LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016679.D
Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW203D1-20210918

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: BN016679.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	16413	22364	10.01%	0.775%
2	3.253	16	19	28	rBV	30429	78169	34.99%	2.708%
3	3.364	28	31	46	rVB	38741	120890	54.11%	4.188%
4	3.816	76	80	87	rBV	11699	38313	17.15%	1.327%
5	3.908	87	90	105	rVB2	27280	93959	42.06%	3.255%
6	4.821	185	189	203	rVB	34397	81987	36.70%	2.840%
7	5.263	234	237	245	rVB	7027	18491	8.28%	0.641%
8	5.678	279	282	297	rVB	2187	8707	3.90%	0.302%
9	6.646	383	387	401	rVV	3818	10121	4.53%	0.351%
10	6.822	403	406	418	rVB	5494	15010	6.72%	0.520%
11	7.264	450	454	460	rBV2	7671	17595	7.88%	0.609%
12	7.633	490	494	500	rVB	51467	108630	48.63%	3.763%
13	7.864	515	519	525	rBV	8919	18367	8.22%	0.636%
14	8.168	549	552	560	rVV	5286	16428	7.35%	0.569%
15	8.306	564	567	569	rVB	8982	11088	4.96%	0.384%
16	8.784	601	605	610	rBV	23654	47595	21.31%	1.649%
17	10.191	713	716	727	rBV	118452	204161	91.39%	7.072%
18	10.407	729	733	736	rBV	112645	192679	86.25%	6.674%
19	12.003	920	931	942	rBV	44628	72526	32.46%	2.512%
20	12.886	1071	1074	1078	rBV	92426	156864	70.22%	5.434%
21	13.177	1094	1097	1106	rBV	68981	109322	48.94%	3.787%
22	14.269	1180	1183	1186	rBV	147393	213038	95.36%	7.380%
23	14.434	1193	1196	1201	rBV	4157	8167	3.66%	0.283%
24	15.715	1294	1297	1299	rBV	8739	12792	5.73%	0.443%
25	15.766	1299	1301	1307	rVB2	12826	20998	9.40%	0.727%
26	17.017	1400	1403	1409	rBV	114616	178121	79.73%	6.170%
27	17.723	1457	1461	1468	rBV2	3238	7166	3.21%	0.248%
28	18.015	1483	1485	1495	rVB5	2333	3752	1.68%	0.130%
29	19.063	1687	1696	1716	rBV	156930	223398	100.00%	7.738%
30	19.241	1727	1732	1745	rBV	1973	3004	1.34%	0.104%
31	19.430	1765	1770	1782	rVB	5333	7998	3.58%	0.277%
32	19.678	1813	1820	1841	rBV	137345	181030	81.03%	6.271%
33	20.006	1885	1886	1890	rBV3	2633	6972	3.12%	0.242%
34	20.070	1890	1892	1897	rVV	4803	9064	4.06%	0.314%
35	20.378	1919	1921	1924	rBV	3984	6094	2.73%	0.211%
36	20.994	1976	1979	1980	rBV2	3549	7510	3.36%	0.260%

LSC Area Percent Report

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Misc :
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Instrument : BNA_N
ClientSampleId : MW203D1-20210918

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	21.025	1980	1982	1992	rVB	4285	8838	3.96%	0.306%
38	21.164	1993	1995	1998	rBV	35421	45121	20.20%	1.563%
39	21.227	1998	2001	2010	rVB	138644	212354	95.06%	7.356%
40	22.311	2100	2103	2108	rBV	4376	9861	4.41%	0.342%
41	22.841	2232	2239	2261	rVB	4142	6629	2.97%	0.230%
42	23.341	2378	2385	2397	rVB	2341	4129	1.85%	0.143%
43	23.423	2400	2409	2415	rVV	5609	9621	4.31%	0.333%
44	23.481	2415	2426	2474	rVB	109105	220993	98.92%	7.655%
45	24.083	2593	2602	2618	rBV	6142	11969	5.36%	0.415%
46	24.853	2817	2827	2847	rVB2	5392	12439	5.57%	0.431%
47	25.757	3074	3091	3114	rBV	1815	5304	2.37%	0.184%
48	26.818	3383	3401	3426	rBV	1296	4661	2.09%	0.161%
49	28.085	3751	3771	3796	rBV2	671	2558	1.15%	0.089%

