LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016648.D
Acq On : 01 Oct 2021 22:36
Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW203D-20210918

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: BN016648.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	6	9	11	rVB	39939	48813	25.25%	2.002%
2	3.364	29	31	45	rVB	16803	50170	25.96%	2.058%
3	3.816	76	80	97	rVB	12125	48861	25.28%	2.004%
4	4.821	185	189	207	rVB	38659	90085	46.61%	3.695%
5	5.273	234	238	246	rVB2	6542	17109	8.85%	0.702%
6	6.379	355	358	368	rVB	2803	6421	3.32%	0.263%
7	6.647	383	387	391	rBV	3458	7655	3.96%	0.314%
8	6.831	403	407	420	rVB2	4970	14503	7.50%	0.595%
9	7.264	450	454	460	rVB2	7148	16402	8.49%	0.673%
10	7.642	490	495	500	rVB	44712	92474	47.84%	3.793%
11	7.864	515	519	525	rBV	7694	15860	8.21%	0.651%
12	8.168	549	552	560	rVV	4450	15437	7.99%	0.633%
13	8.306	564	567	569	rVB	8420	10366	5.36%	0.425%
14	8.784	601	605	610	rBV	22696	43577	22.55%	1.788%
15	10.191	713	716	727	rBV	109994	187473	96.99%	7.690%
16	10.407	729	733	737	rBV	96673	165813	85.79%	6.802%
17	11.205	793	796	802	rBV	3534	6960	3.60%	0.285%
18	12.003	918	931	943	rBV	40152	66156	34.23%	2.714%
19	12.886	1071	1074	1078	rBV2	82485	150023	77.62%	6.154%
20	13.178	1094	1097	1105	rBV	36163	60361	31.23%	2.476%
21	14.269	1180	1183	1186	rBV	127626	183280	94.82%	7.518%
22	15.715	1294	1297	1299	rBV	7788	11993	6.20%	0.492%
23	15.766	1299	1301	1305	rVB2	13434	22318	11.55%	0.915%
24	17.018	1400	1403	1406	rBV	92764	151805	78.54%	6.227%
25	17.955	1477	1480	1483	rBV	4709	9435	4.88%	0.387%
26	18.015	1483	1485	1499	rVB3	3686	5501	2.85%	0.226%
27	19.063	1687	1696	1715	rBV	132077	186538	96.51%	7.652%
28	19.242	1728	1732	1748	rBV	4745	7558	3.91%	0.310%
29	19.678	1813	1820	1838	rBV	137728	174493	90.28%	7.158%
30	20.006	1885	1886	1889	rBV2	2942	5974	3.09%	0.245%
31	20.378	1918	1921	1924	rBV	9849	12283	6.35%	0.504%
32	20.972	1975	1977	1980	rBV	6004	9990	5.17%	0.410%
33	21.164	1993	1995	1999	rBV	61343	87485	45.26%	3.589%
34	21.227	1999	2001	2010	rVB	117252	180664	93.47%	7.411%
35	22.109	2081	2084	2089	rVB	4820	7112	3.68%	0.292%
36	22.321	2101	2104	2108	rBV	3825	6341	3.28%	0.260%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016648.D
Acq On : 01 Oct 2021 22:36
Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW203D-20210918

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	22.841	2232	2239	2256	rVB	5488	8065	4.17%	0.331%
38	23.419	2400	2408	2415	rBV	7663	12618	6.53%	0.518%
39	23.481	2415	2426	2473	rVB	98017	193288	100.00%	7.929%
40	24.083	2593	2602	2620	rVB2	8087	15187	7.86%	0.623%
41	24.854	2817	2827	2844	rVB	7295	15958	8.26%	0.655%
42	25.761	3076	3092	3115	rBV2	2169	6383	3.30%	0.262%
43	26.822	3382	3402	3426	rBV2	1579	5756	2.98%	0.236%
44	28.088	3749	3772	3793	rBV	883	3294	1.70%	0.135%

