LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016660.D
Acq On : 02 Oct 2021 07:33
Operator : CG/JU
Sample : M3829-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D2-20210917

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: BN016660.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	5	9	12	rBV	1064029	1619194	100.00%	32.703%
2	3.253	17	19	29	rVB	339256	1127085	69.61%	22.764%
3	3.364	29	31	46	rVB	49792	121945	7.53%	2.463%
4	3.816	77	80	97	rVB	9666	37523	2.32%	0.758%
5	4.821	185	189	202	rVB	58046	124057	7.66%	2.506%
6	5.264	234	237	245	rVB	6926	17122	1.06%	0.346%
7	6.822	403	406	418	rVB3	4535	17639	1.09%	0.356%
8	7.633	489	494	500	rBV2	60208	120938	7.47%	2.443%
9	7.864	515	519	526	rBV	17166	34043	2.10%	0.688%
10	8.168	549	552	560	rVV2	10347	26296	1.62%	0.531%
11	8.306	563	567	569	rVB	14136	18692	1.15%	0.378%
12	8.784	601	605	610	rBV	22704	47029	2.90%	0.950%
13	10.191	713	716	726	rBV	15096	30875	1.91%	0.624%
14	10.407	729	733	736	rBV	109014	191479	11.83%	3.867%
15	12.003	918	931	942	rBV	46251	74955	4.63%	1.514%
16	12.886	1071	1074	1078	rBV	92049	153061	9.45%	3.091%
17	14.269	1180	1183	1186	rBV	140675	205142	12.67%	4.143%
18	15.766	1298	1301	1305	rVB3	14083	27108	1.67%	0.548%
19	17.018	1400	1403	1405	rBV	112765	169236	10.45%	3.418%
20	17.066	1405	1407	1410	rVB	25323	38804	2.40%	0.784%
21	19.063	1688	1696	1713	rBV	135973	183715	11.35%	3.711%
22	19.679	1813	1820	1839	rBV	120027	156195	9.65%	3.155%
23	21.164	1992	1995	1998	rBV	21714	26653	1.65%	0.538%
24	21.227	1998	2001	2011	rVV	129874	187578	11.58%	3.789%
25	23.481	2414	2426	2466	rVB	96003	194817	12.03%	3.935%

Sum of corrected areas: 4951181

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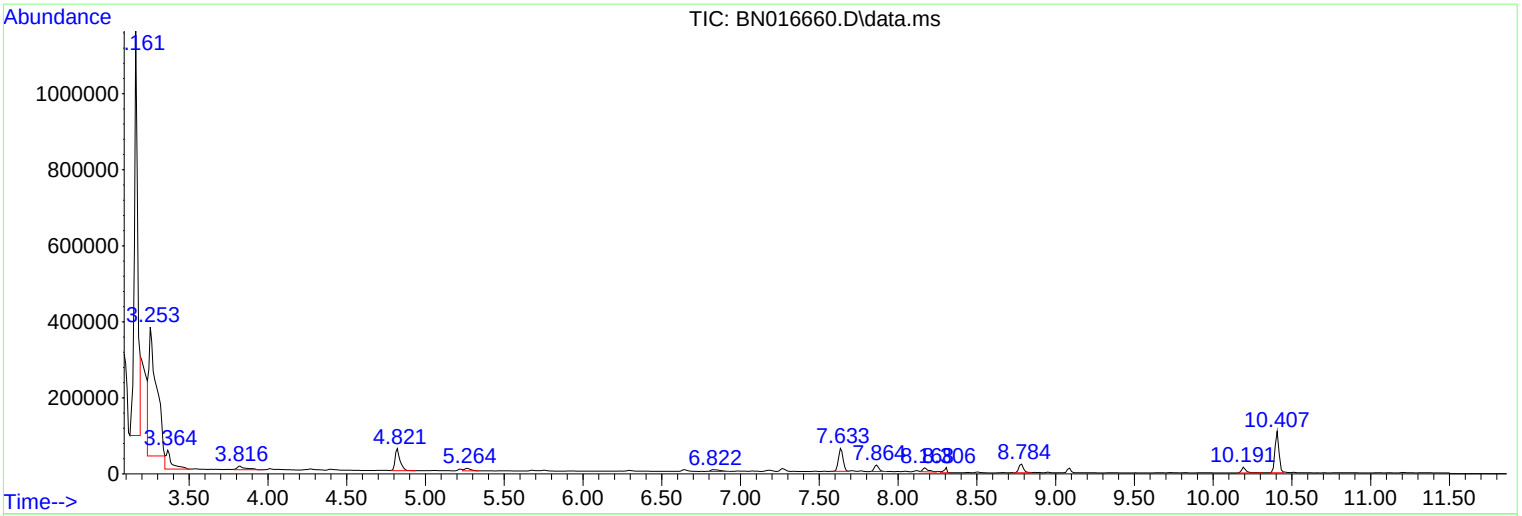
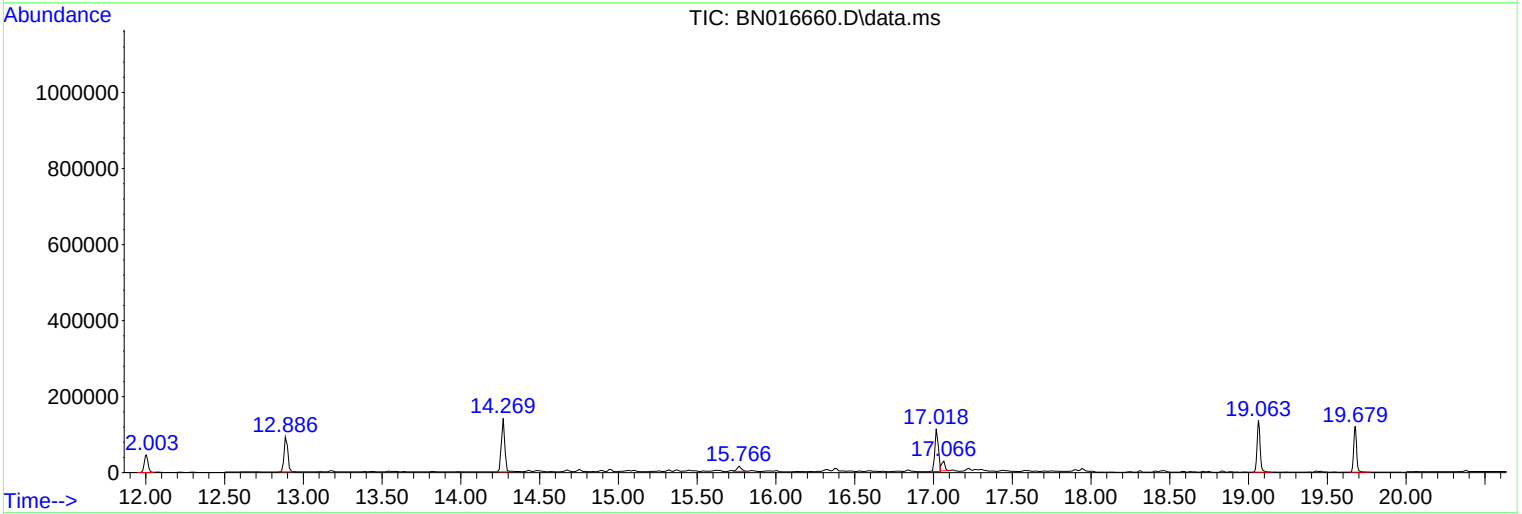
Misc :
ALS Vial : 28 Sample Multiplier: 1