Sum of corrected areas: 2886847

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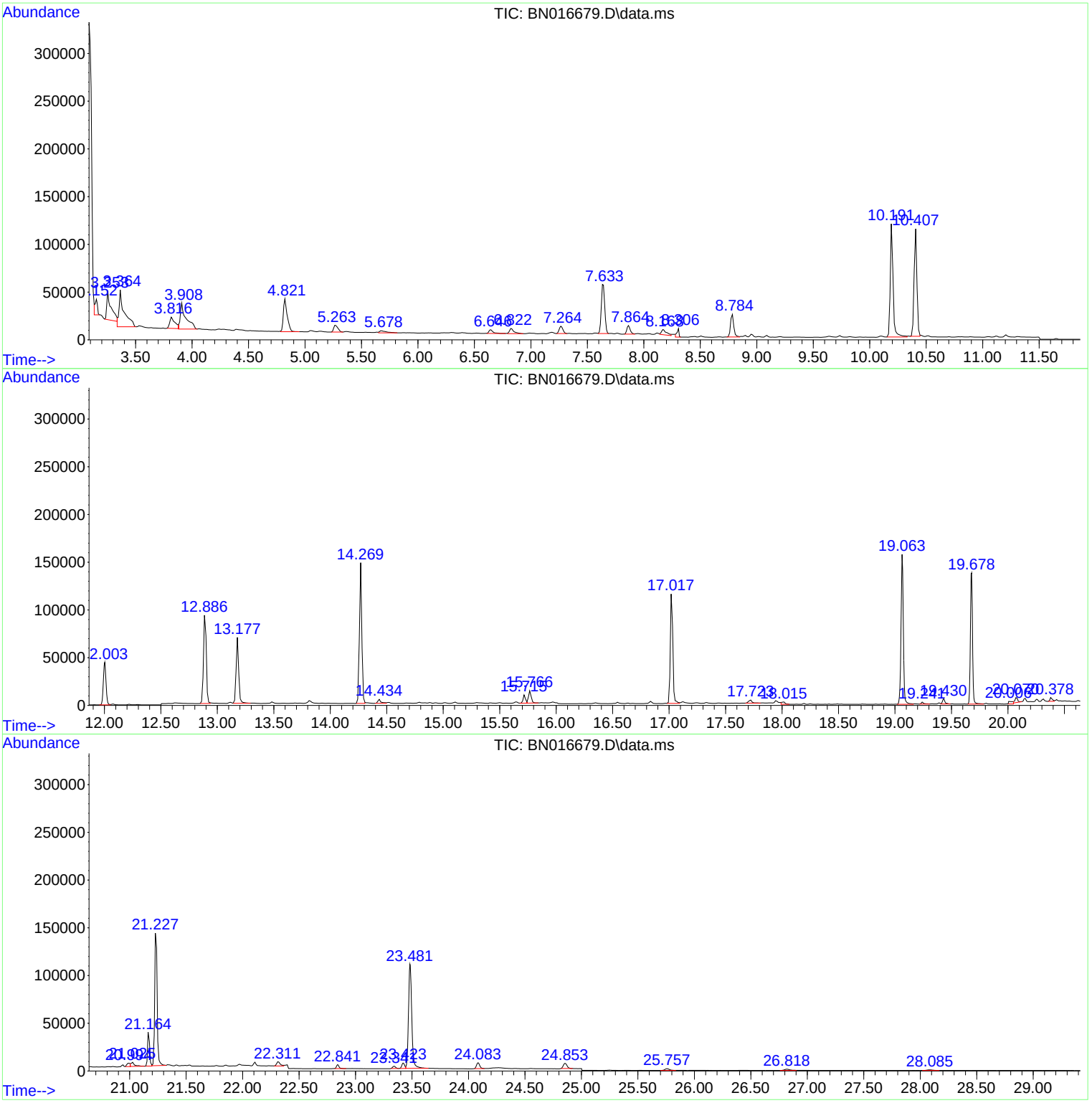
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

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 : BN016679.D
Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