Sum of corrected areas: 2437838

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Instrument :
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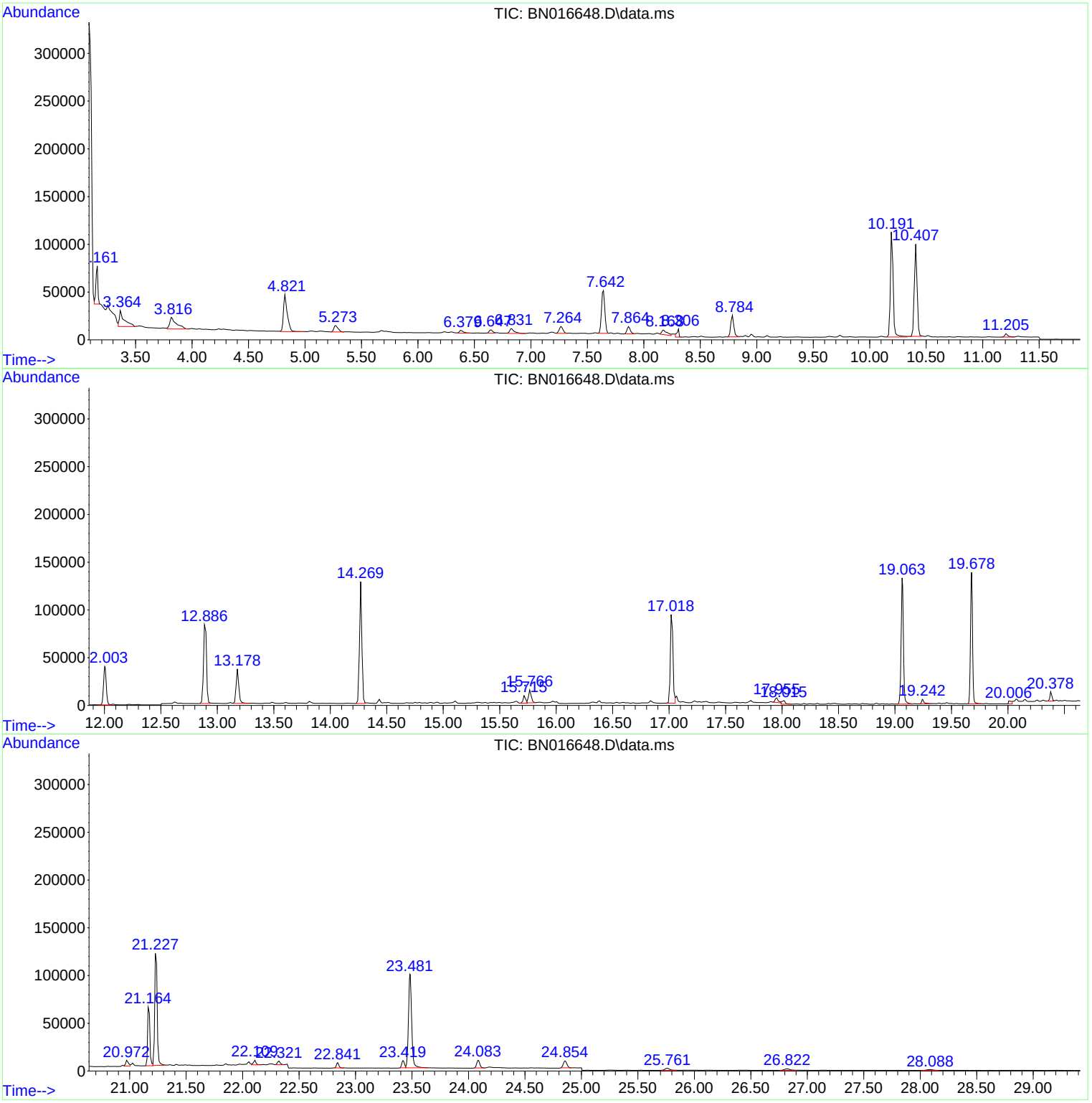
ClientSampleId :
MW203D-20210918

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 : BN016648.D
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Instrument : BNA_N
ClientSampleId : MW203D-20210918

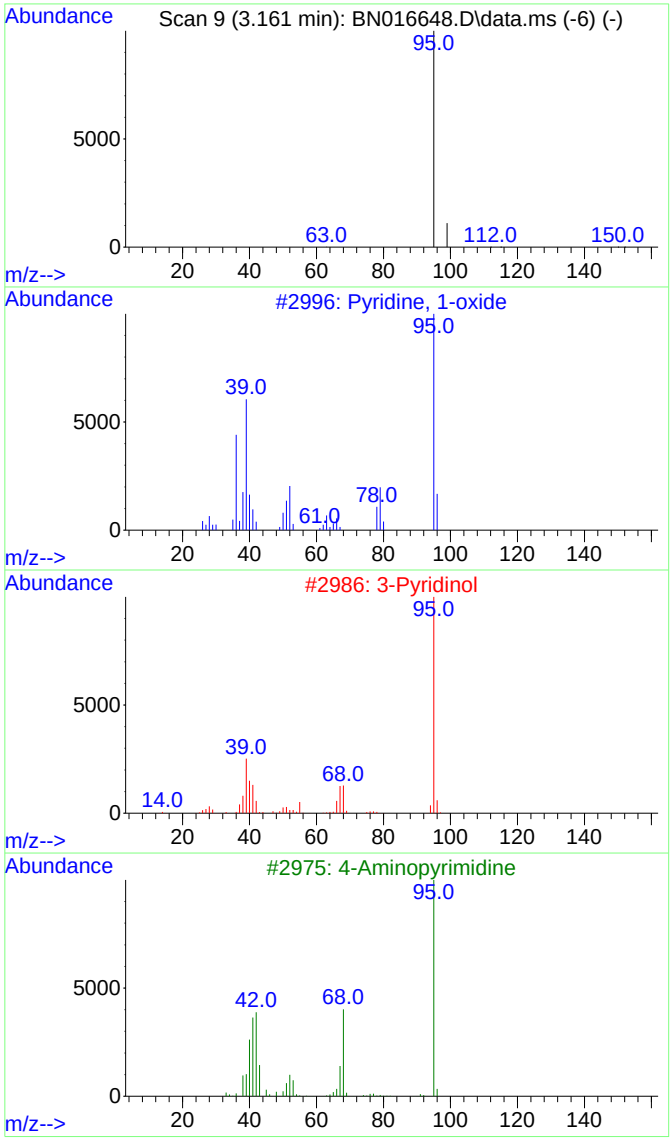
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

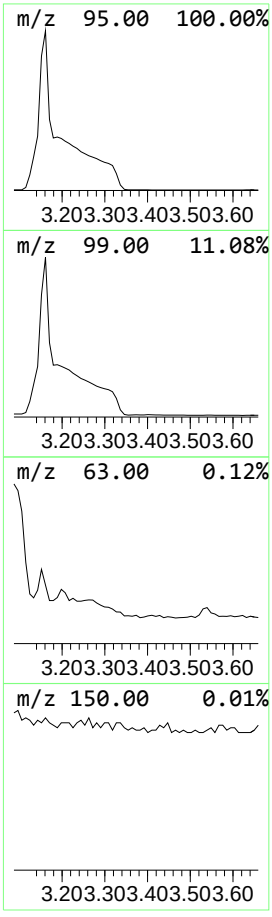
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pyridine, 1-oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	0.21 ng	48813	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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Operator : CG/JU
Sample : M3829-18
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Instrument : BNA_N
ClientSampleId : MW203D-20210918

