LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016691.D
Acq On : 03 Oct 2021 04:36
Operator : CG/JU
Sample : M3915-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : TT101D1-20210921

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: BN016691.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	672659	1035841	100.00%	25.216%
2	3.253	17	19	29	rVB	225913	773357	74.66%	18.826%
3	3.364	29	31	48	rVB2	46898	132015	12.74%	3.214%
4	3.825	77	81	88	rBV	9795	28788	2.78%	0.701%
5	4.821	185	189	204	rVB	42801	90652	8.75%	2.207%
6	5.272	234	238	245	rVB	7830	19982	1.93%	0.486%
7	6.296	345	349	354	rBV	15472	32587	3.15%	0.793%
8	6.831	403	407	415	rVB2	5270	16694	1.61%	0.406%
9	7.080	430	434	440	rVB	5686	11698	1.13%	0.285%
10	7.264	450	454	460	rBV	8913	18027	1.74%	0.439%
11	7.633	490	494	500	rBV	55830	116058	11.20%	2.825%
12	7.725	500	504	513	rVB3	3986	10880	1.05%	0.265%
13	8.784	601	605	610	rBV	24782	48864	4.72%	1.190%
14	10.191	713	716	726	rBV	10943	25955	2.51%	0.632%
15	10.406	729	733	737	rBV	112048	195506	18.87%	4.759%
16	12.002	921	931	943	rBV	52634	85756	8.28%	2.088%
17	12.886	1071	1074	1078	rBV	99728	173181	16.72%	4.216%
18	14.268	1180	1183	1186	rBV	143056	206926	19.98%	5.037%
19	14.484	1197	1200	1207	rVB	29388	46573	4.50%	1.134%
20	15.766	1299	1301	1305	rVB2	11762	18643	1.80%	0.454%
21	17.017	1400	1403	1406	rBV	105164	168516	16.27%	4.102%
22	19.063	1689	1696	1720	rBV	145442	203607	19.66%	4.956%
23	19.430	1765	1770	1783	rVB	7046	10687	1.03%	0.260%
24	19.678	1813	1820	1845	rBV	129190	164494	15.88%	4.004%
25	21.163	1992	1995	1998	rBV	30120	42255	4.08%	1.029%
26	21.227	1998	2001	2011	rVB	122943	194942	18.82%	4.746%
27	23.423	2400	2409	2415	rBV	6376	10651	1.03%	0.259%
