423%
8	6.296	345	349	357	rVB	6533	14207	2.46%	0.426%
9	6.647	383	387	396	rVB	4696	11788	2.04%	0.353%
10	6.831	403	407	418	rVB3	4368	17712	3.07%	0.531%
11	7.181	440	445	450	rBV2	3012	8908	1.54%	0.267%
12	7.264	450	454	460	rVB2	7681	18216	3.15%	0.546%
13	7.633	490	494	500	rVB	49109	102967	17.82%	3.087%
14	7.864	515	519	527	rBV	15780	32106	5.56%	0.963%
15	8.113	543	546	549	rBV	2767	6101	1.06%	0.183%
16	8.168	549	552	560	rVV	10688	29547	5.11%	0.886%
17	8.306	563	567	569	rVB	13670	18020	3.12%	0.540%
18	8.785	601	605	610	rBV	21177	43625	7.55%	1.308%
19	10.191	713	716	729	rBV	86077	144318	24.98%	4.327%
20	10.407	729	733	736	rBV	101600	178291	30.86%	5.346%
21	12.003	920	931	942	rBV	43191	70187	12.15%	2.105%
22	12.886	1071	1074	1078	rBV	93365	153805	26.62%	4.612%
23	13.178	1094	1097	1104	rVB	4827	8886	1.54%	0.266%
24	14.269	1180	1183	1186	rBV	133051	193470	33.48%	5.801%
25	14.434	1193	1196	1198	rBV	4952	7245	1.25%	0.217%
26	15.639	1286	1291	1294	rVB4	2290	6647	1.15%	0.199%
27	15.715	1294	1297	1299	rBV	6852	11288	1.95%	0.338%
28	15.766	1299	1301	1305	rVB2	12577	21635	3.74%	0.649%
29	16.324	1343	1346	1349	rBV3	2376	6615	1.14%	0.198%
30	16.835	1386	1388	1397	rVB	4183	8516	1.47%	0.255%
31	17.018	1400	1403	1405	rBV	106232	159627	27.63%	4.786%
32	17.066	1405	1407	1410	rVB	12942	19599	3.39%	0.588%
33	17.225	1417	1420	1422	rBV2	3741	7820	1.35%	0.234%
34	17.444	1434	1438	1446	rVB3	1599	6437	1.11%	0.193%
35	17.711	1457	1460	1463	rBV2	3578	7383	1.28%	0.221%
36	17.943	1477	1479	1483	rVB	4016	6287	1.09%	0.189%

LSC Area Percent Report

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Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW179D1-20210916

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	19.063	1689	1696	1714	rBV	134688	182511	31.59%	5.473%
38	19.674	1813	1819	1836	rBV	143112	179423	31.05%	5.380%
39	20.006	1884	1886	1890	rBV2	2856	7188	1.24%	0.216%
40	20.983	1975	1978	1980	rBV	2695	6302	1.09%	0.189%
41	21.164	1992	1995	1998	rBV	29797	35623	6.17%	1.068%
42	21.228	1998	2001	2011	rVB	136295	188582	32.64%	5.655%
43	22.311	2100	2103	2109	rBV	4258	8870	1.54%	0.266%
44	23.420	2399	2408	2414	rBV	5338	8966	1.55%	0.269%
45	23.481	2414	2426	2464	rVB	99055	197529	34.19%	5.923%
46	24.080	2592	2601	2621	rBV2	5523	10912	1.89%	0.327%
47	24.850	2816	2826	2851	rVB	5569	13275	2.30%	0.398%

Sum of corrected areas: 3335018

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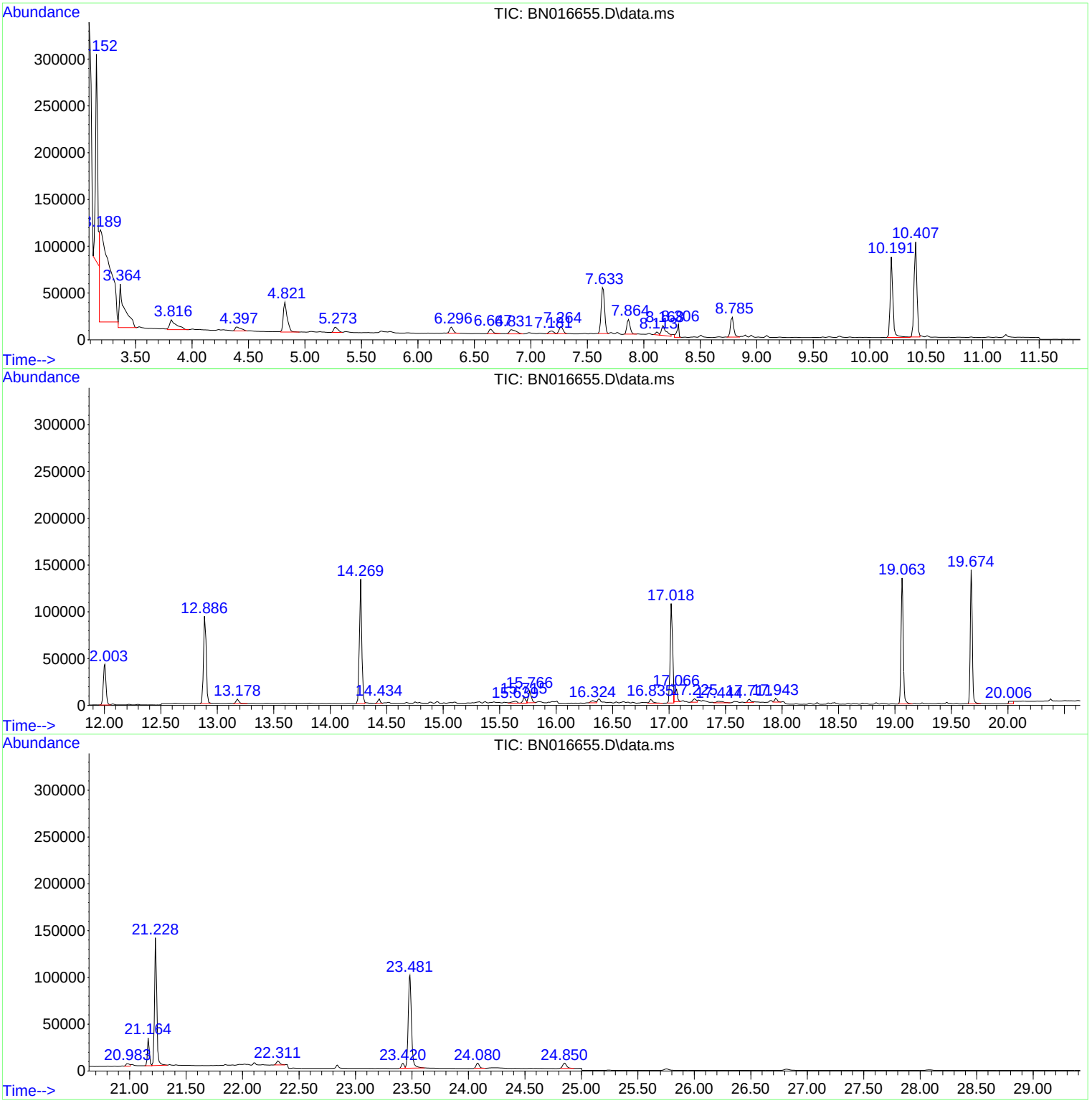
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 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