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

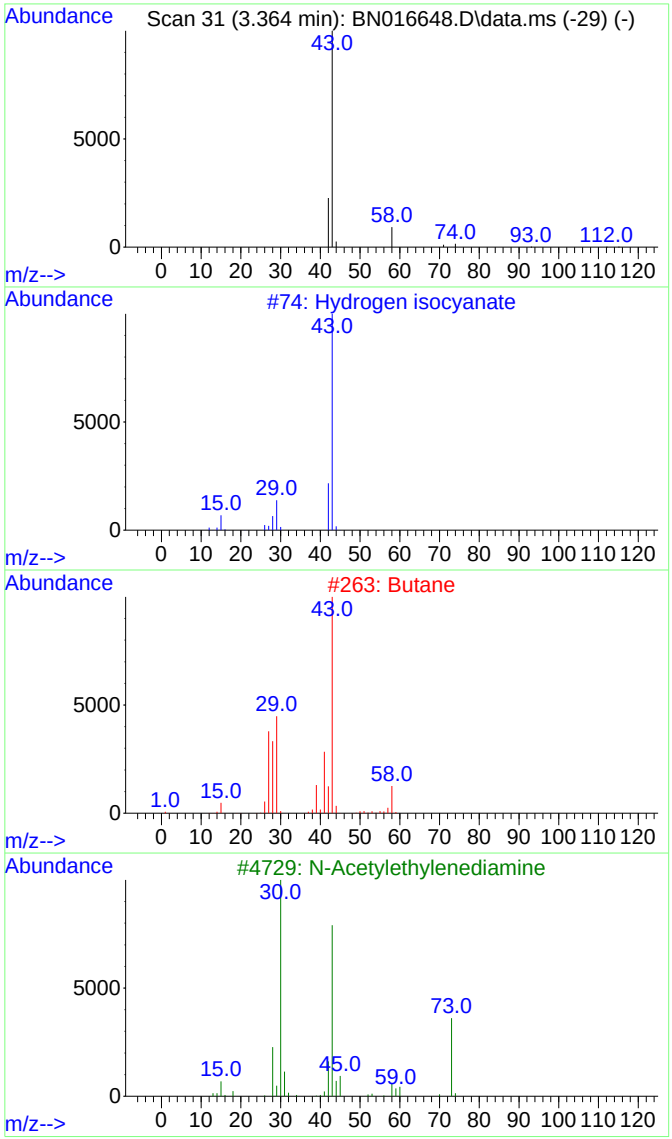
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

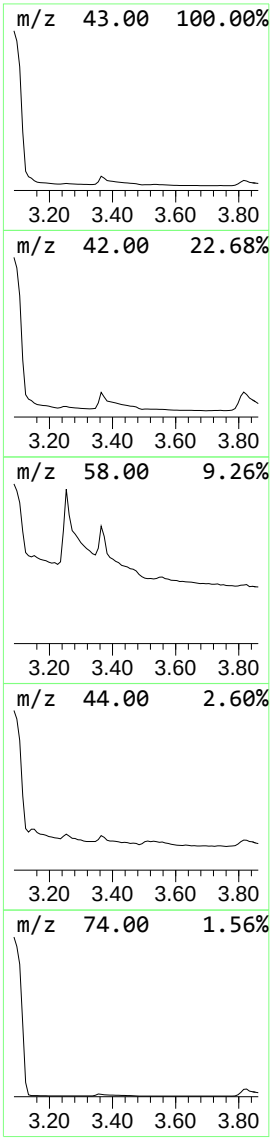
****

Peak Number 2 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.22 ng	50170	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	Butane	58	C4H10	000106-97-8	4
3	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	2
4	1-Tetrazol-2-ylethanone	112	C3H4N4O	051410-11-8	2
5	Hydrogen azide	43	HN3	007782-79-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016648.D
Acq On : 01 Oct 2021 22:36
Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D-20210918

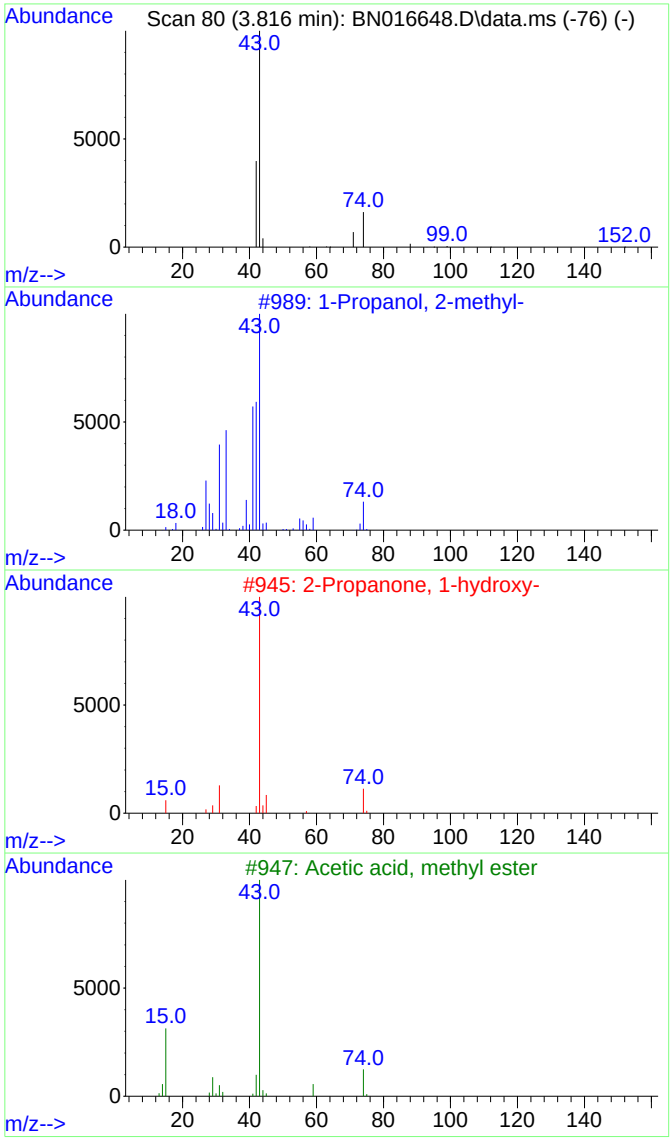
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