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

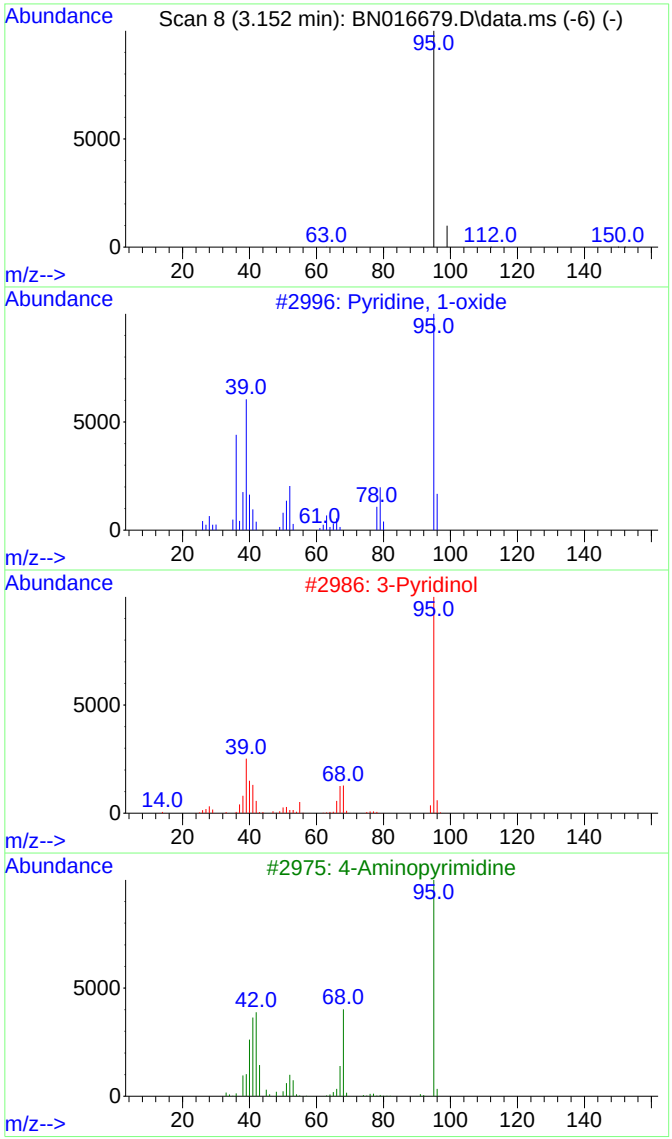
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

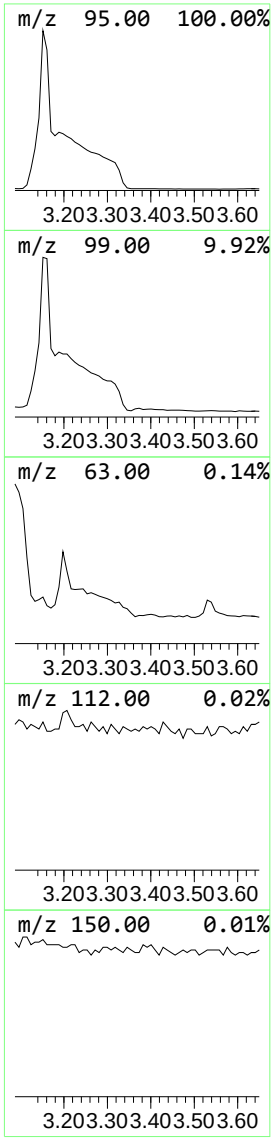
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.08 ng	22364	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016679.D
Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

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

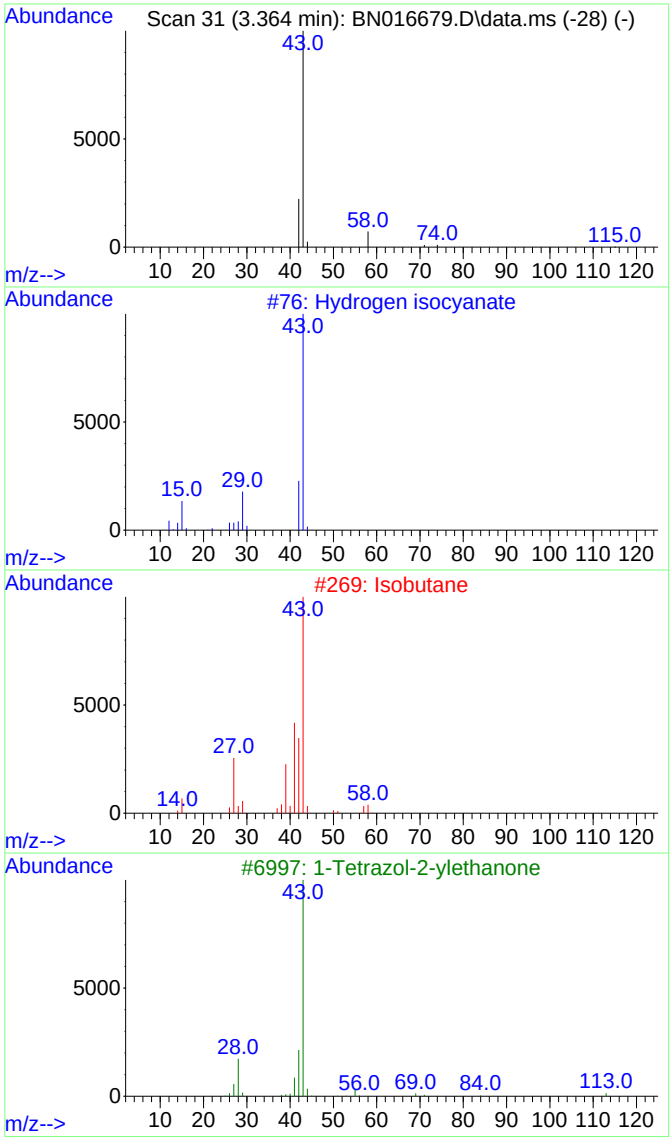
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