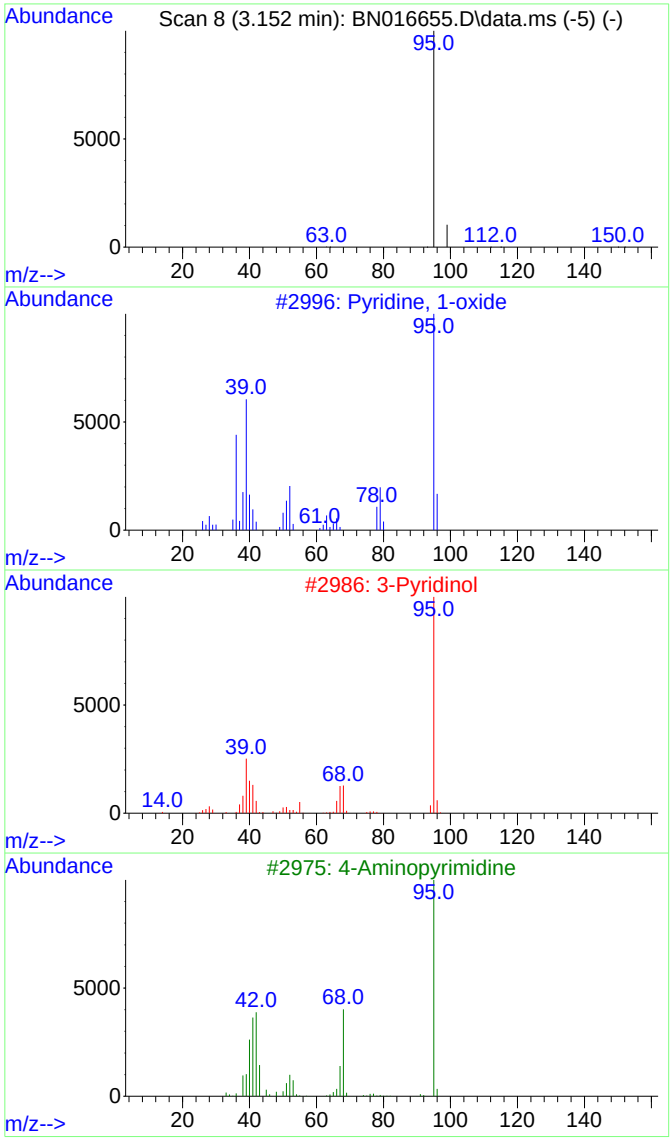
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

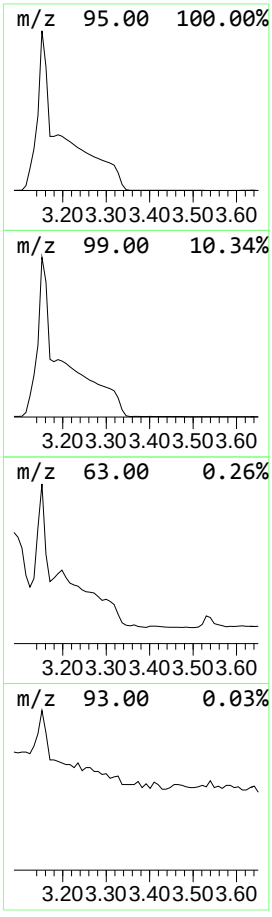
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	1.16 ng	298148	1,4-Dichlorobenzene-d4	7.643

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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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW179D1-20210916

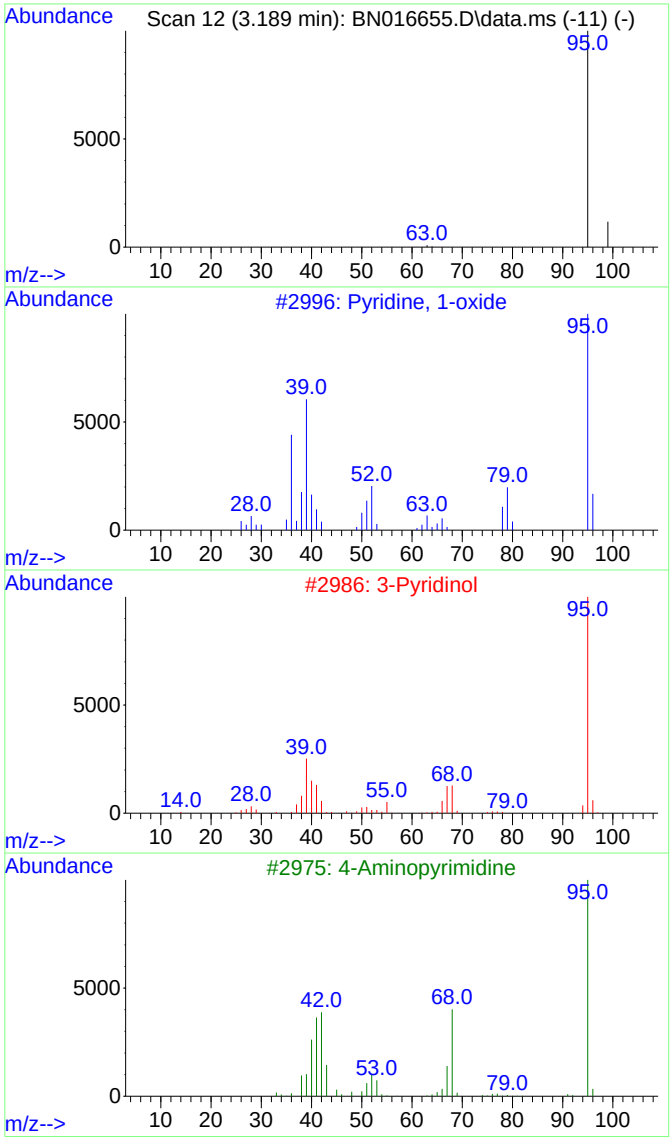
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

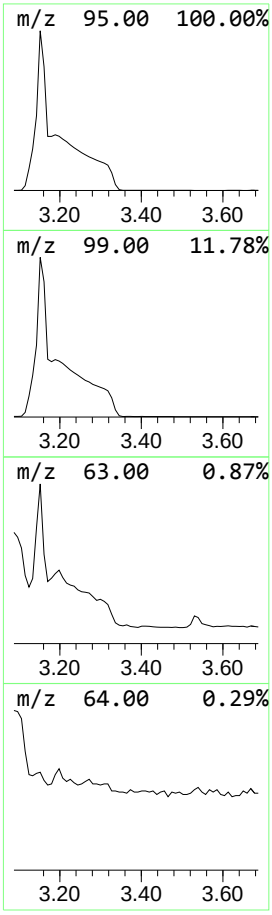
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	2.24 ng	577818	1,4-Dichlorobenzene-d4	7.643