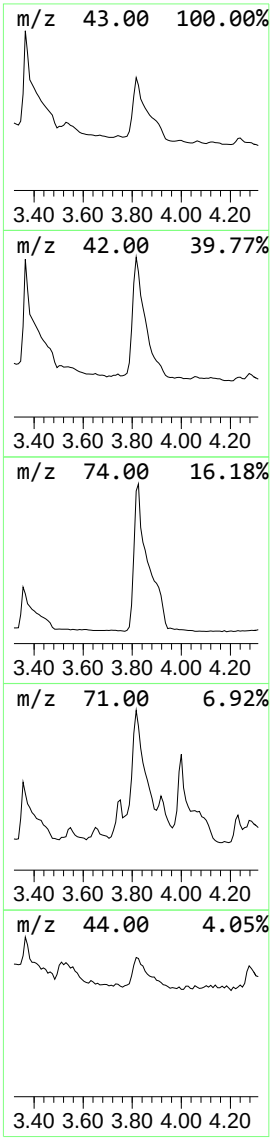
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.21 ng	48861	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	3
5	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D-20210918

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

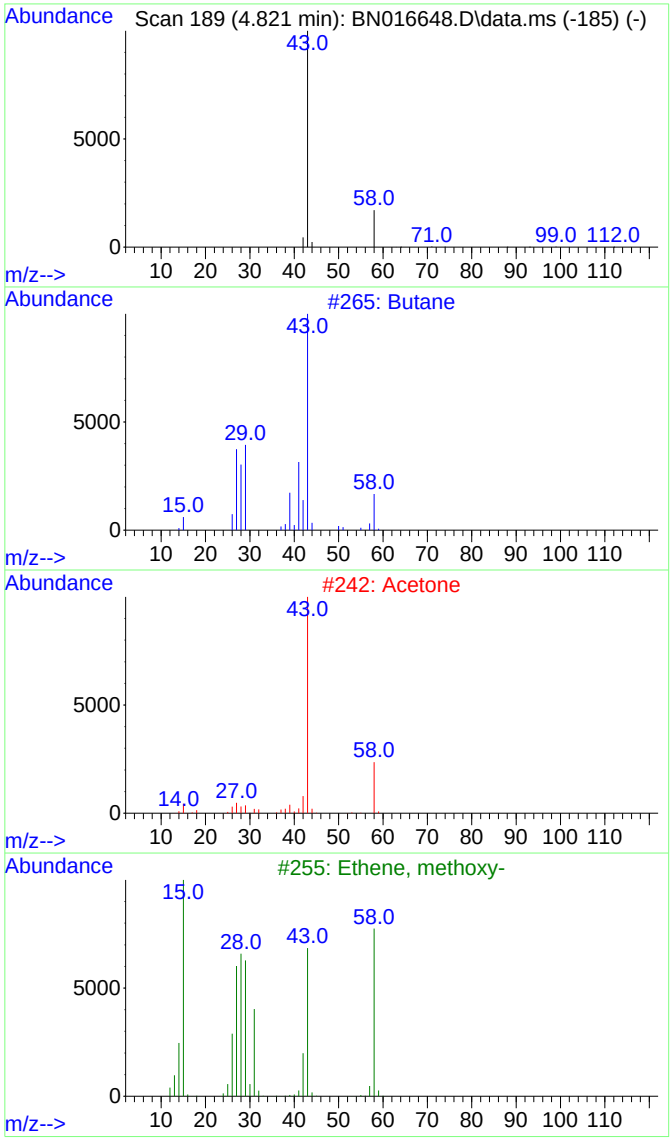
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

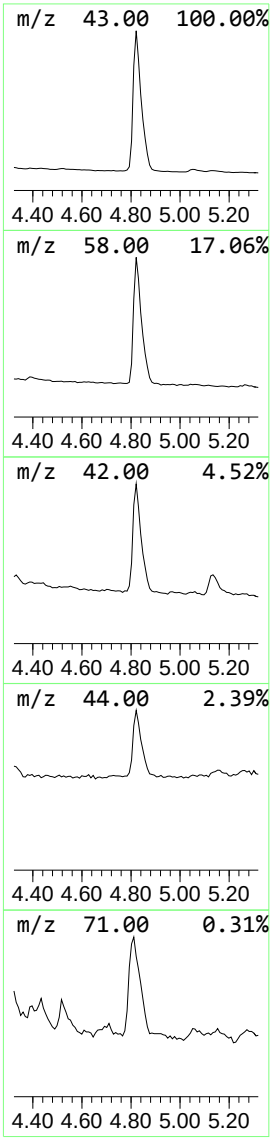
****

Peak Number 4 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.39 ng	90085	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\
Data File : BN016648.D
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Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D-20210918