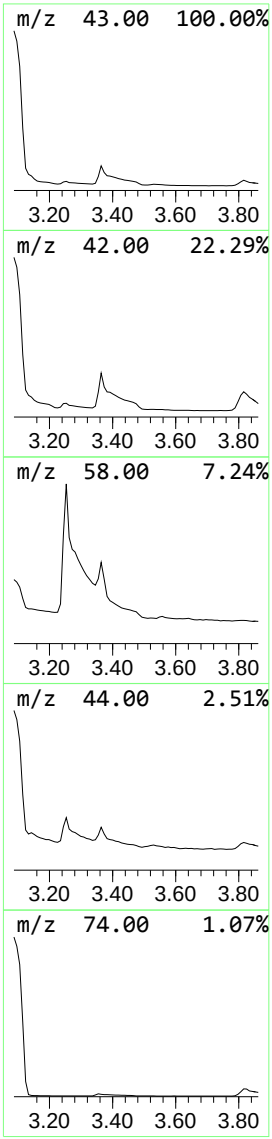
****

Peak Number 2 Hydrogen isocyanate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.45 ng	120890	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	Isobutane	58	C4H10	000075-28-5	3
3	1-Tetrazol-2-ylethanone	112	C3H4N4O	051410-11-8	2
4	Hydrogen azide	43	HN3	007782-79-8	2
5	Butane	58	C4H10	000106-97-8	2





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Data File : BN016679.D
Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

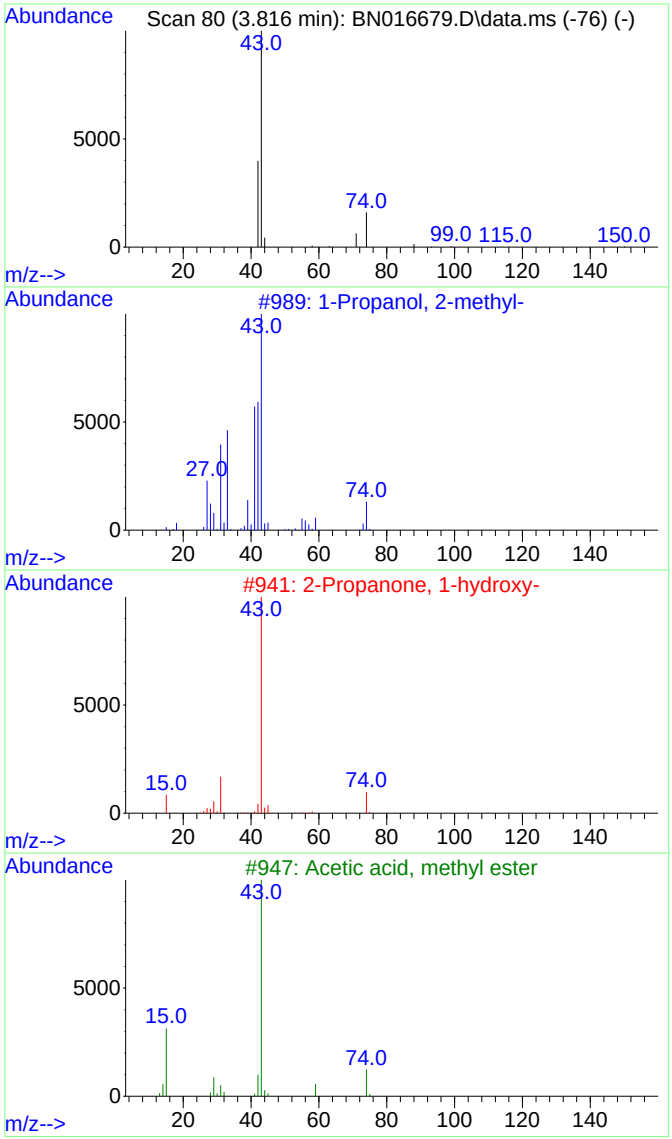
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