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 : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW179D1-20210916

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

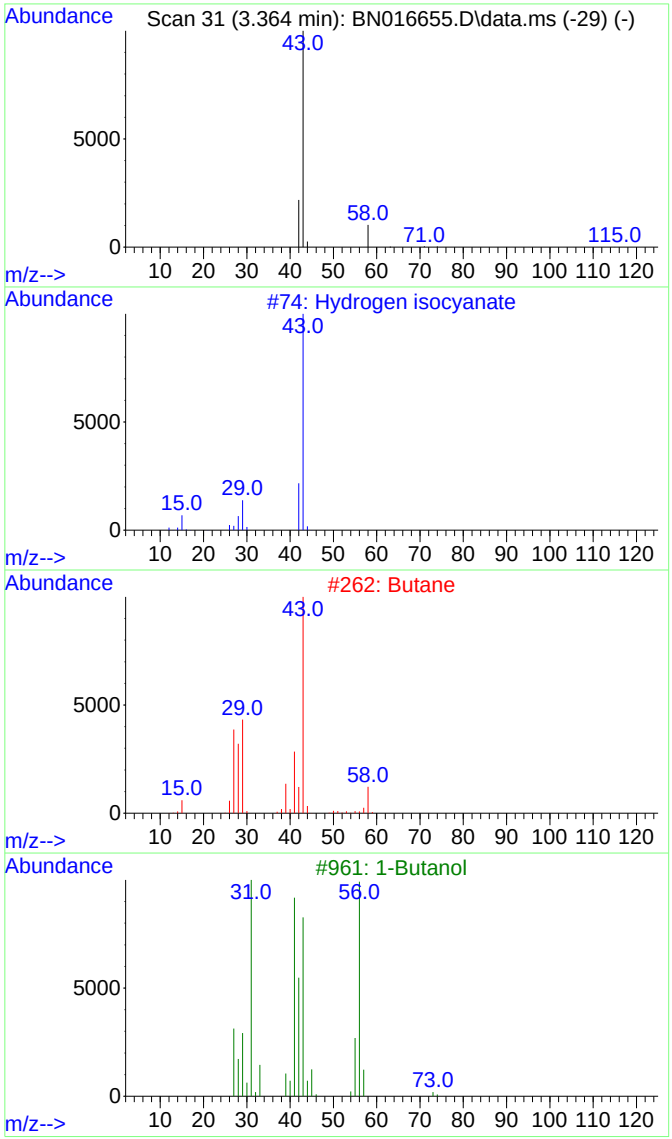
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

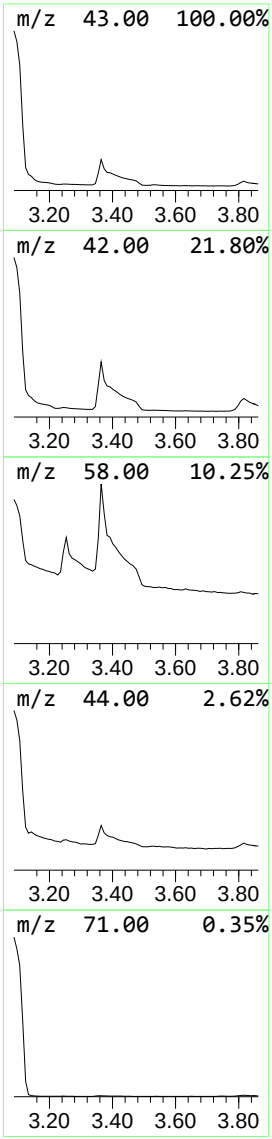
****

Peak Number 3 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.58 ng	150389	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	4
2	Butane	58	C4H10	000106-97-8	4
3	1-Butanol	74	C4H10O	000071-36-3	3
4	Hydrogen azide	43	HN3	007782-79-8	2
5	O-Methylisourea	74	C2H6N2O	002440-60-0	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW179D1-20210916

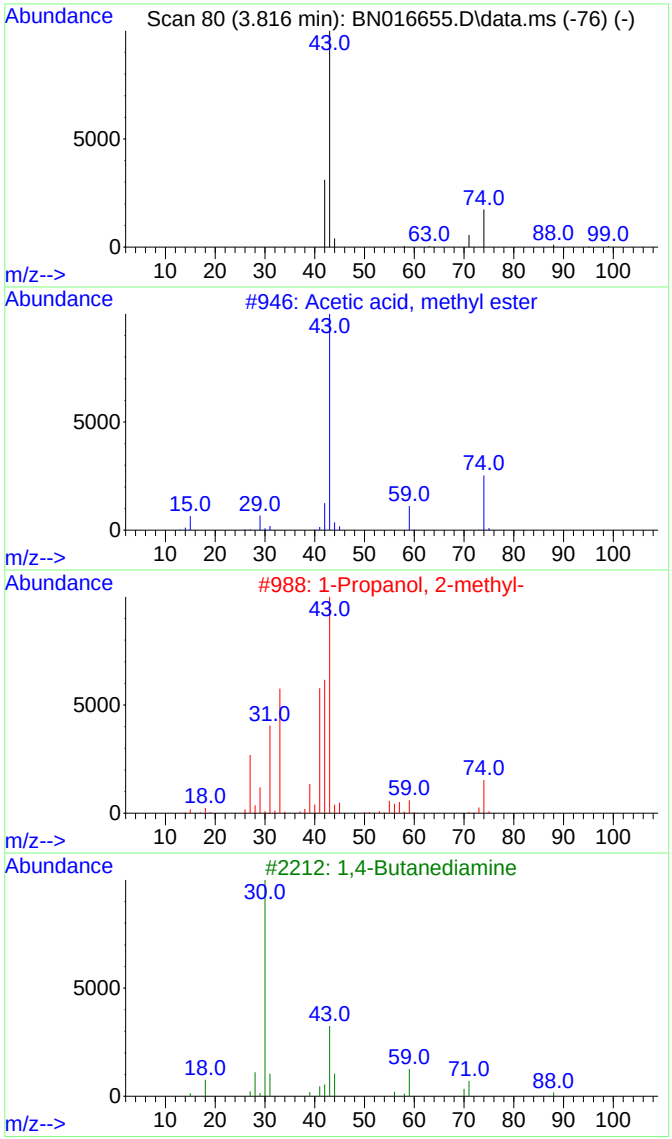
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

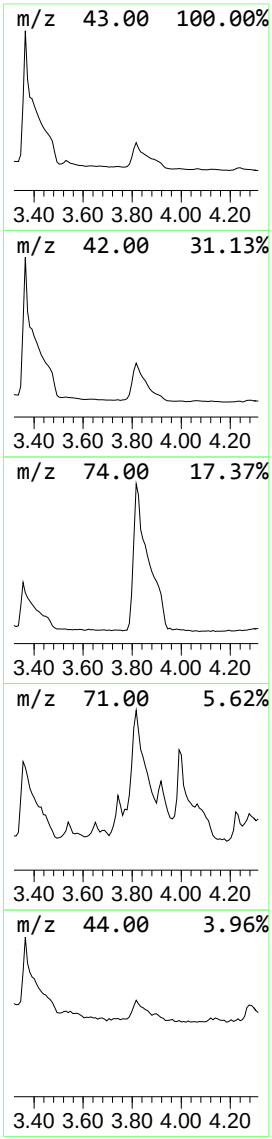
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.17 ng	44194	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	5
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3