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

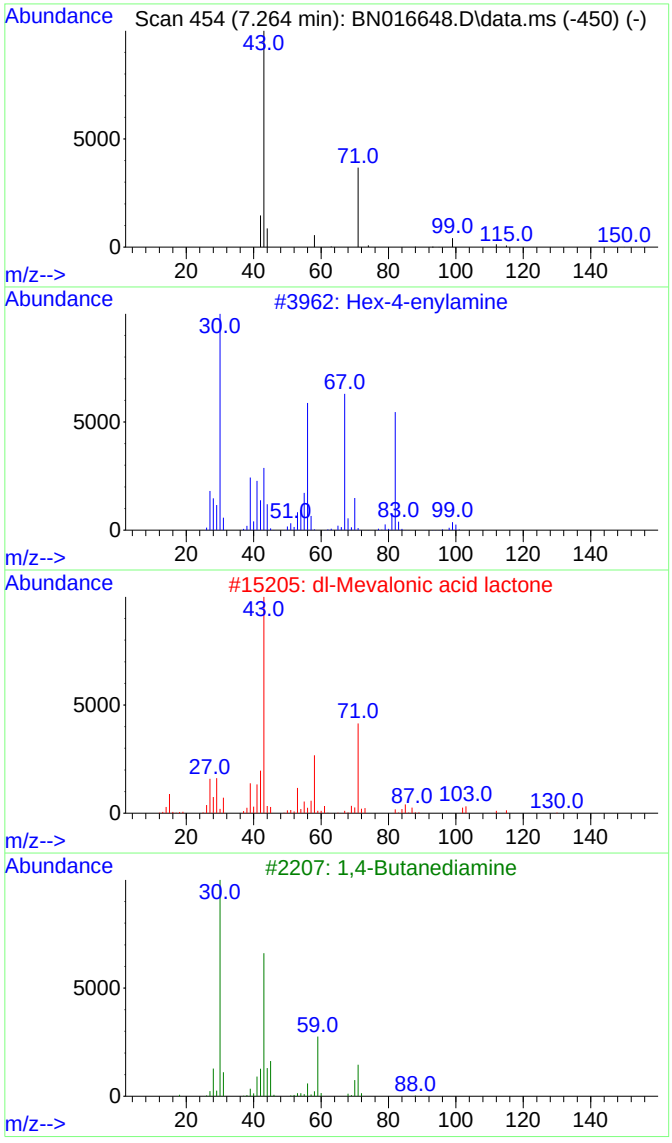
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

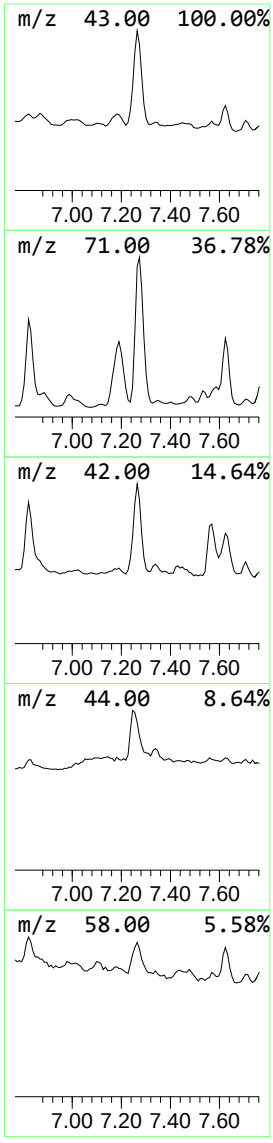
****

Peak Number 5 Hex-4-enylamine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.07 ng	16402	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	1,4-Butanediamine	88	C4H12N2	000110-60-1	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





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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

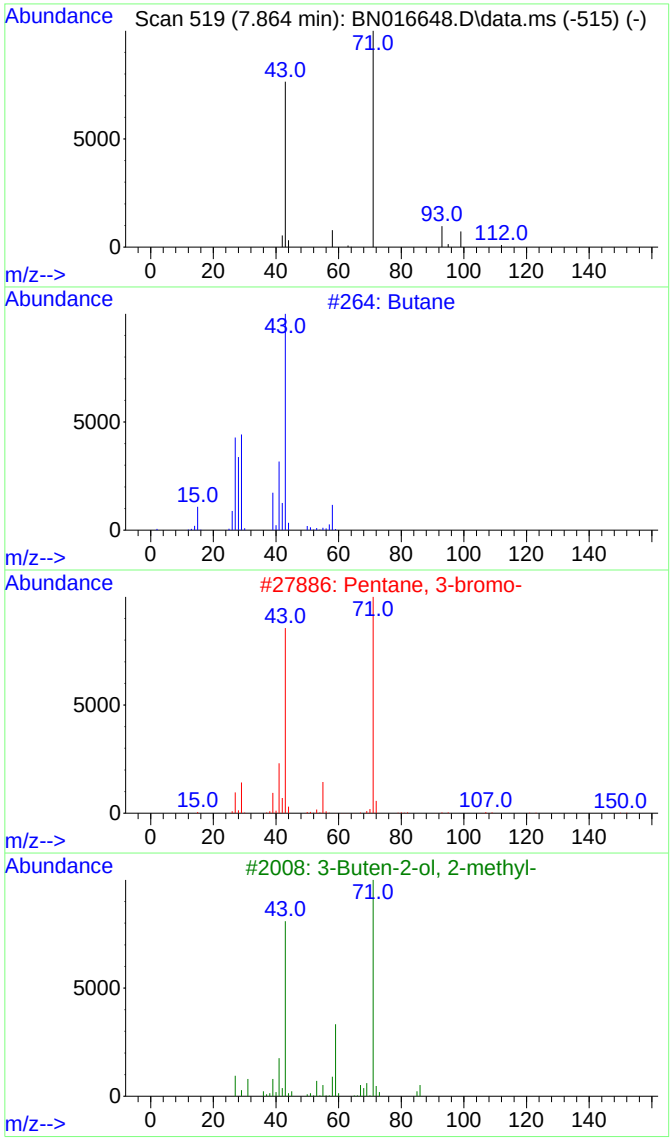
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