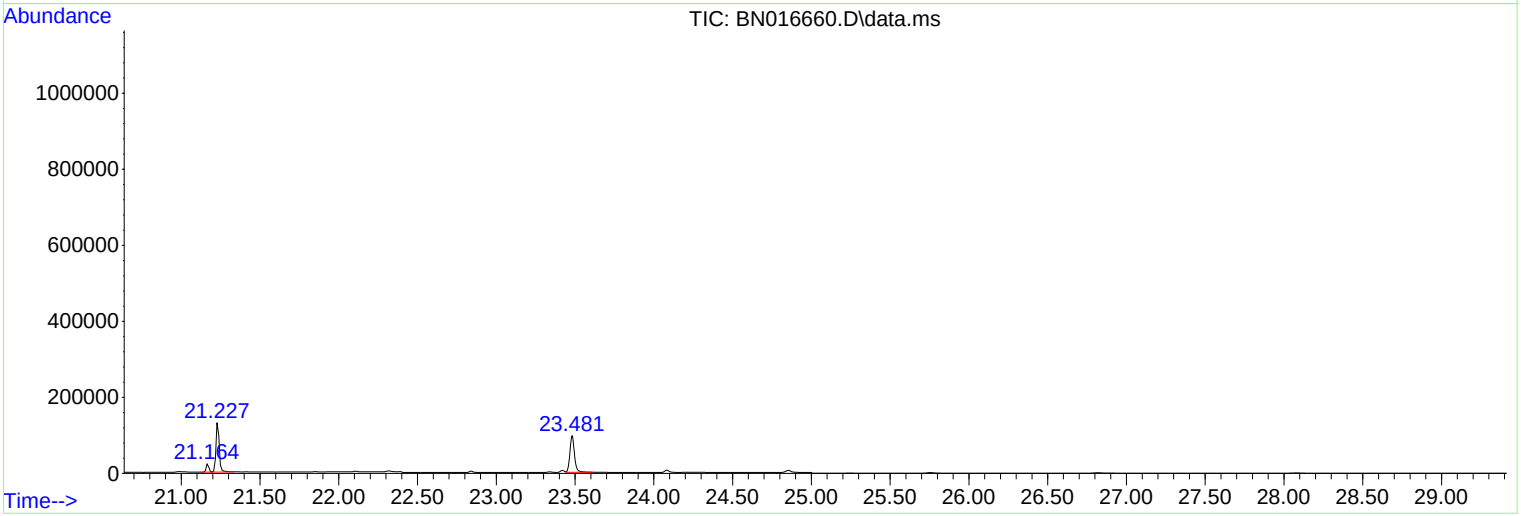
Instrument :
BNA_N
ClientSampleId :
RE125D2-20210917