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Data File : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW179D1-20210916

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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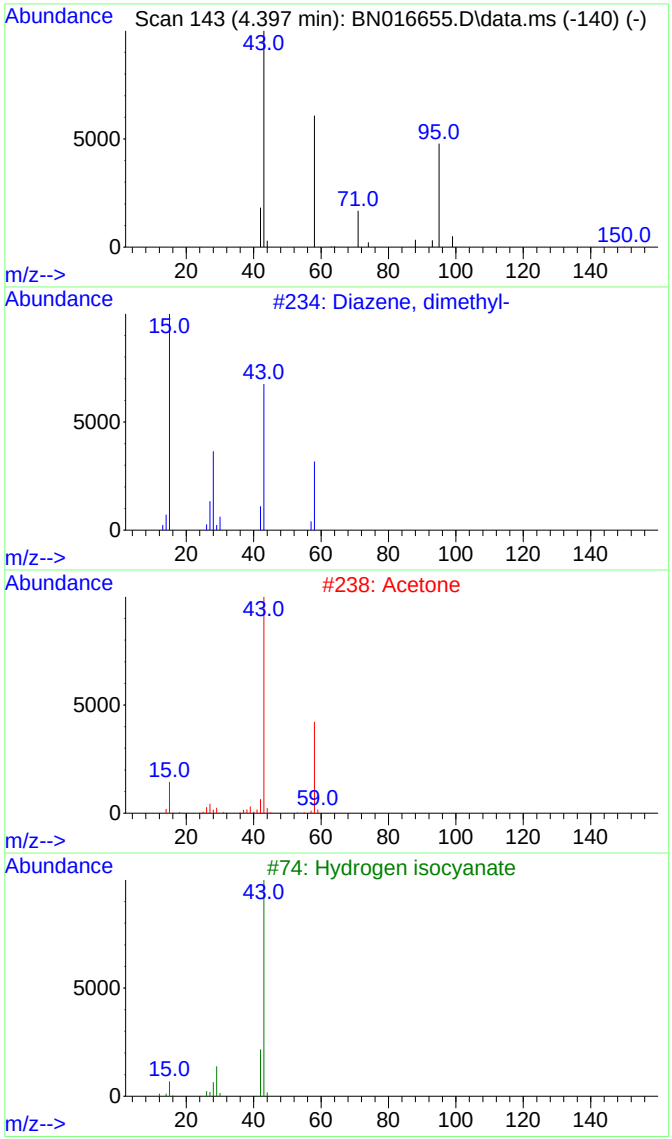
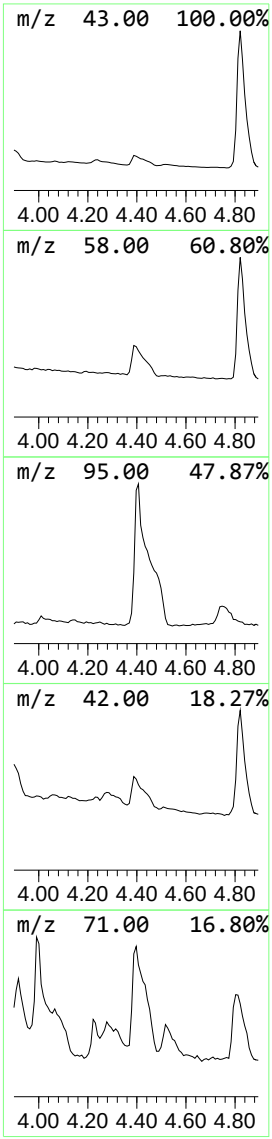
****

Peak Number 5 Diazene, dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.397	0.06 ng	14512	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5
2	Acetone	58	C3H6O	000067-64-1	5
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Ethene, methoxy-	58	C3H6O	000107-25-5	4
5	1,2-Ethanediamine, N,N-dimethyl-	88	C4H12N2	000108-00-9	4





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Operator : CG/JU
Sample : M3829-01
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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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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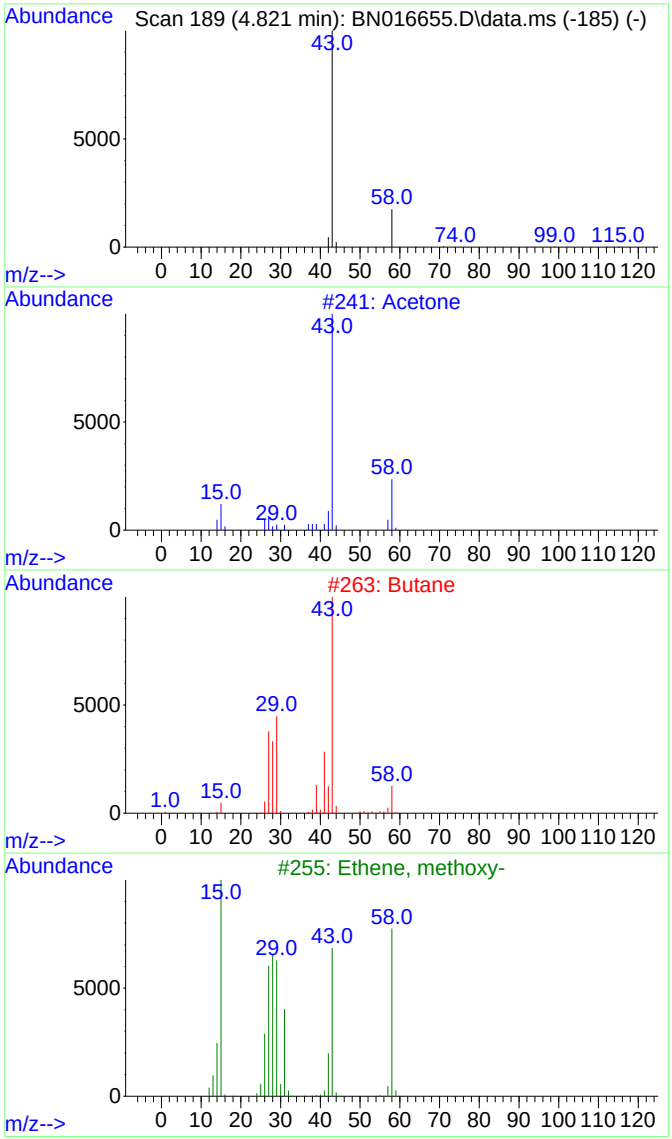
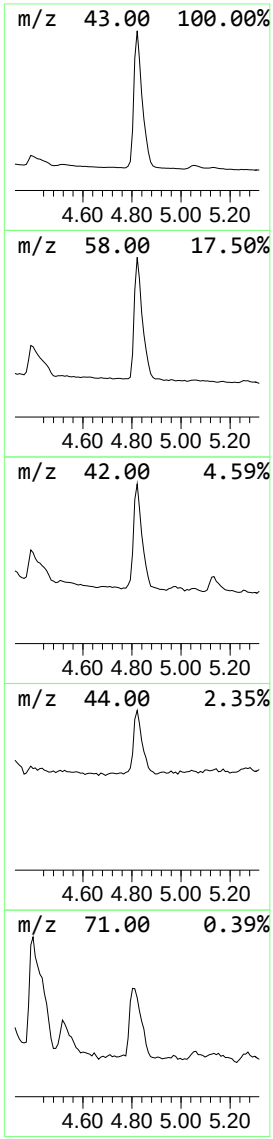
Peak Number 6 Acetone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.29 ng	75425	1,4-Dichlorobenzene-d4	7.643