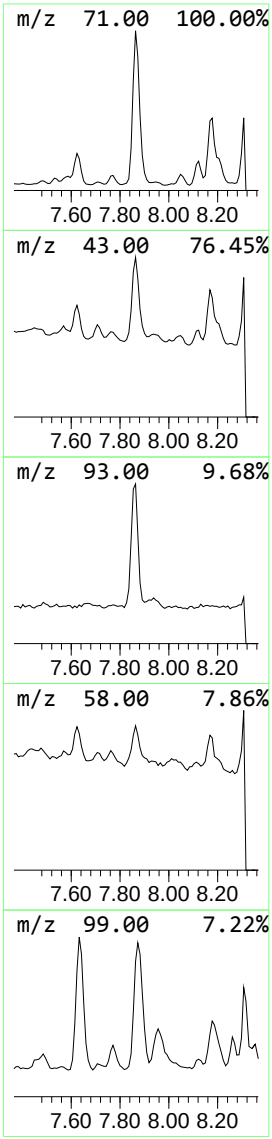
****

Peak Number 6 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.07 ng	15860	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
4	3-Penten-2-ol	86	C5H10O	001569-50-2	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW203D-20210918

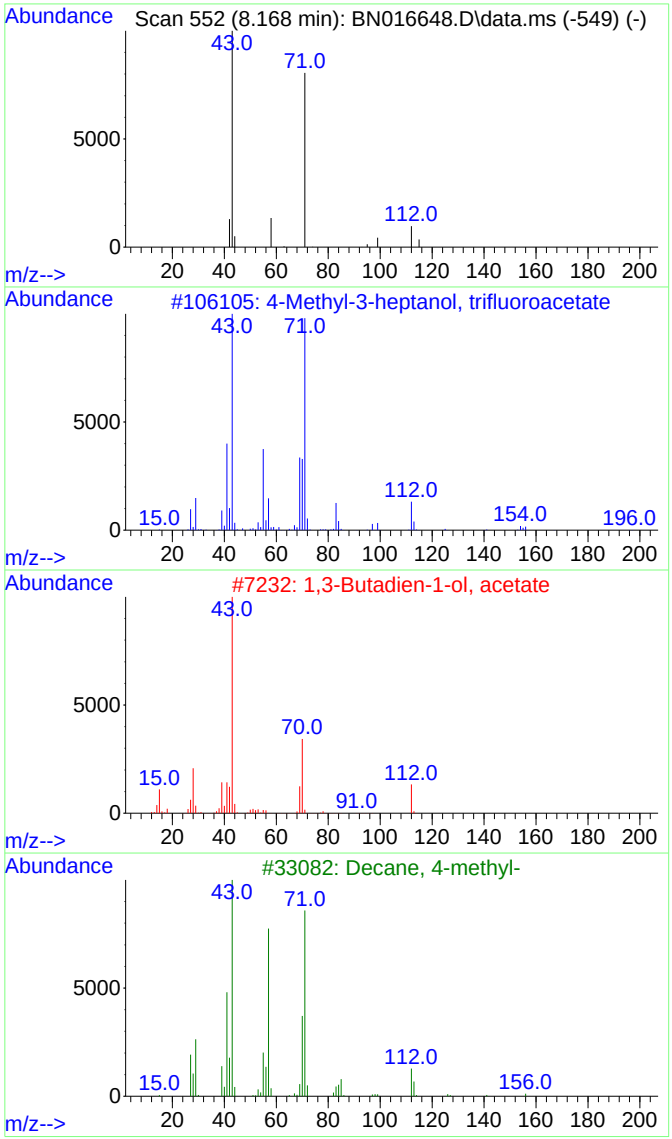
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

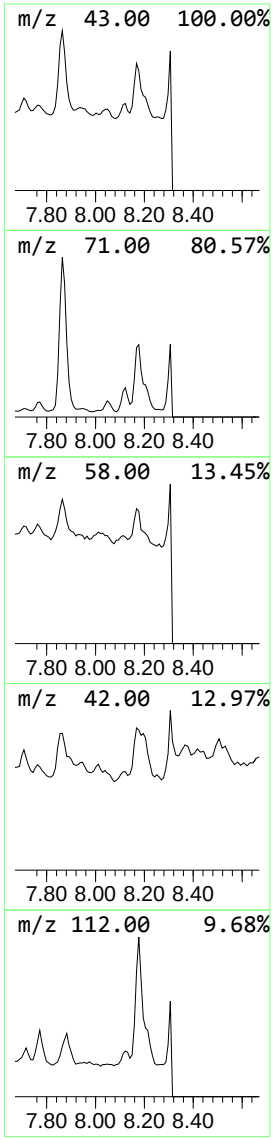
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Methyl-3-heptanol, triflu... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	15437	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	Decane, 4-methyl-	156	C11H24	002847-72-5	9
4	Octane, 3-ethyl-	142	C10H22	005881-17-4	9
5	Butane	58	C4H10	000106-97-8	7