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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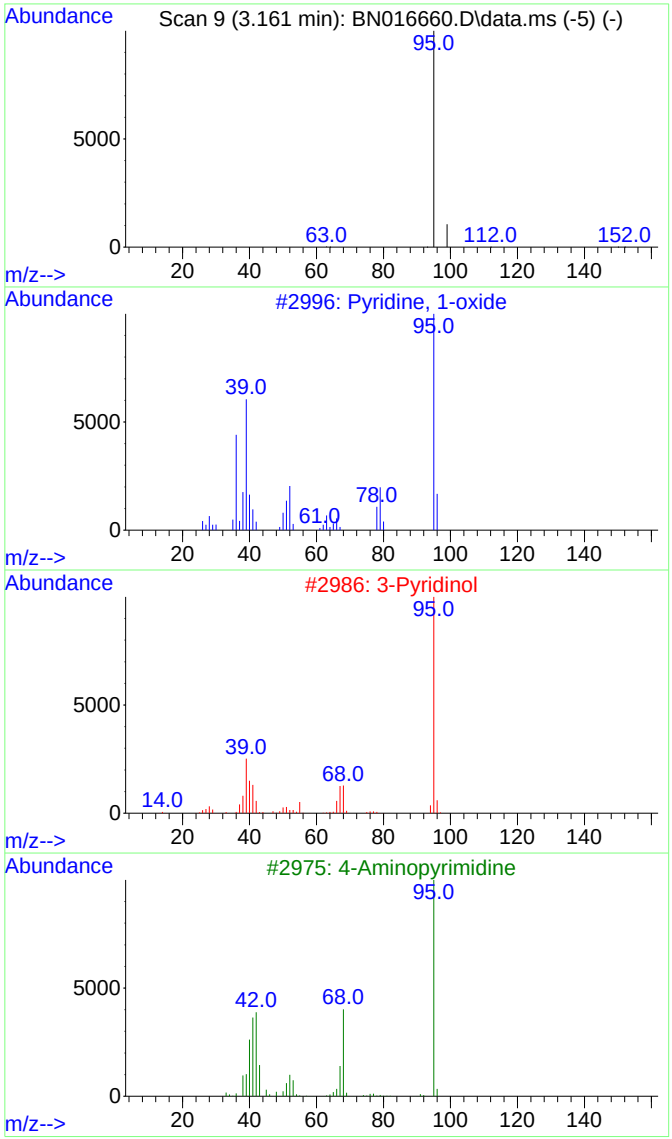
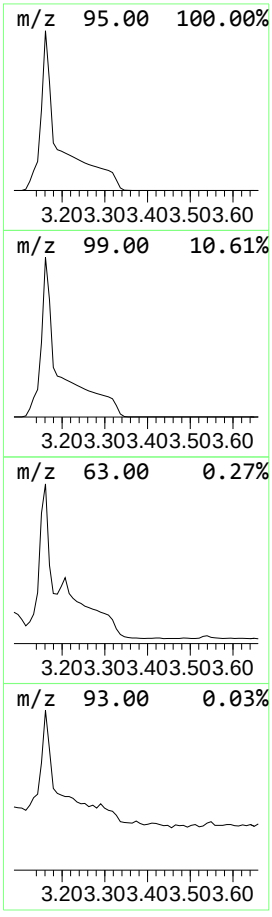
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	5.36 ng	1619190	1,4-Dichlorobenzene-d4	7.633

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 : BN016660.D
Acq On : 02 Oct 2021 07:33
Operator : CG/JU
Sample : M3829-08
Misc :
ALS Vial : 28 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

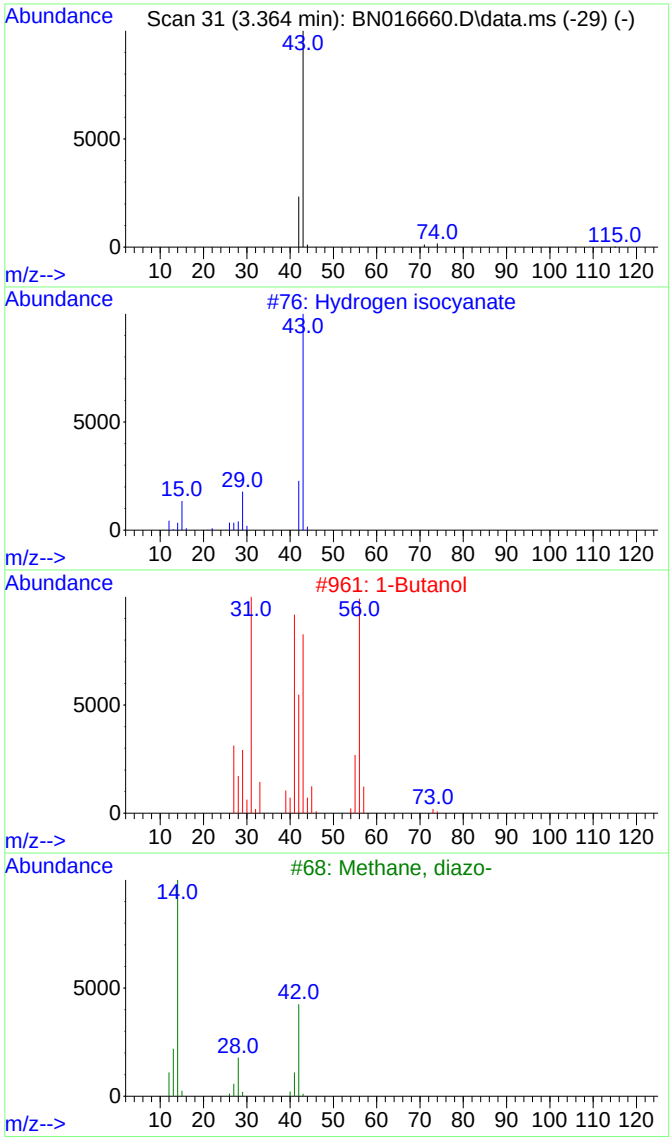
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