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 : 23 Sample Multiplier: 1

Instrument :
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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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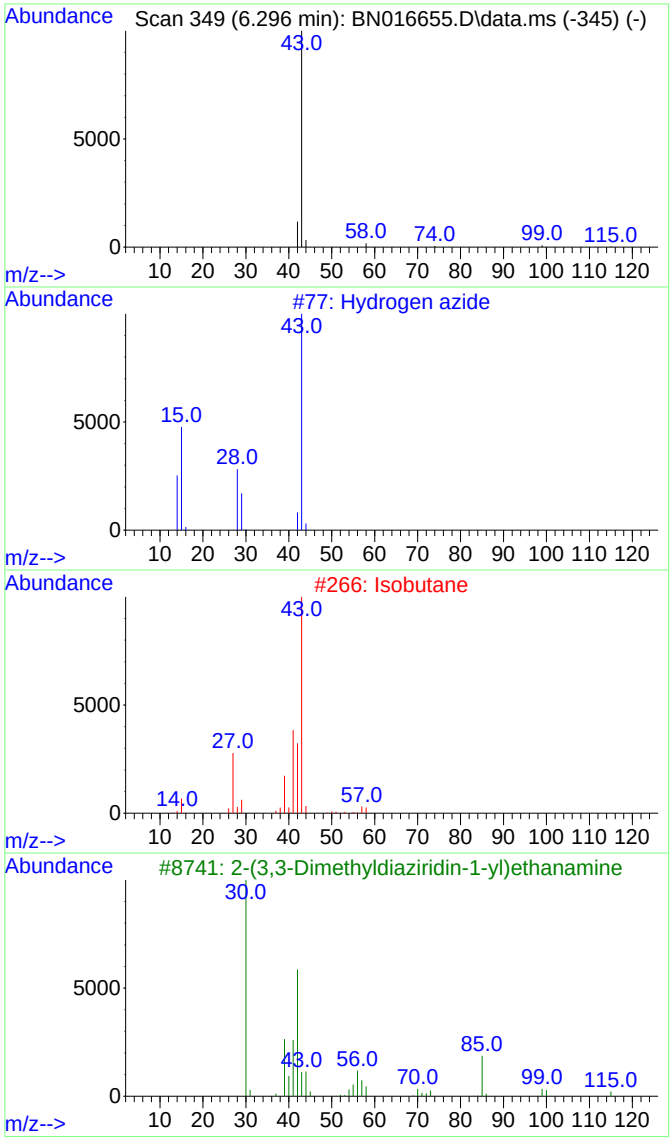
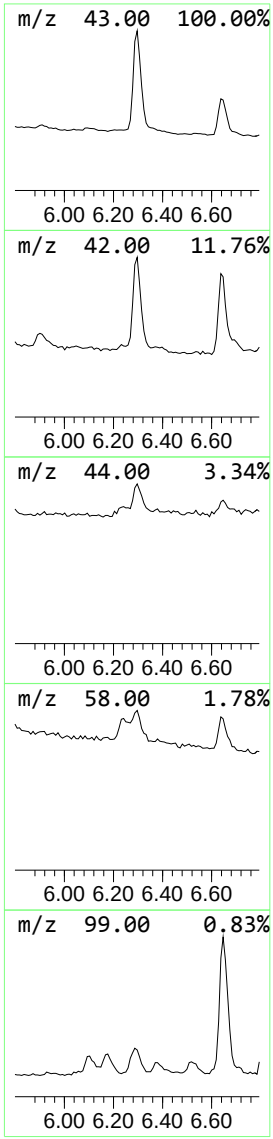
Peak Number 7 Hydrogen azide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.06 ng	14207	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen azide	43	HN3	007782-79-8	4
2	Isobutane	58	C4H10	000075-28-5	3
3	2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	3
4	Hydrogen isocyanate	43	CHNO	000075-13-8	2
5	1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-66-3	2





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ALS Vial : 23 Sample Multiplier: 1

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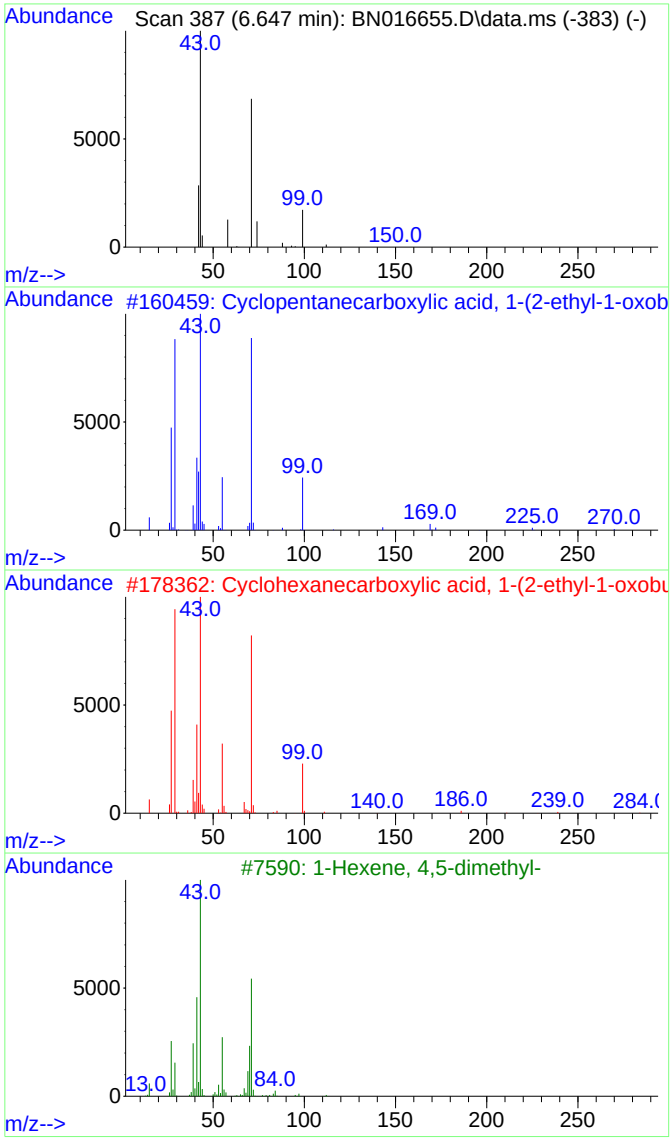
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