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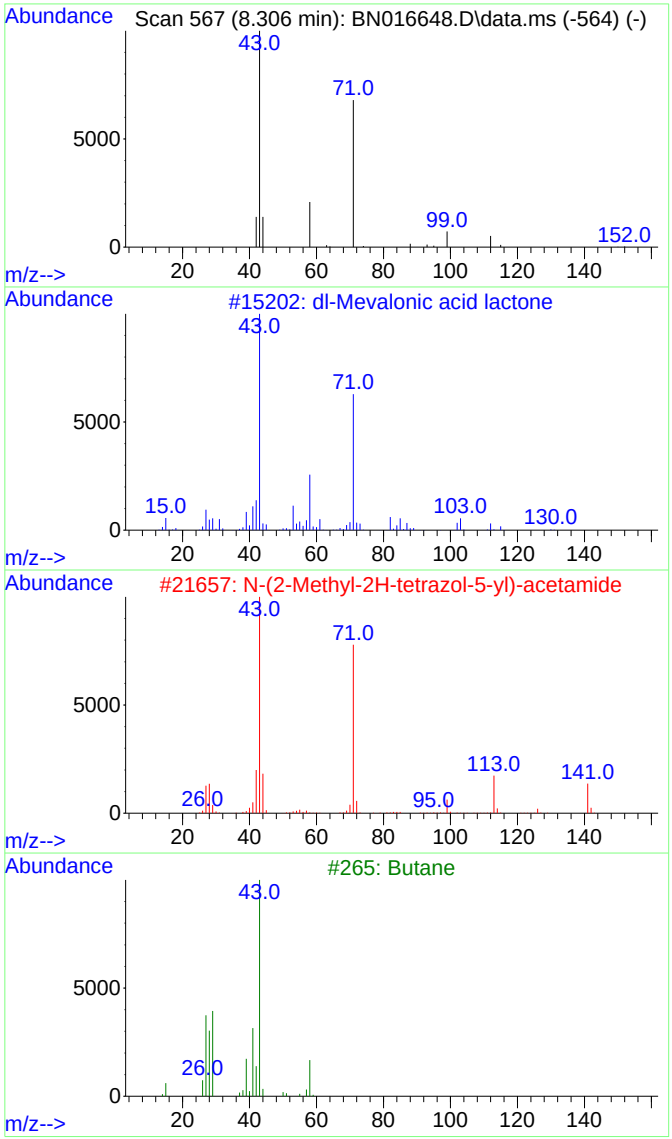
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

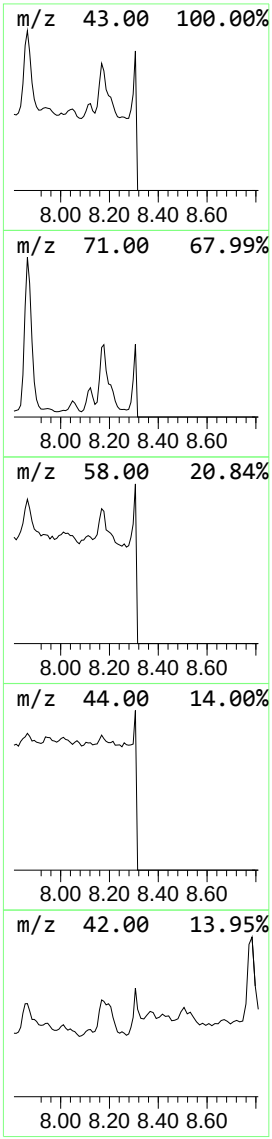
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 dl-Mevalonic acid lactone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.04 ng	10366	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	39
2	N-(2-Methyl-2H-tetrazol-5-yl)-ac...	141	C4H7N5O	006154-06-9	36
3	Butane	58	C4H10	000106-97-8	5
4	Acetone	58	C3H6O	000067-64-1	5
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	5





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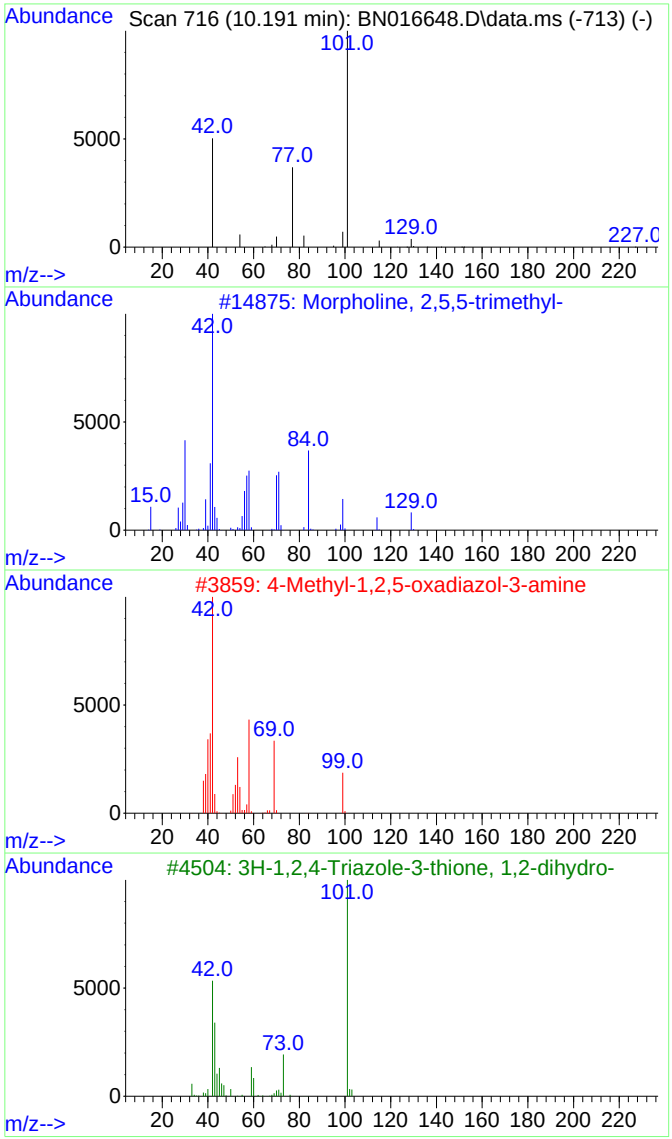
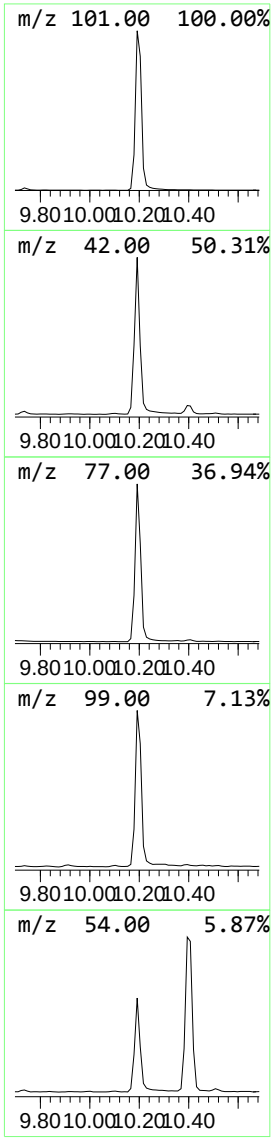
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Morpholine, 2,5,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.45 ng	187473	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
2	4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	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	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016648.D
Acq On : 01 Oct 2021 22:36
Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D-20210918