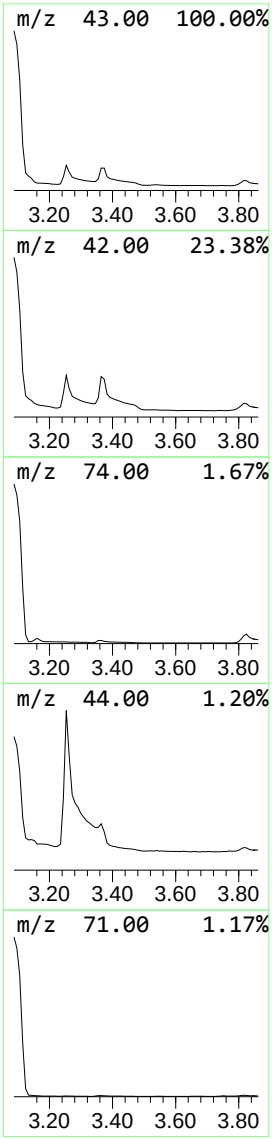
****

Peak Number 2 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.40 ng	121945	1,4-Dichlorobenzene-d4	7.633

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	2
3	Methane, diazo-	42	CH2N2	000334-88-3	2
4	Diazirine	42	CH2N2	1000305-84-1	2
5	Borane carbonyl	42	CH3BO	013205-44-2	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 07:33
Operator : CG/JU
Sample : M3829-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE125D2-20210917

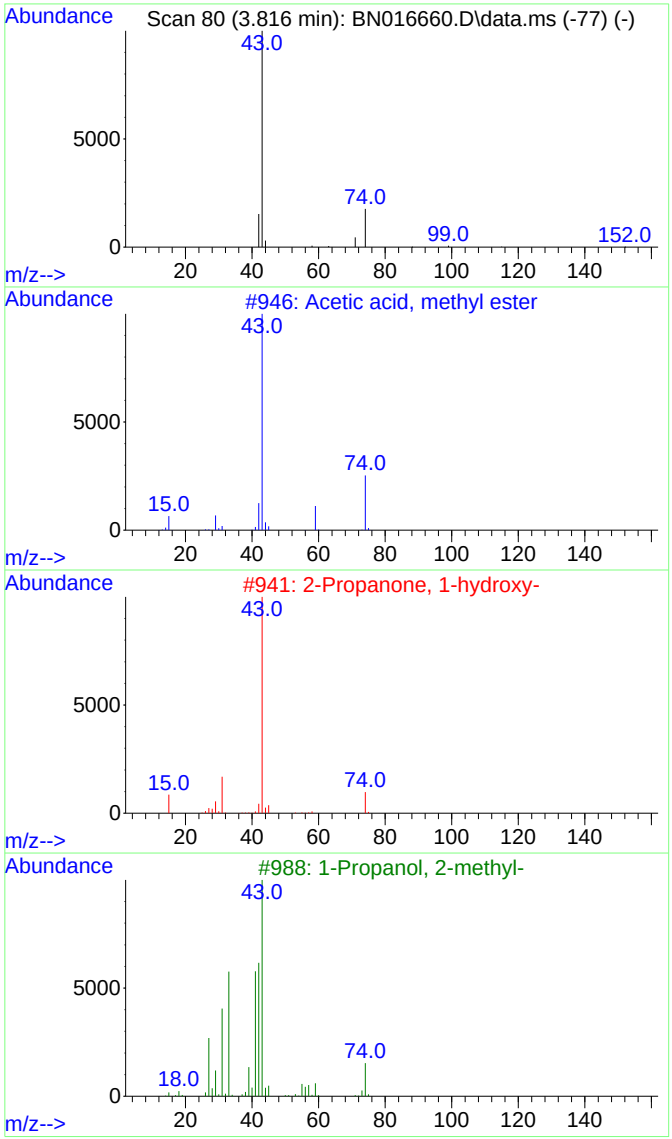
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