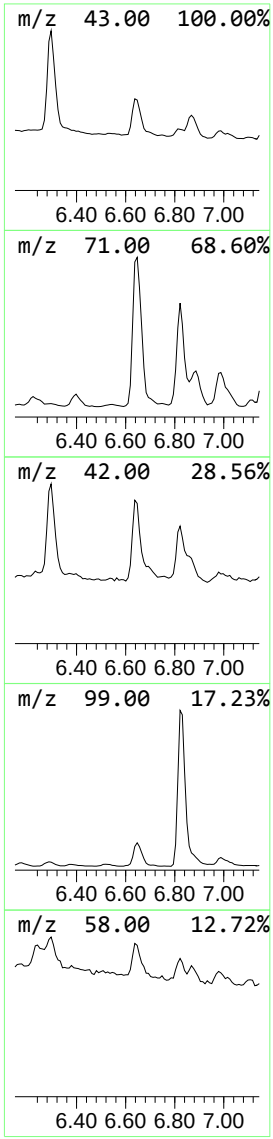
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentanecarboxylic acid... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.647	0.05 ng	11788	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 1-(...	270	C14H22O5	1000460-66-4	39
2	Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	9
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 :
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ClientSampleId :
MW179D1-20210916

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

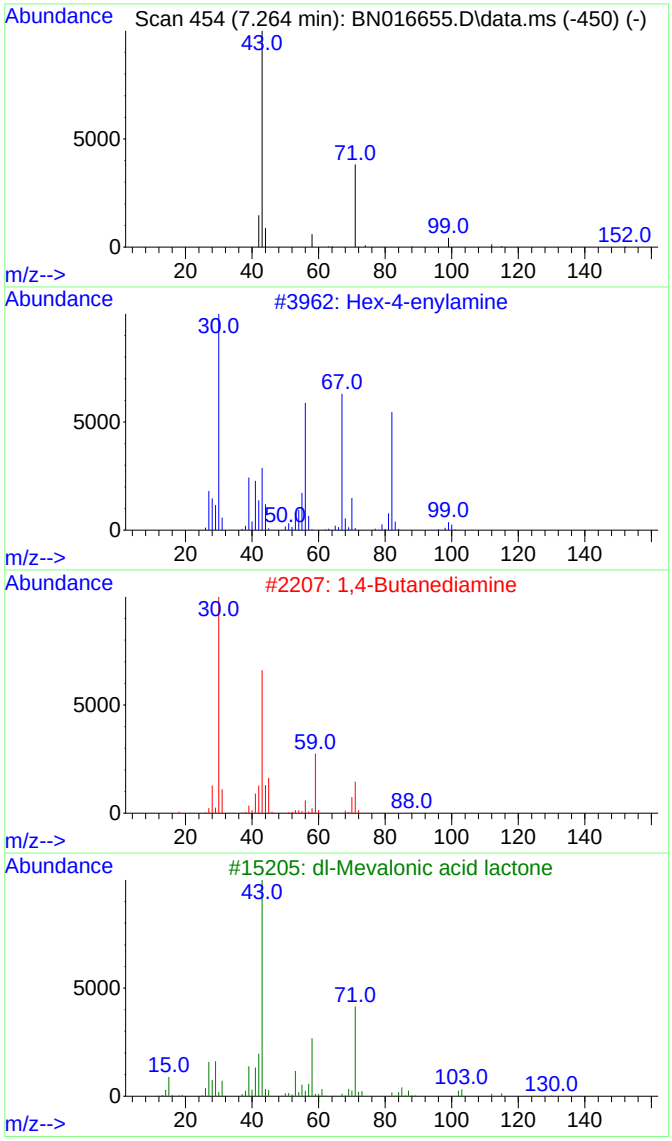
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

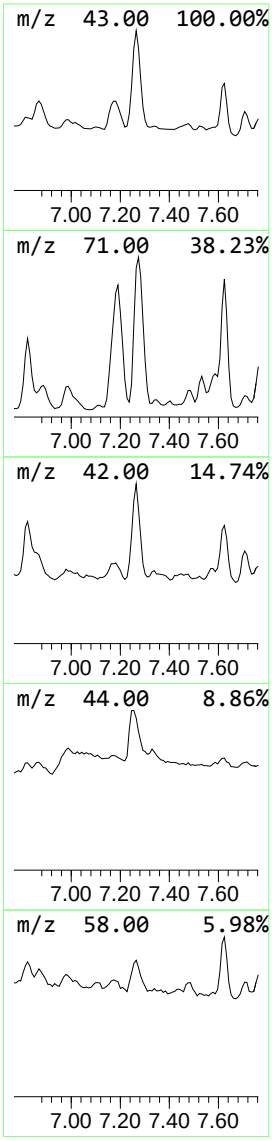
****

Peak Number 9 Hex-4-enylamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.07 ng	18216	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hex-4-enylamine	99	C6H13N	055108-01-5	4
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
3	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
4	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
5	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016655.D
Acq On : 02 Oct 2021 04:34
Operator : CG/JU
Sample : M3829-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW179D1-20210916

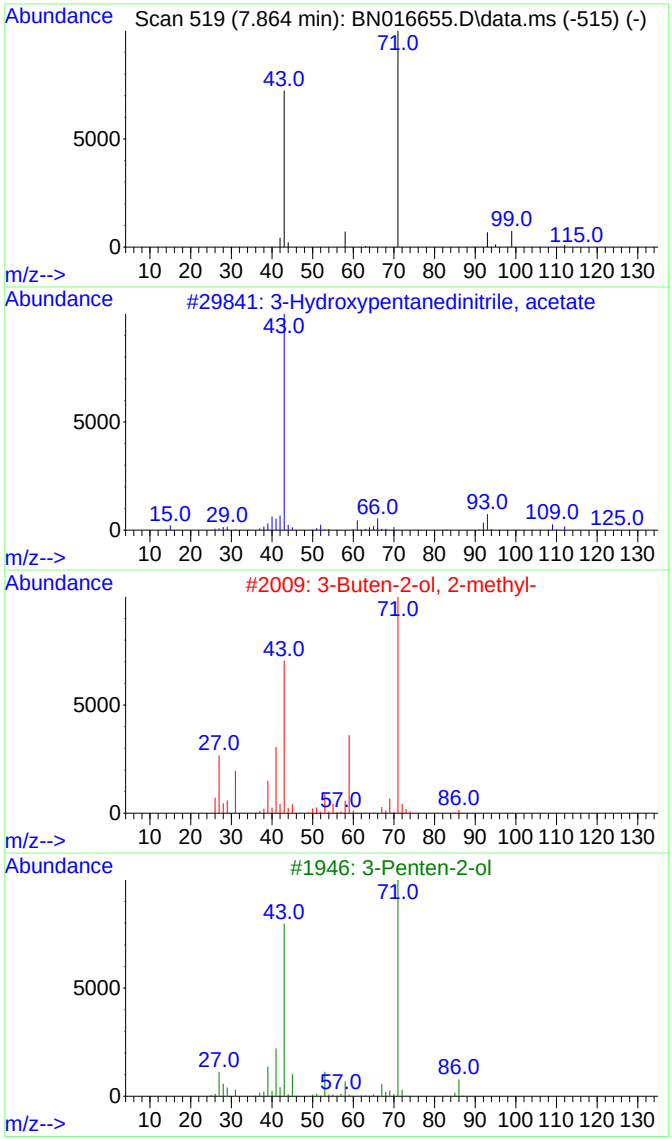
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