28	23.484	2415	2427	2476	rVB	99114	196111	18.93%	4.774%
29	24.087	2593	2603	2626	rBV	6971	13865	1.34%	0.338%
30	24.857	2817	2828	2855	rVB	6355	14781	1.43%	0.360%

Sum of corrected areas: 4107892

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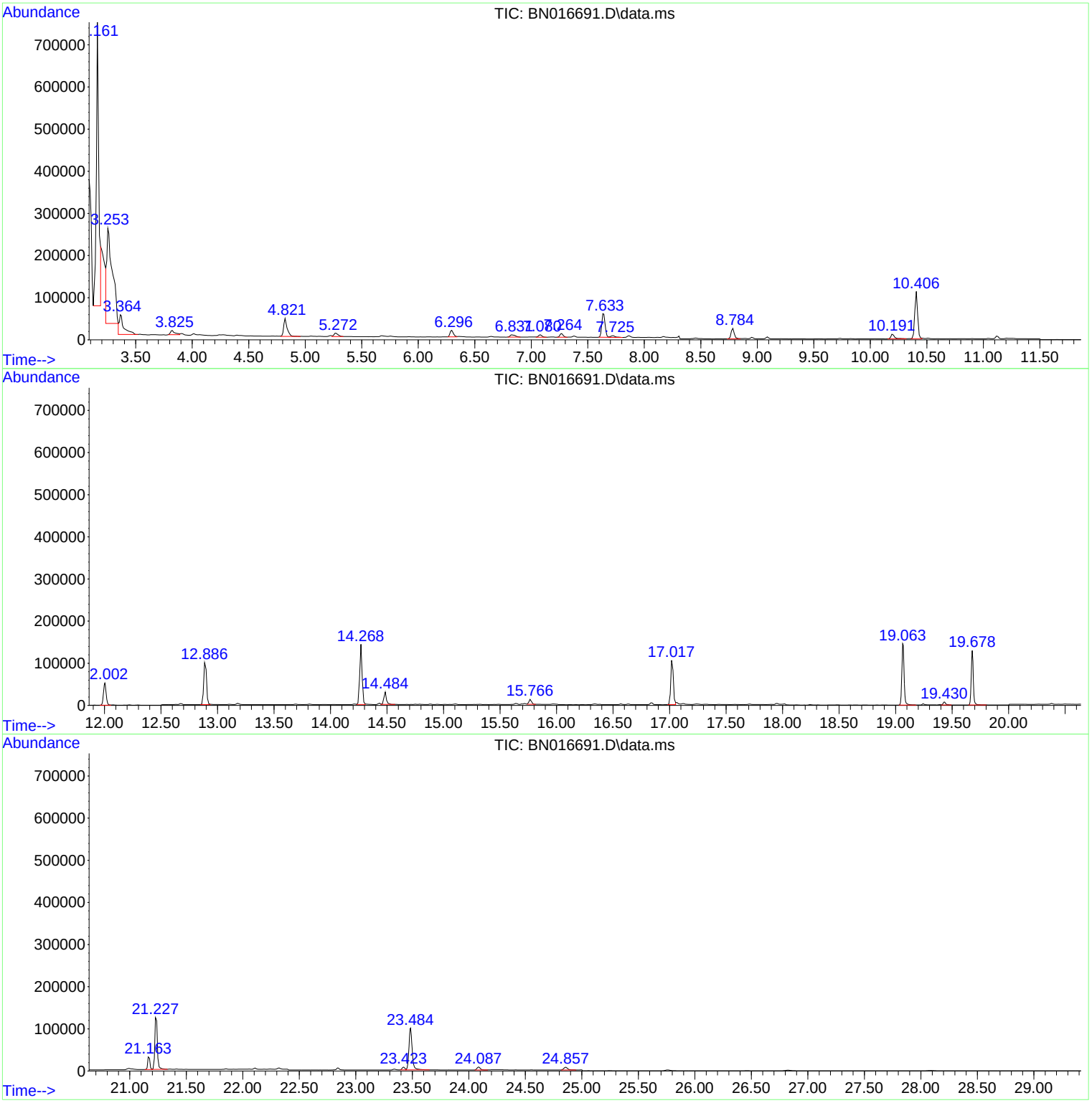
Instrument :
BNA_N
ClientSampleId :
TT101D1-20210921

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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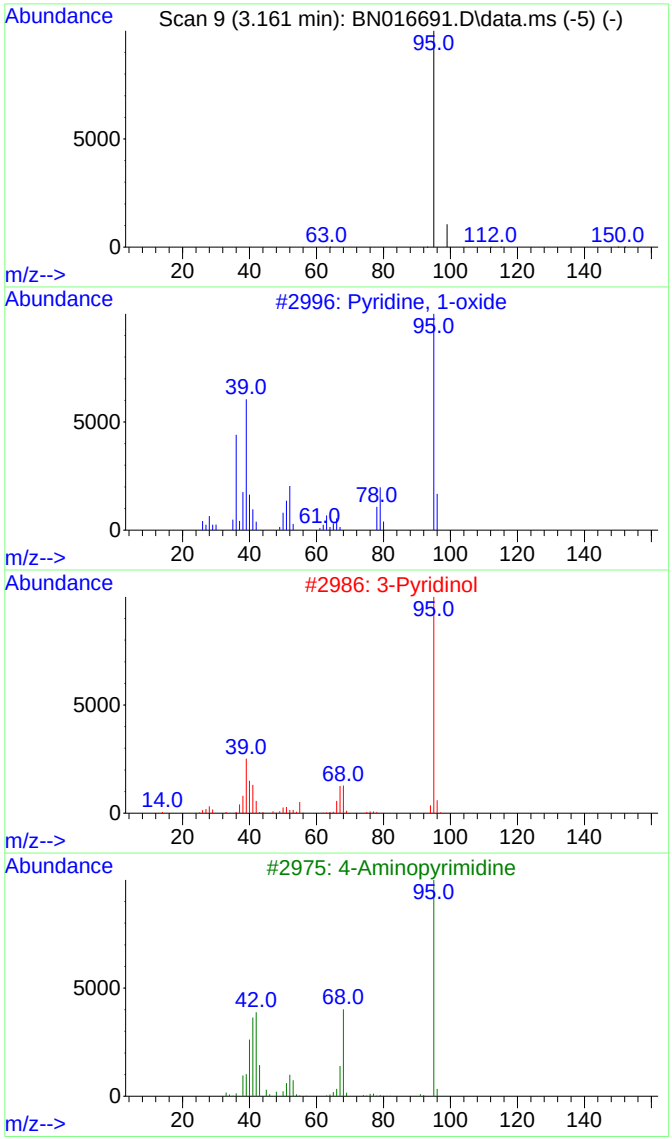
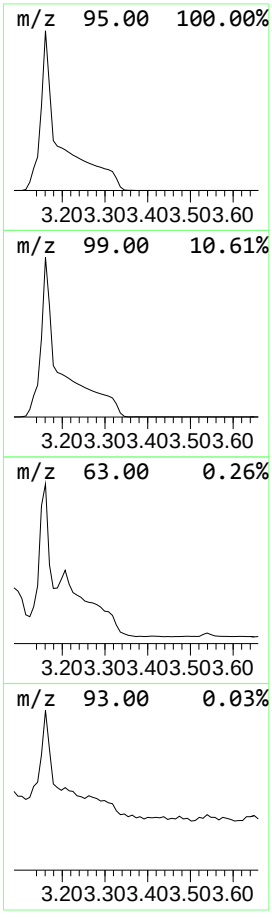
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	3.57 ng	1035840	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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Instrument : BNA_N
ClientSampleId : TT101D1-20210921

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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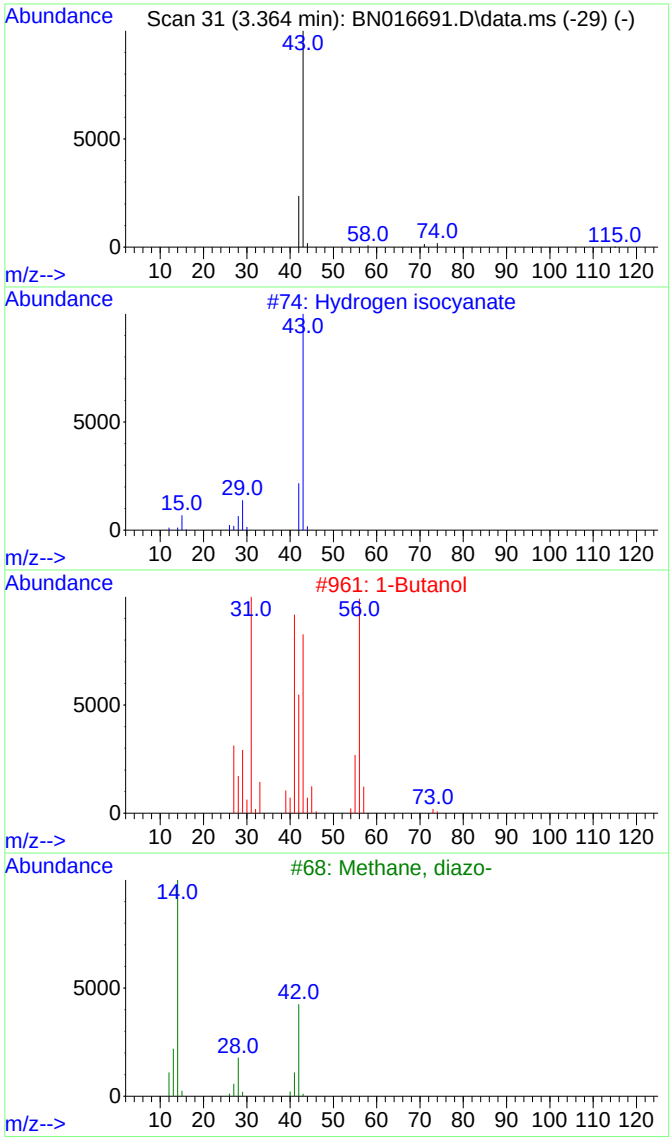