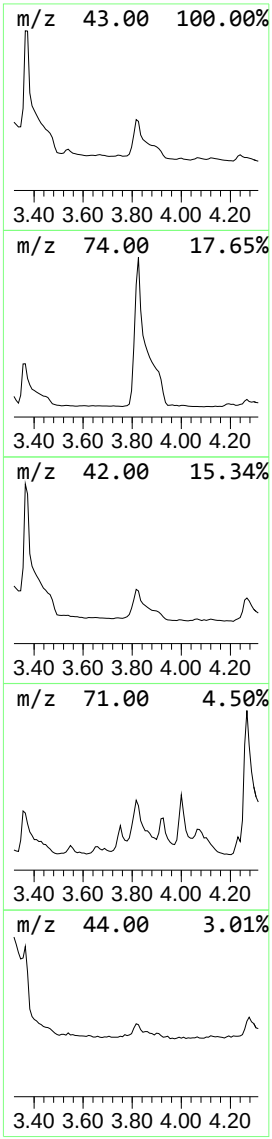
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Acetic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.12 ng	37523	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	5
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016660.D
Acq On : 02 Oct 2021 07:33
Operator : CG/JU
Sample : M3829-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE125D2-20210917

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

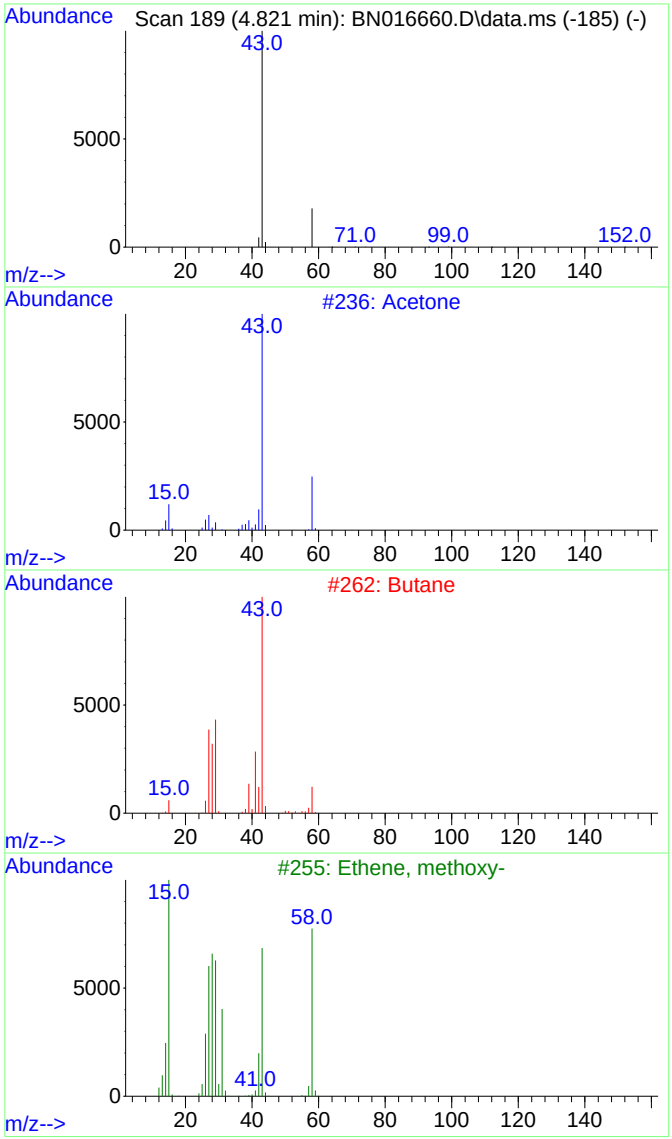
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

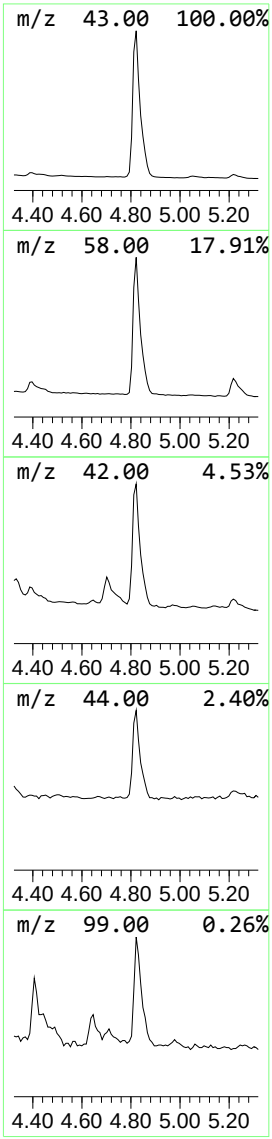
****

Peak Number 4 Acetone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.41 ng	124057	1,4-Dichlorobenzene-d4	7.633

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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Data File : BN016660.D
Acq On : 02 Oct 2021 07:33
Operator : CG/JU
Sample : M3829-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D2-20210917