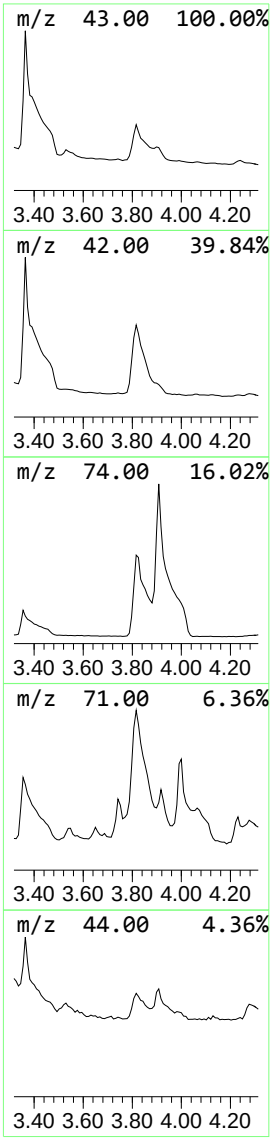
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.14 ng	38313	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	5
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	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

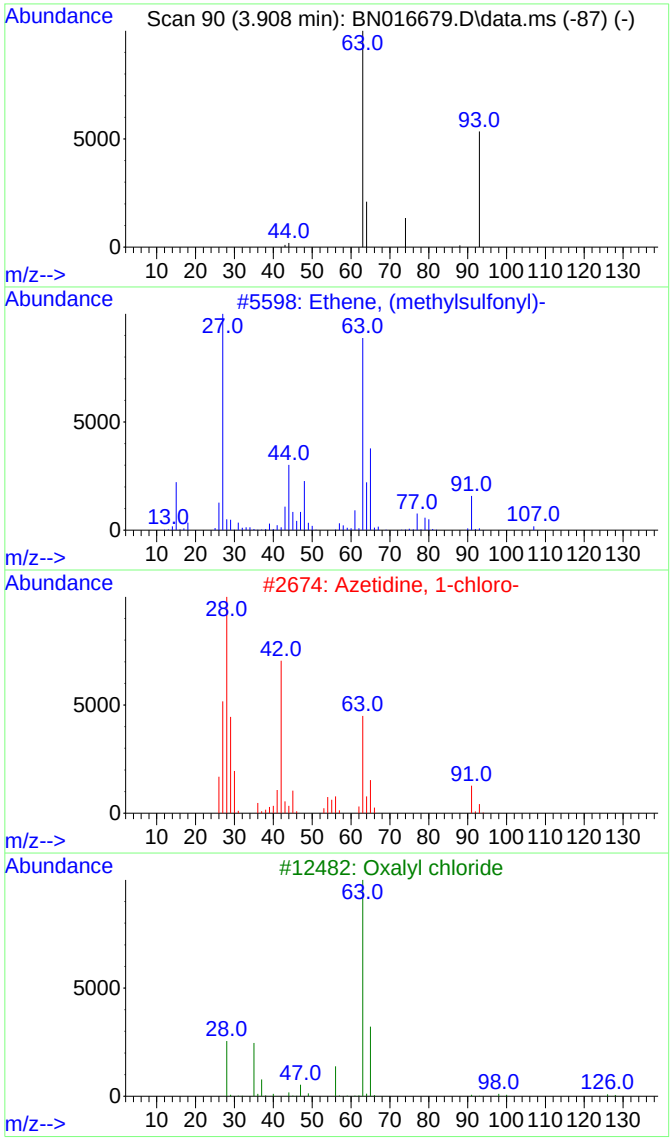
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