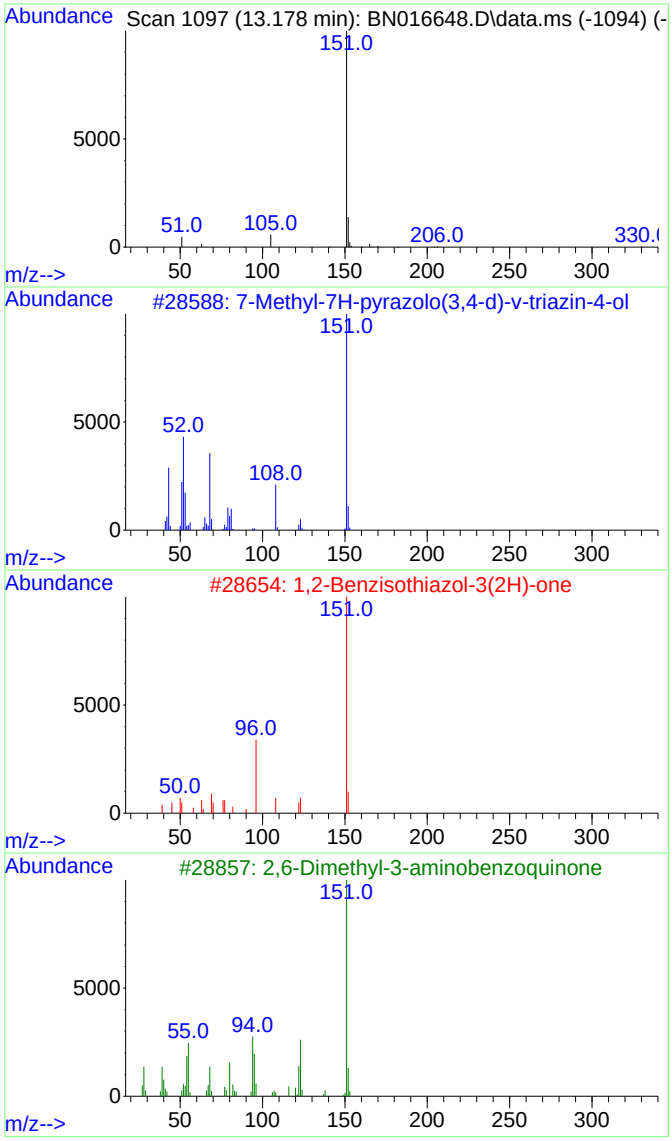
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

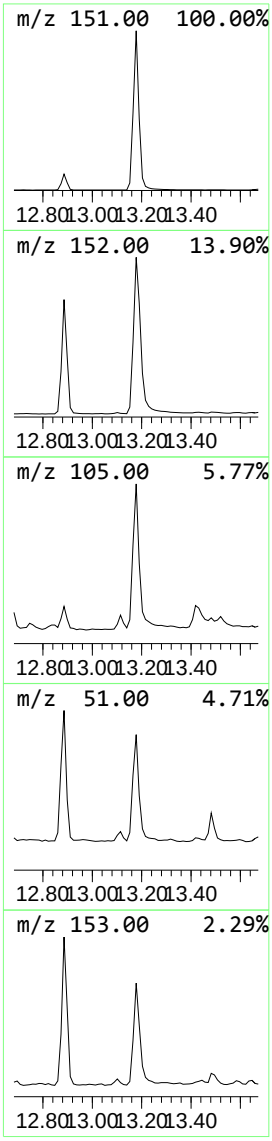
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7-Methyl-7H-pyrazolo(3,4-d)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.13 ng	60361	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
3	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
4	Vanillin	152	C8H8O3	000121-33-5	5
5	Butane-1,3-dione, 1-(pyrrol-2-yl)-	151	C8H9NO2	022441-25-4	5





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016648.D
Acq On : 01 Oct 2021 22:36
Operator : CG/JU
Sample : M3829-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW203D-20210918

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	3.161	0.2	ng	48813	1	7.642	92474	0.4
Hydrogen isocya...	3.364	0.2	ng	50170	1	7.642	92474	0.4
1-Propanol, 2-m...	3.816	0.2	ng	48861	1	7.642	92474	0.4
Butane	4.821	0.4	ng	90085	1	7.642	92474	0.4
Hex-4-enylamine	7.264	0.1	ng	16402	1	7.642	92474	0.4
Butane	7.864	0.1	ng	15860	1	7.642	92474	0.4
4-Methyl-3-hept...	8.168	0.1	ng	15437	1	7.642	92474	0.4
dl-Mevalonic ac...	8.306	0.0	ng	10366	1	7.642	92474	0.4
Morpholine, 2,5...	10.191	0.5	ng	187473	2	10.407	165813	0.4
7-Methyl-7H-pyr...	13.178	0.1	ng	60361	3	14.269	183280	0.4