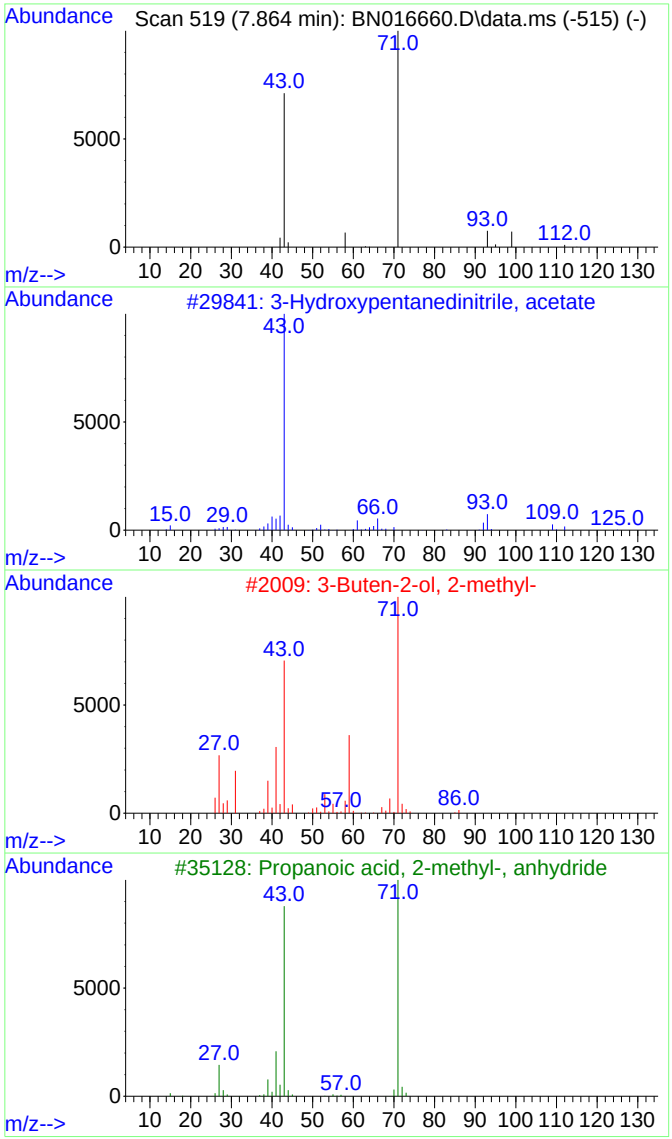
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

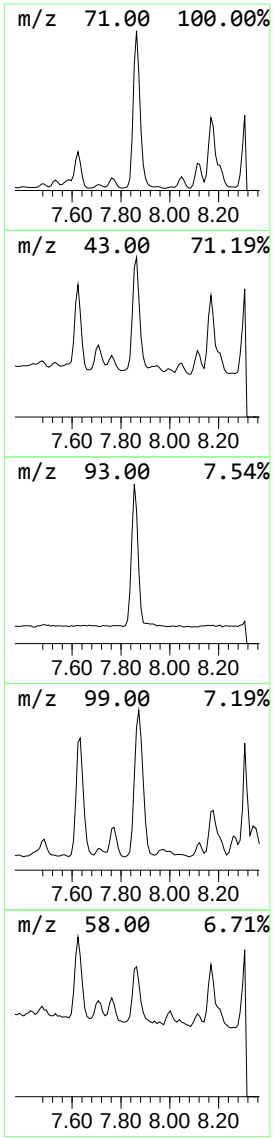
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Hydroxypentanedinitrile, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.11 ng	34043	1,4-Dichlorobenzene-d4	7.633

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	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
4	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
5	3-Penten-2-ol	86	C5H10O	001569-50-2	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
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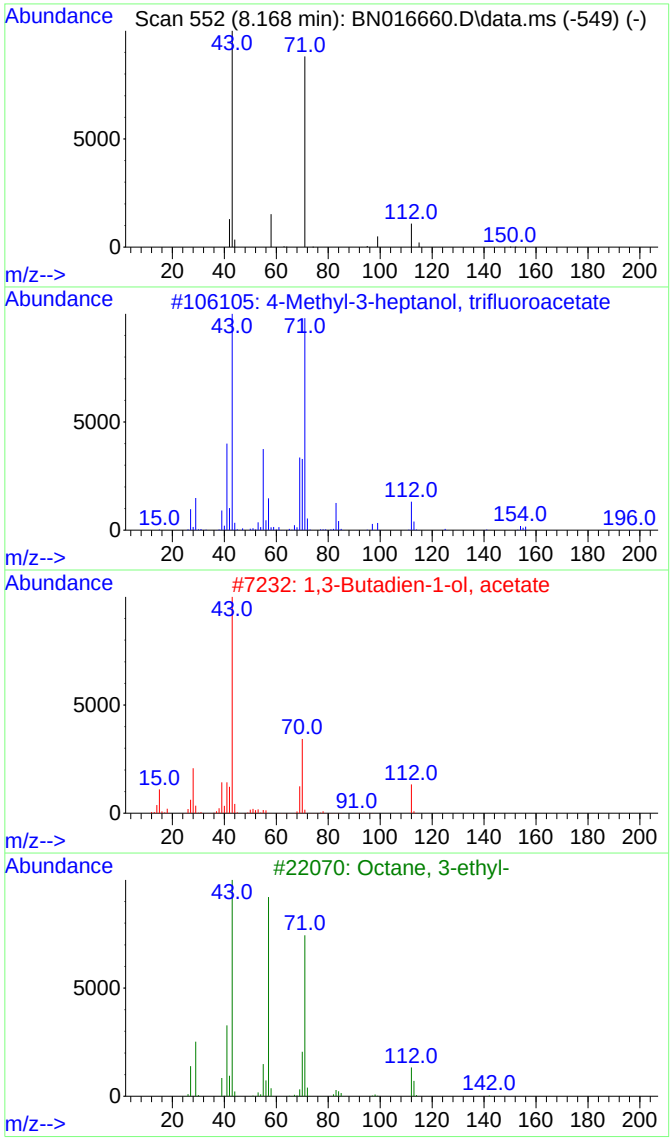
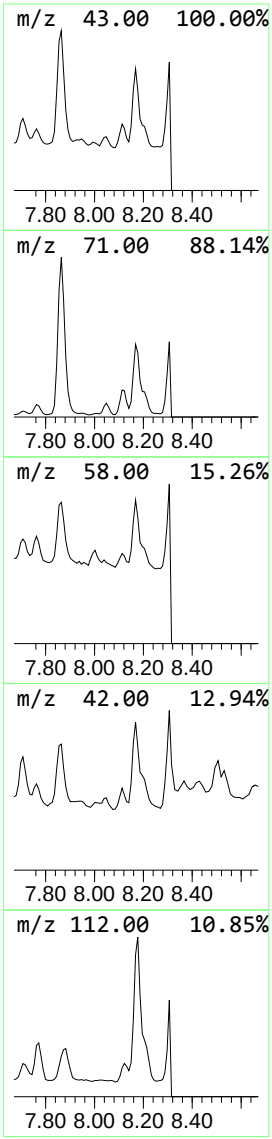
****
Peak Number 6 4-Methyl-3-heptanol, triflu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.09 ng	26296	1,4-Dichlorobenzene-d4	7.633