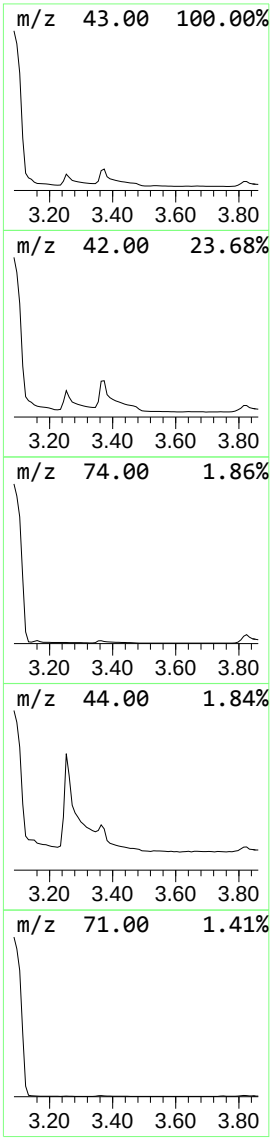
Peak Number 2 Hydrogen isocyanate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.45 ng	132015	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	2
3	Methane, diazo-	42	CH2N2	000334-88-3	2
4	Diazirine	42	CH2N2	1000305-84-1	2
5	Ketene	42	C2H2O	000463-51-4	2





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Data File : BN016691.D
Acq On : 03 Oct 2021 04:36
Operator : CG/JU
Sample : M3915-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : TT101D1-20210921

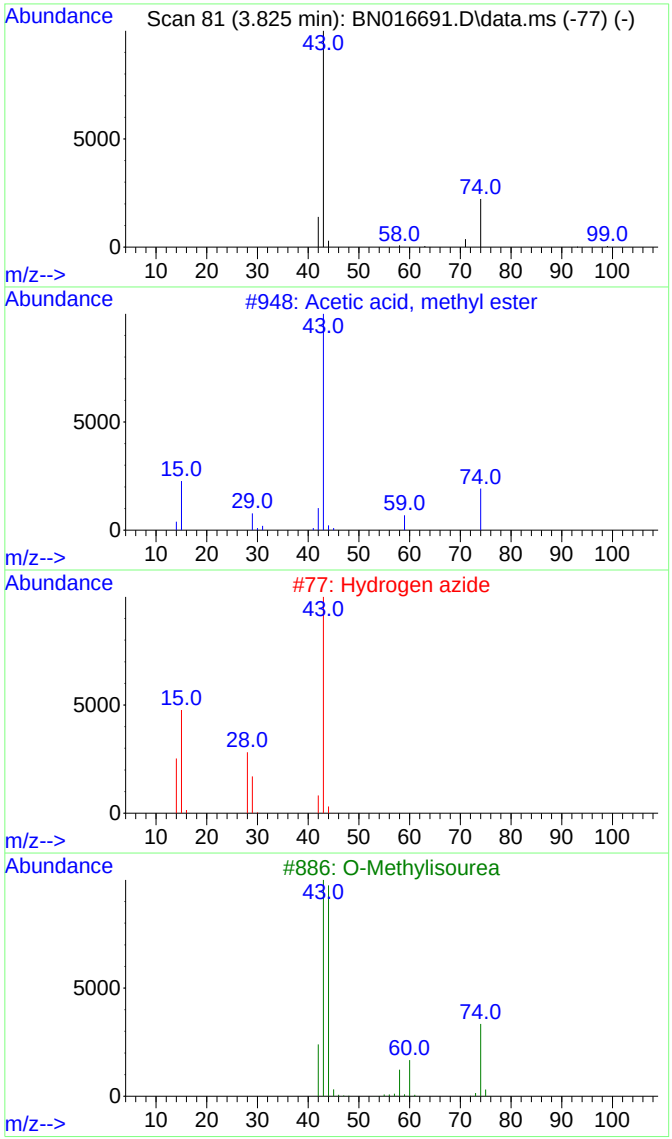
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

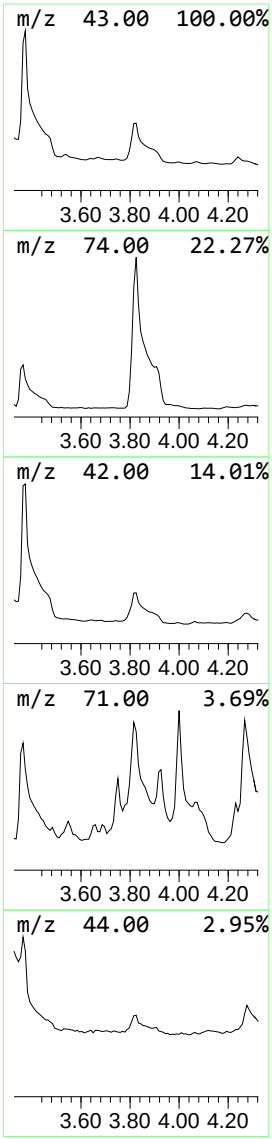
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.10 ng	28788	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 azide	43	HN3	007782-79-8	4
3	O-Methylisourea	74	C2H6N2O	002440-60-0	4