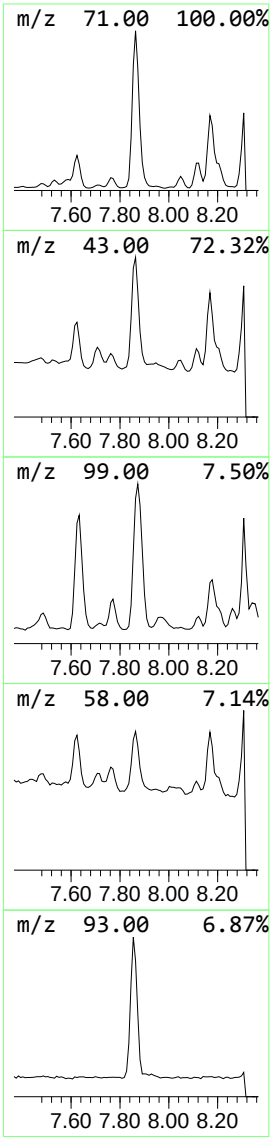
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3-Hydroxypentanedinitrile, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.12 ng	32106	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	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	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4





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ClientSampleId :
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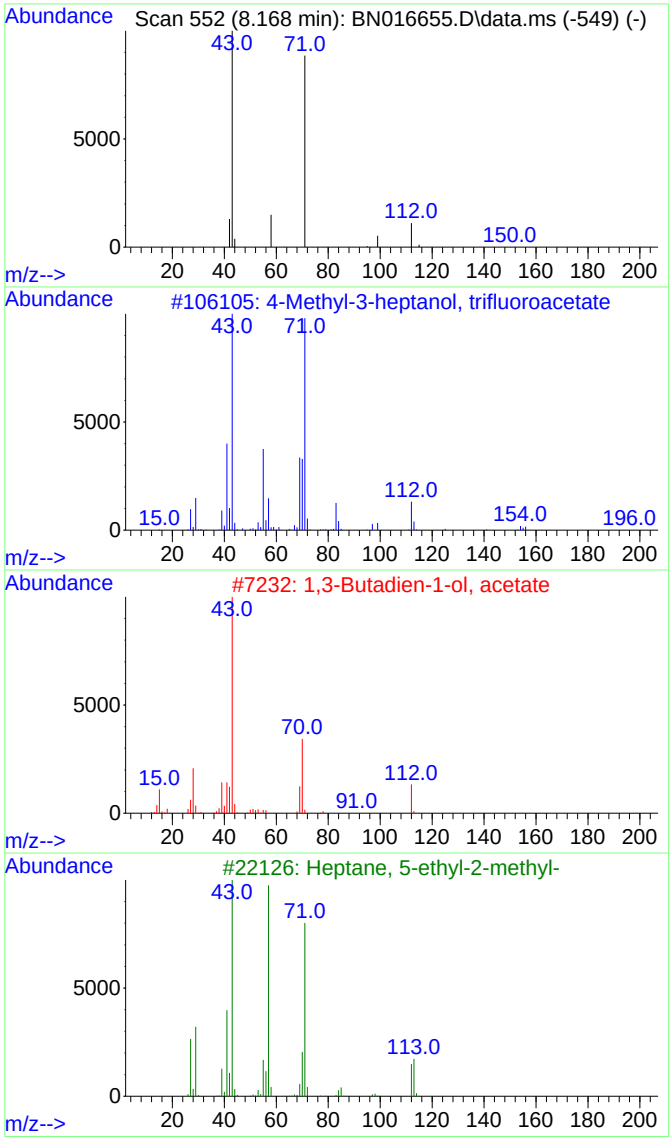
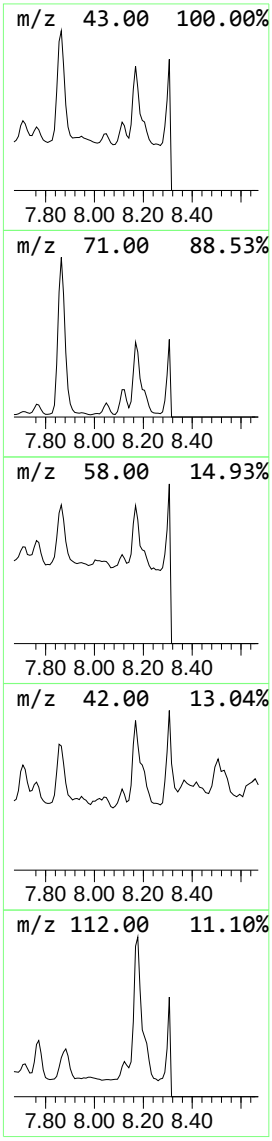
****
Peak Number 11 4-Methyl-3-heptanol, triflu... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.11 ng	29547	1,4-Dichlorobenzene-d4	7.643

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	Octane, 3-ethyl-	142	C10H22	005881-17-4	9
5	Decane, 4-methyl-	156	C11H24	002847-72-5	9





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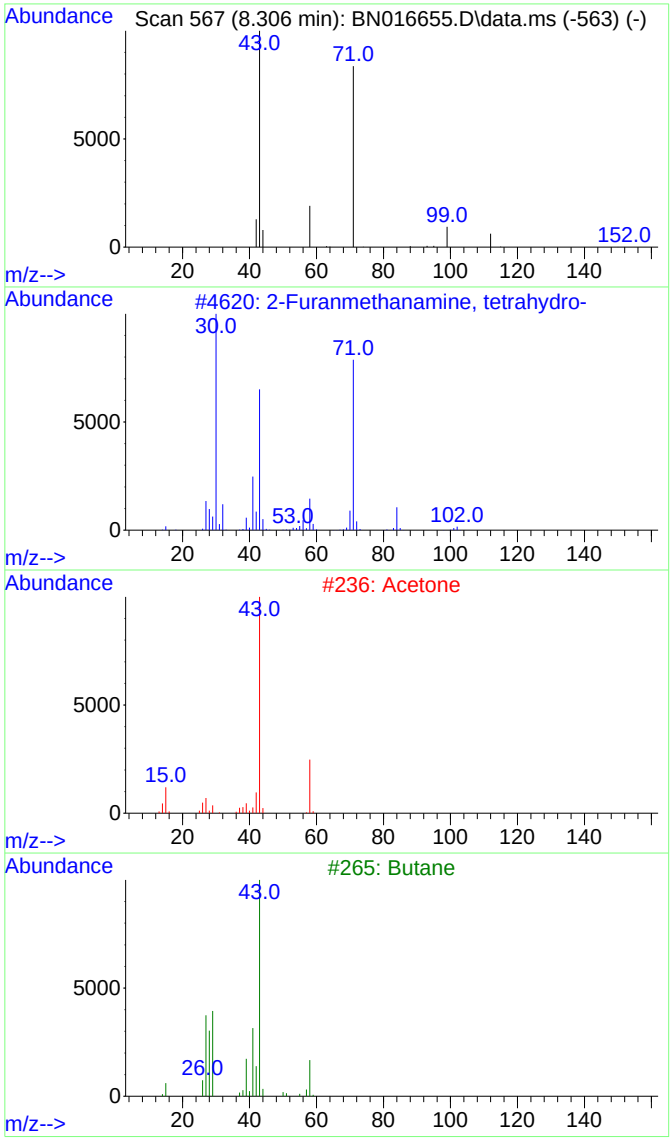
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