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	Octane, 3-ethyl-	142	C10H22	005881-17-4	9
4	Decane, 4-methyl-	156	C11H24	002847-72-5	9
5	Butane	58	C4H10	000106-97-8	7





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ALS Vial : 28 Sample Multiplier: 1

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BNA_N
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RE125D2-20210917

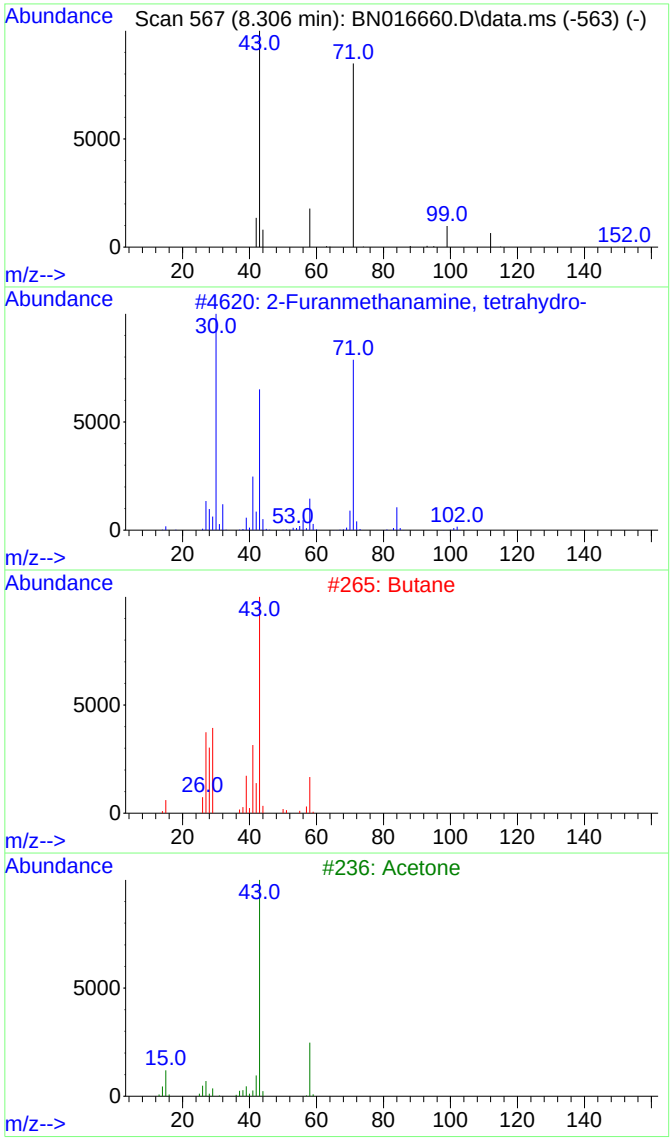
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