4	1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3
5	Urea, methyl-	74	C2H6N2O	000598-50-5	3





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Acq On : 03 Oct 2021 04:36
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Sample : M3915-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : TT101D1-20210921

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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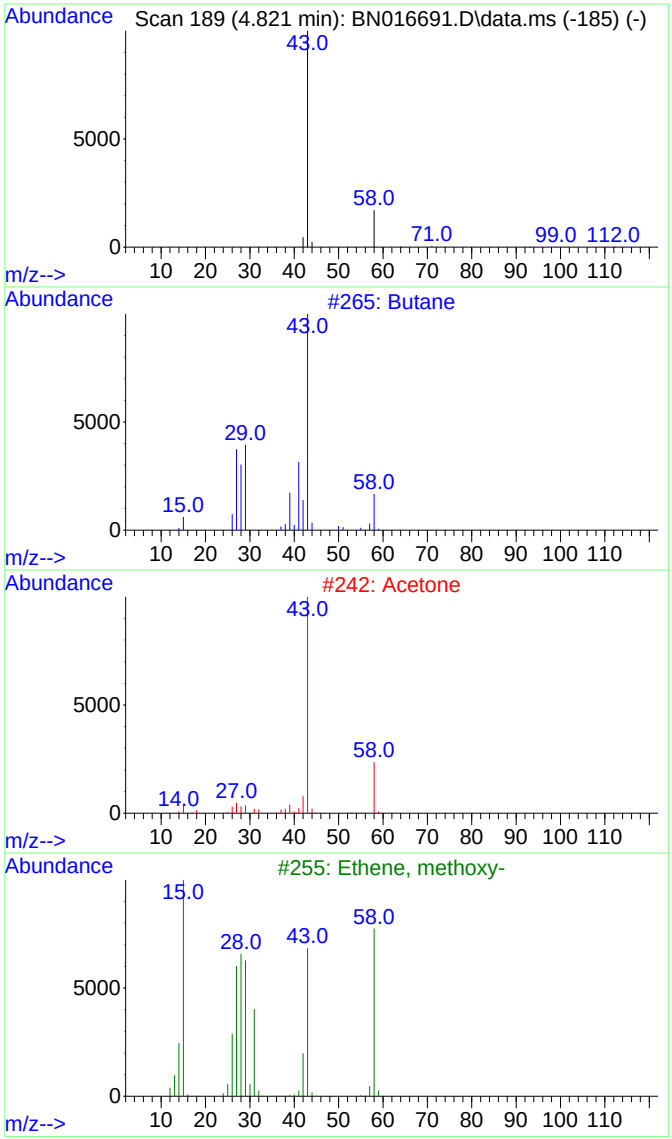
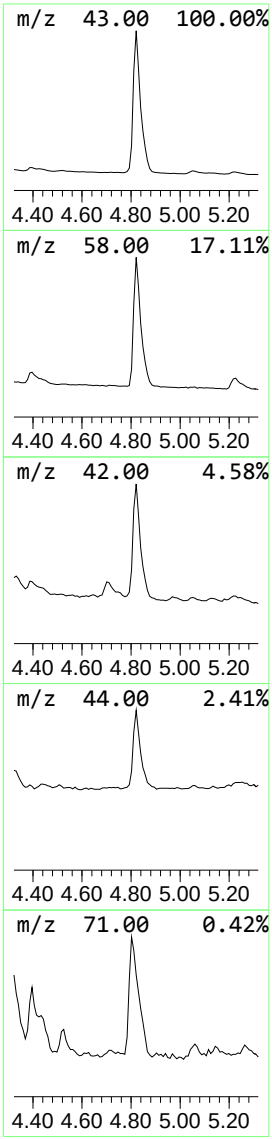
Peak Number 4 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.31 ng	90652	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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Data File : BN016691.D
Acq On : 03 Oct 2021 04:36
Operator : CG/JU
Sample : M3915-01
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : TT101D1-20210921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