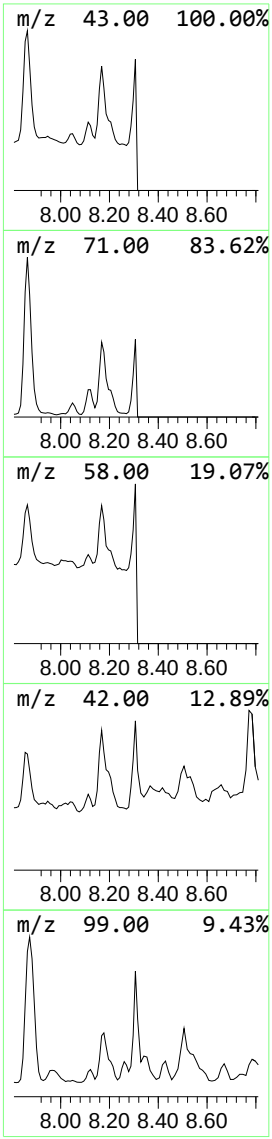
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2-Furanmethanamine, tetrahy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.07 ng	18020	1,4-Dichlorobenzene-d4	7.643

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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Misc :
ALS Vial : 23 Sample Multiplier: 1

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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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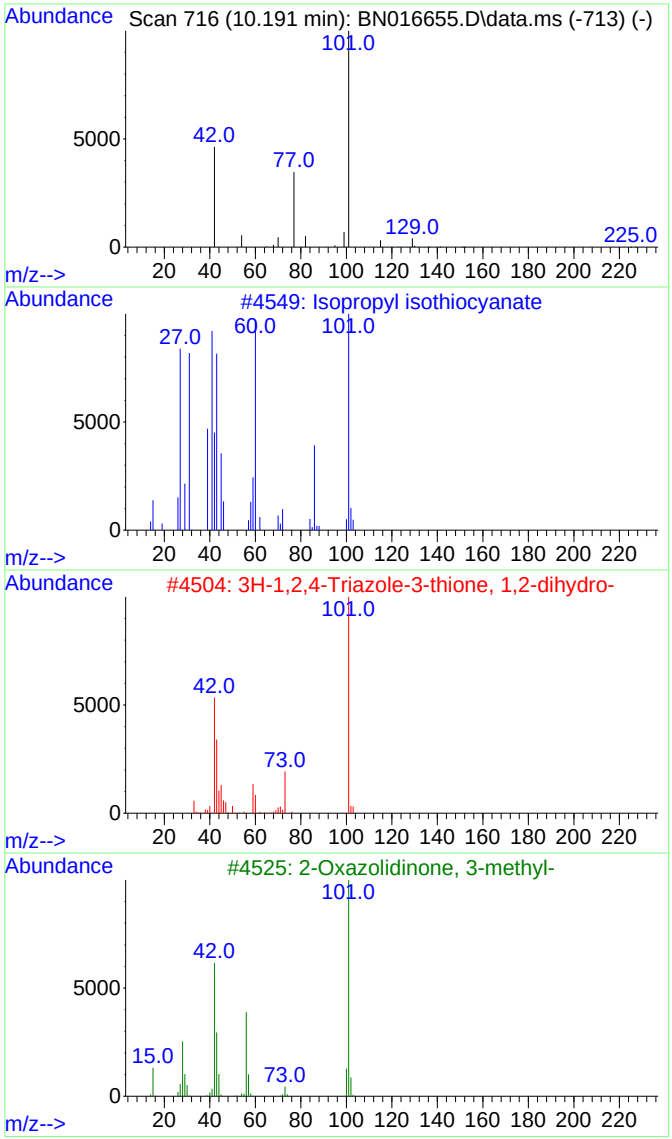
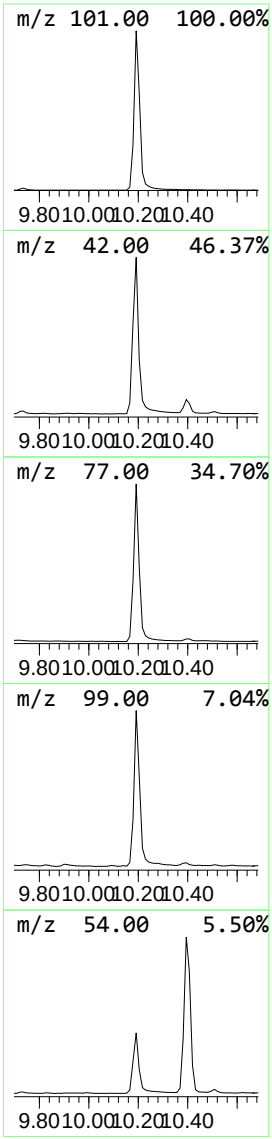
Peak Number 13 Isopropyl isothiocyanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.32 ng	144318	Naphthalene-d8	10.407

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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Operator : CG/JU
Sample : M3829-01
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Instrument :
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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
Pyridine, 1-oxide	3.152	1.2	ng	298148	1	7.643	102967	0.4
Pyridine, 1-oxide	3.189	2.2	ng	577818	1	7.643	102967	0.4
Hydrogen isocya...	3.364	0.6	ng	150389	1	7.643	102967	0.4
Acetic acid, me...	3.816	0.2	ng	44194	1	7.643	102967	0.4
Diazene, dimethyl-	4.397	0.1	ng	14512	1	7.643	102967	0.4
Acetone	4.821	0.3	ng	75425	1	7.643	102967	0.4
Hydrogen azide	6.296	0.1	ng	14207	1	7.643	102967	0.4
Cyclopentanecar...	6.647	0.0	ng	11788	1	7.643	102967	0.4
Hex-4-enylamine	7.264	0.1	ng	18216	1	7.643	102967	0.4
3-Hydroxypentan...	7.864	0.1	ng	32106	1	7.643	102967	0.4
4-Methyl-3-hept...	8.168	0.1	ng	29547	1	7.643	102967	0.4
2-Furanmethanam...	8.306	0.1	ng	18020	1	7.643	102967	0.4
Isopropyl isoth...	10.191	0.3	ng	144318	2	10.407	178291	0.4