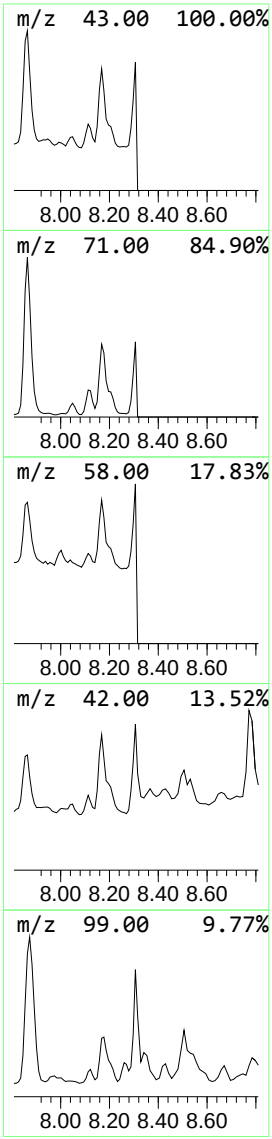
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Furanmethanamine, tetrahy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.06 ng	18692	1,4-Dichlorobenzene-d4	7.633

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





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BNA_N
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

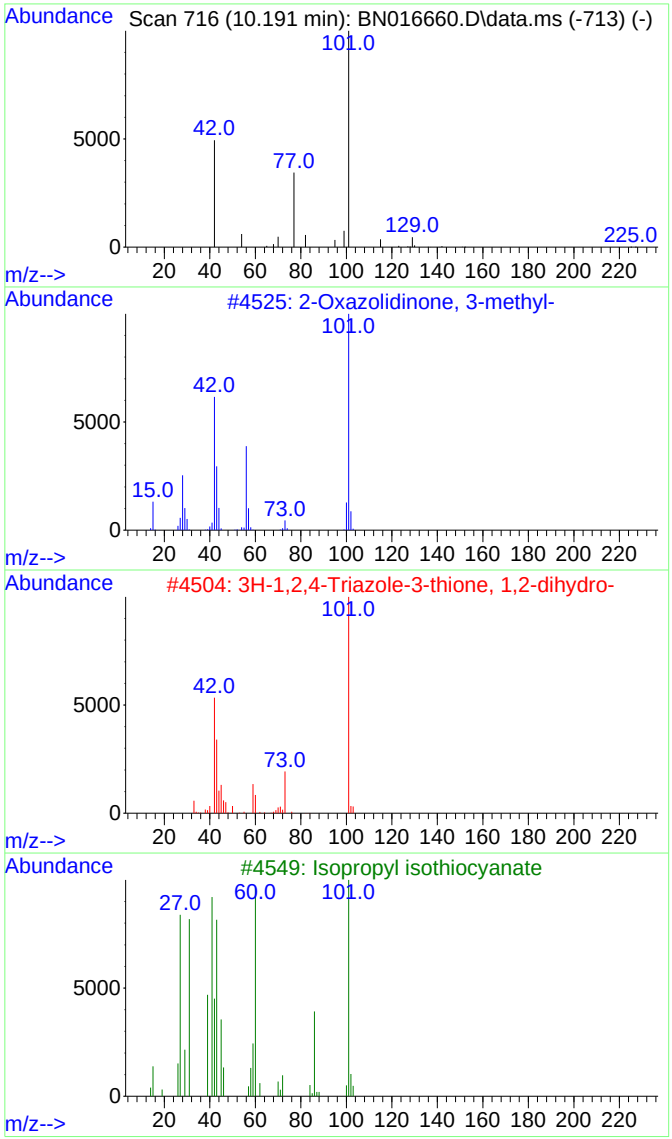
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

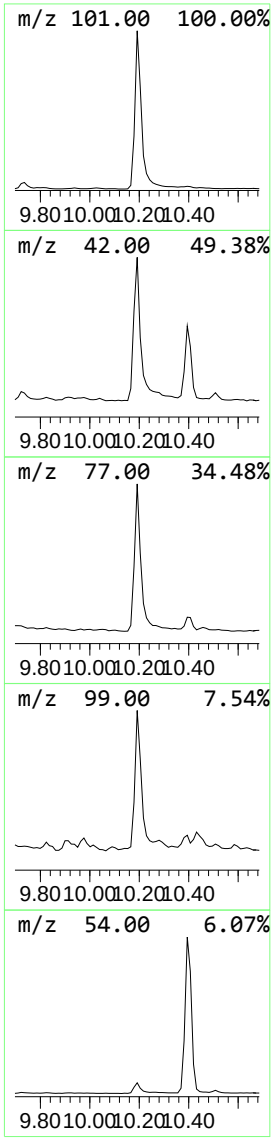
****

Peak Number 8 2-Oxazolidinone, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.06 ng	30875	Naphthalene-d8	10.407

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





Tentatively Identified Compound (LSC) summary

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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	3.161	5.4	ng	1619190	1	7.633	120938	0.4
Hydrogen isocya...	3.364	0.4	ng	121945	1	7.633	120938	0.4
Acetic acid, me...	3.816	0.1	ng	37523	1	7.633	120938	0.4
Acetone	4.821	0.4	ng	124057	1	7.633	120938	0.4
3-Hydroxypentan...	7.864	0.1	ng	34043	1	7.633	120938	0.4
4-Methyl-3-hept...	8.168	0.1	ng	26296	1	7.633	120938	0.4
2-Furanmethanam...	8.306	0.1	ng	18692	1	7.633	120938	0.4
2-Oxazolidinone...	10.191	0.1	ng	30875	2	10.407	191479	0.4