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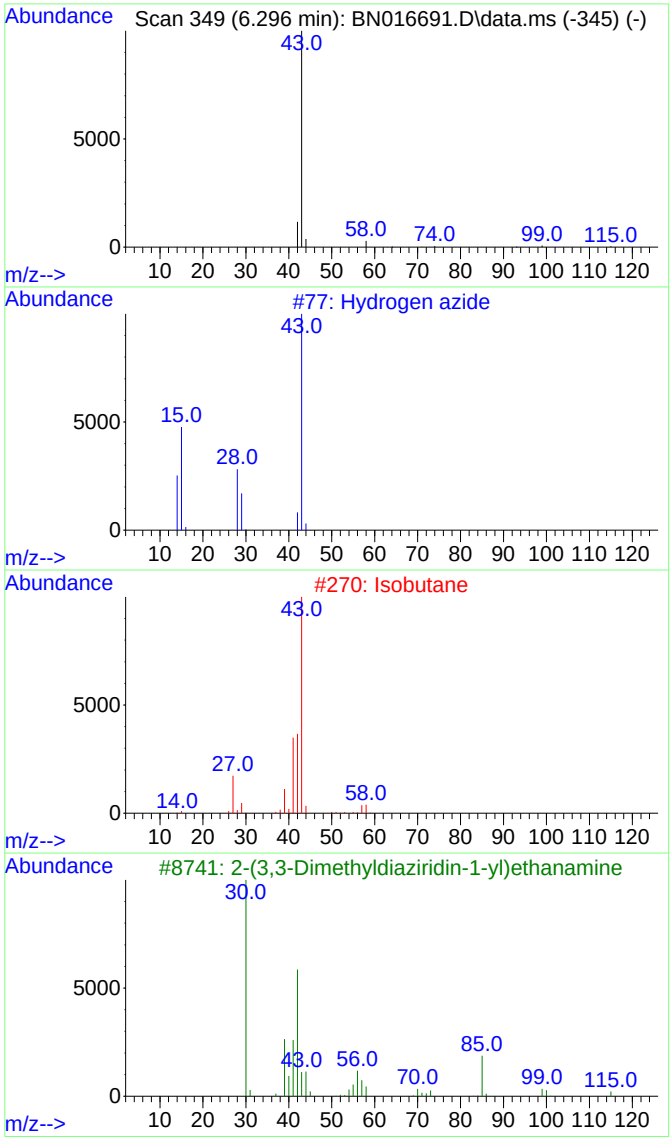
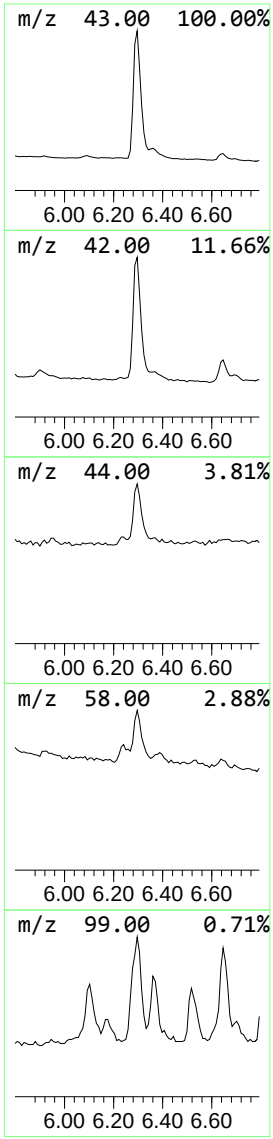
Peak Number 5 Hydrogen azide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.11 ng	32587	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	Isobutane	58	C4H10	000075-28-5	4
3	2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	4
4	2,3-Octanedione	142	C8H14O2	000585-25-1	2
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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TIC Library : C:\Database\NIST20.L
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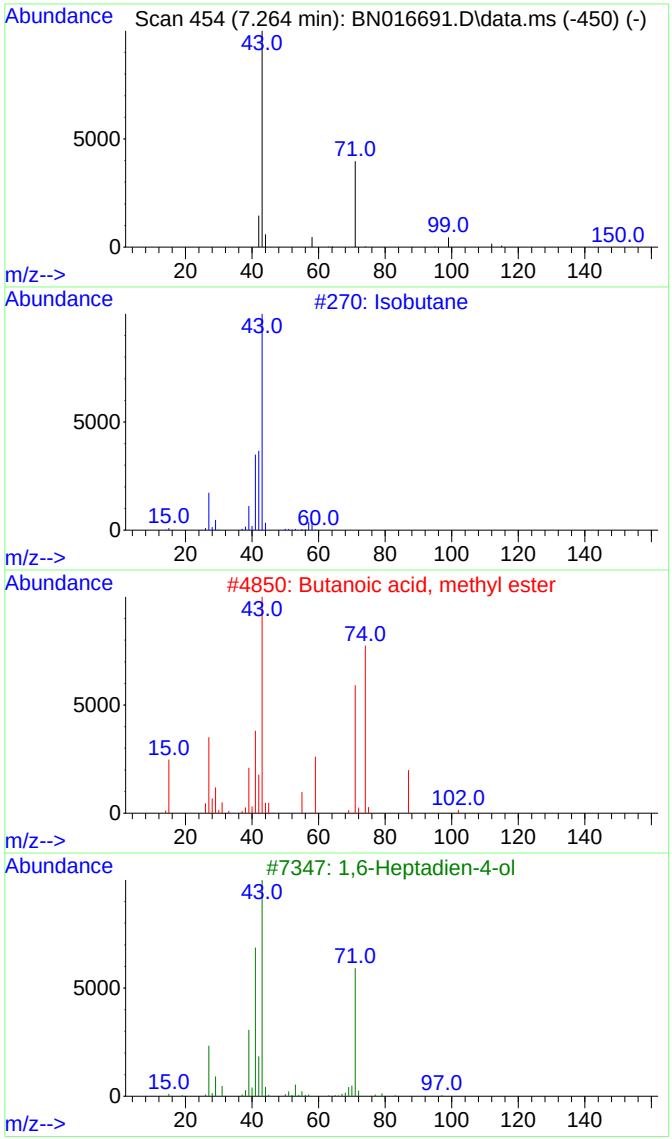
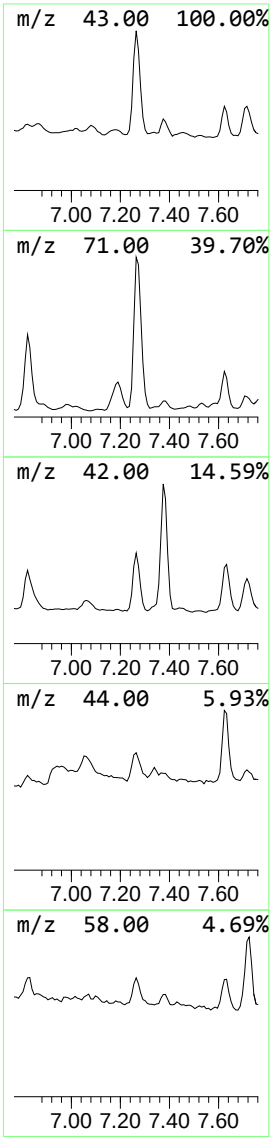
Peak Number 6 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	18027	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	4
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
3	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4





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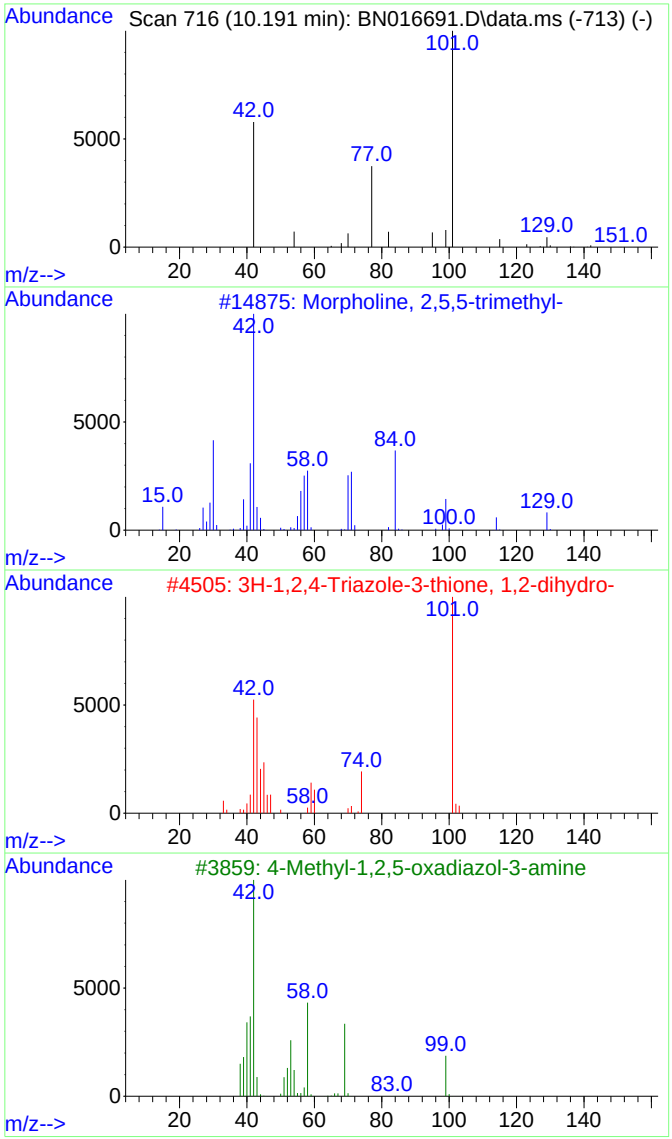
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

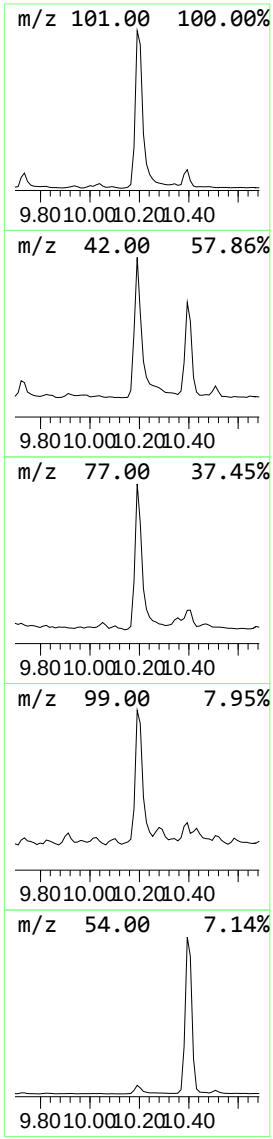
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Morpholine, 2,5,5-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.05 ng	25955	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	7
2	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
3	4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5





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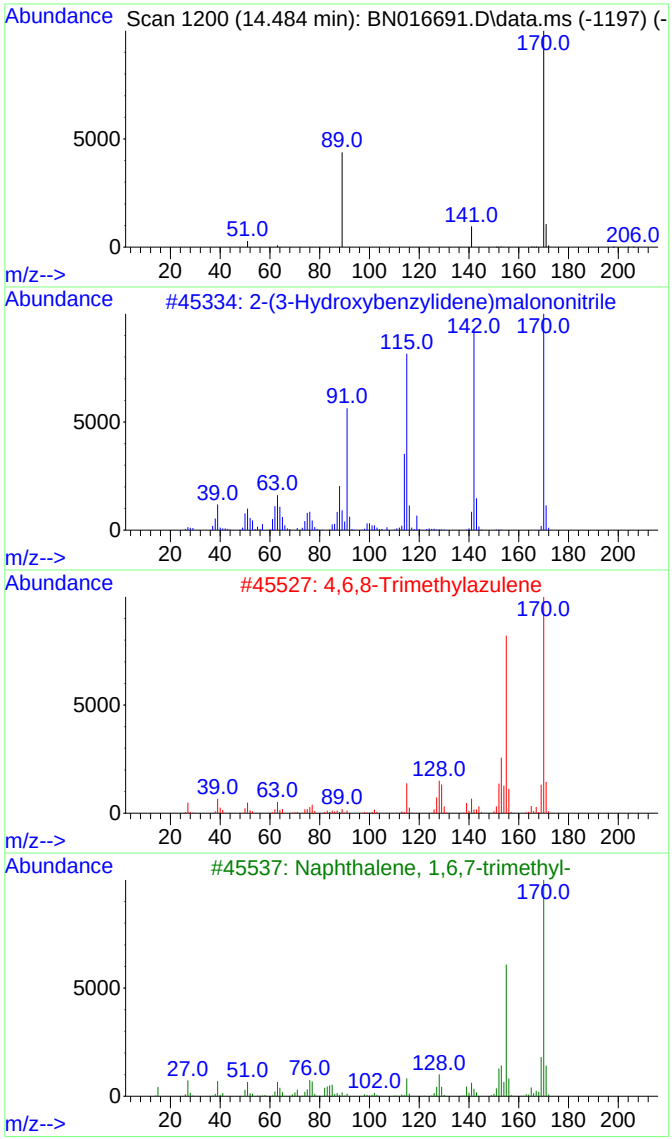
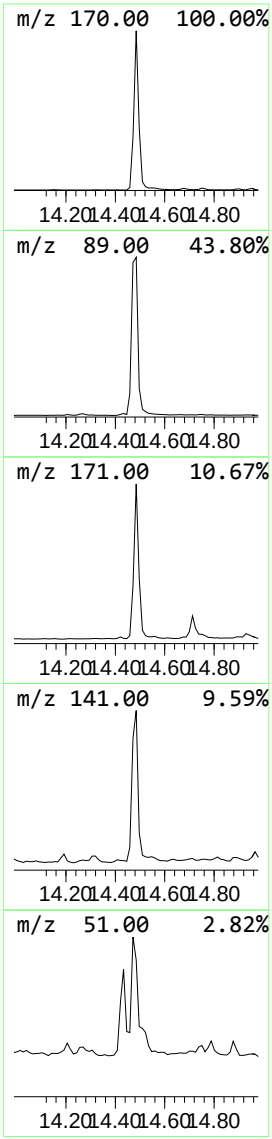
****
Peak Number 8 2-(3-Hydroxybenzylidene)mal... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.484	0.09 ng	46573	Acenaphthene-d10	14.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3-Hydroxybenzylidene)malononi...	170	C10H6N2O	007255-96-1	42
2	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	9
3	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	9
4	8-Hydroxyquinoline-2-carbonitrile	170	C10H6N2O	006759-78-0	9
5	3-Hydroxybiphenyl	170	C12H10O	000580-51-8	9





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	3.6	ng	1035840	1	7.642	116058	0.4
Hydrogen isocya...	3.364	0.5	ng	132015	1	7.642	116058	0.4
Acetic acid, me...	3.825	0.1	ng	28788	1	7.642	116058	0.4
Butane	4.821	0.3	ng	90652	1	7.642	116058	0.4
Hydrogen azide	6.296	0.1	ng	32587	1	7.642	116058	0.4
Isobutane	7.264	0.1	ng	18027	1	7.642	116058	0.4
Morpholine, 2,5...	10.191	0.1	ng	25955	2	10.406	195506	0.4
2-(3-Hydroxyben...	14.484	0.1	ng	46573	3	14.268	206926	0.4