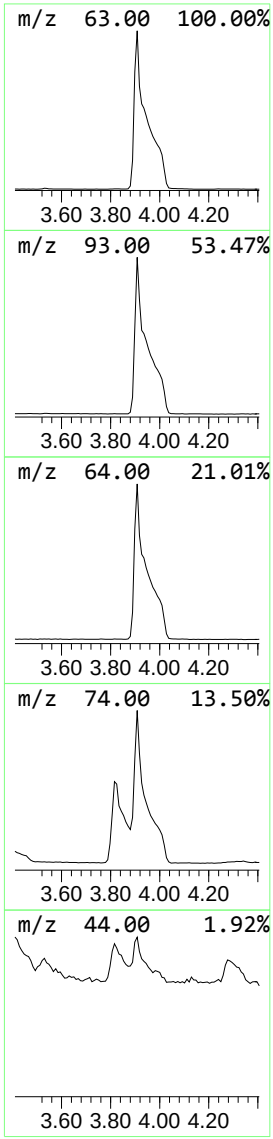
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethene, (methylsulfonyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.908	0.35 ng	93959	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	2
2	Azetidine, 1-chloro-	91	C3H6ClN	032115-53-0	2
3	Oxalyl chloride	126	C2Cl2O2	000079-37-8	1
4	Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
5	2-Propanol, 1-chloro-3-fluoro-	112	C3H6ClFO	189937-18-6	1





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Misc :
ALS Vial : 47 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
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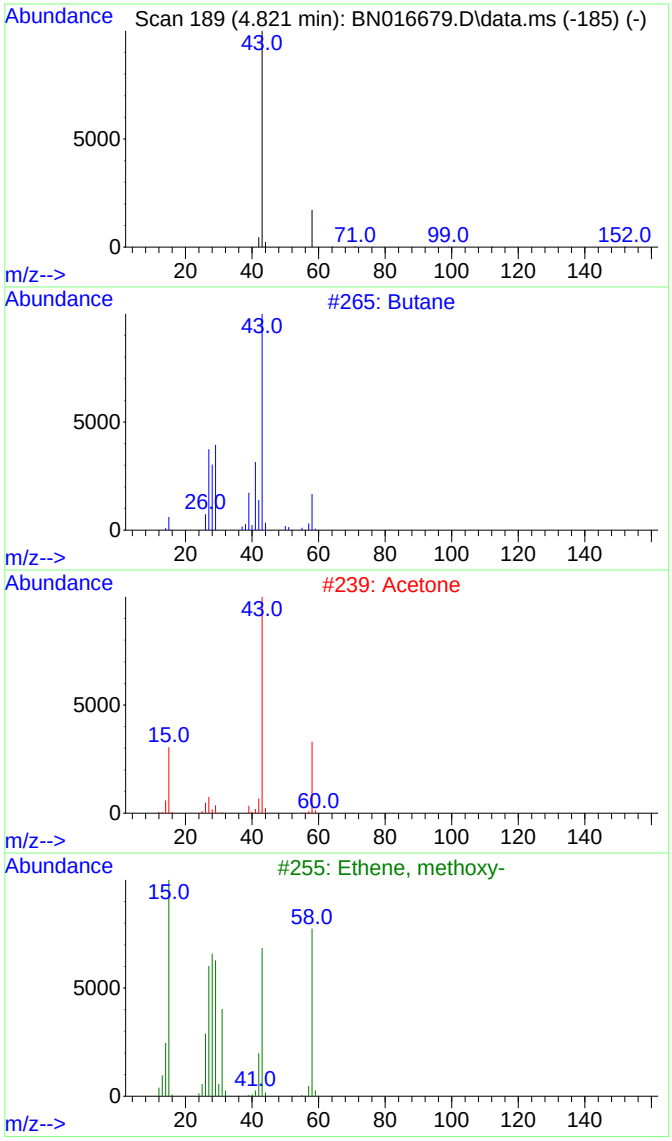
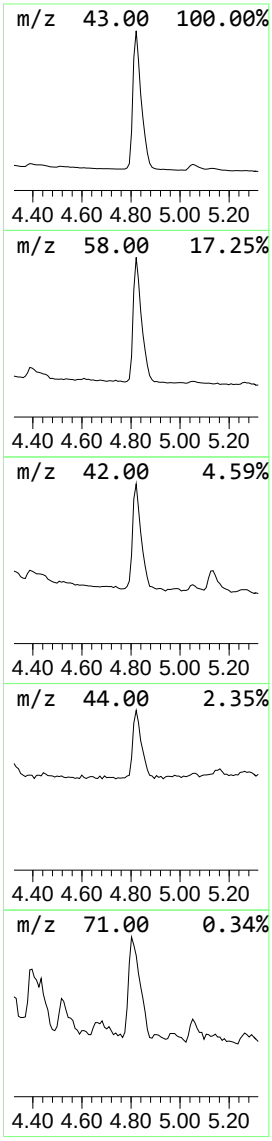
****

Peak Number 5 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.30 ng	81987	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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Instrument :
BNA_N
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MW203D1-20210918

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

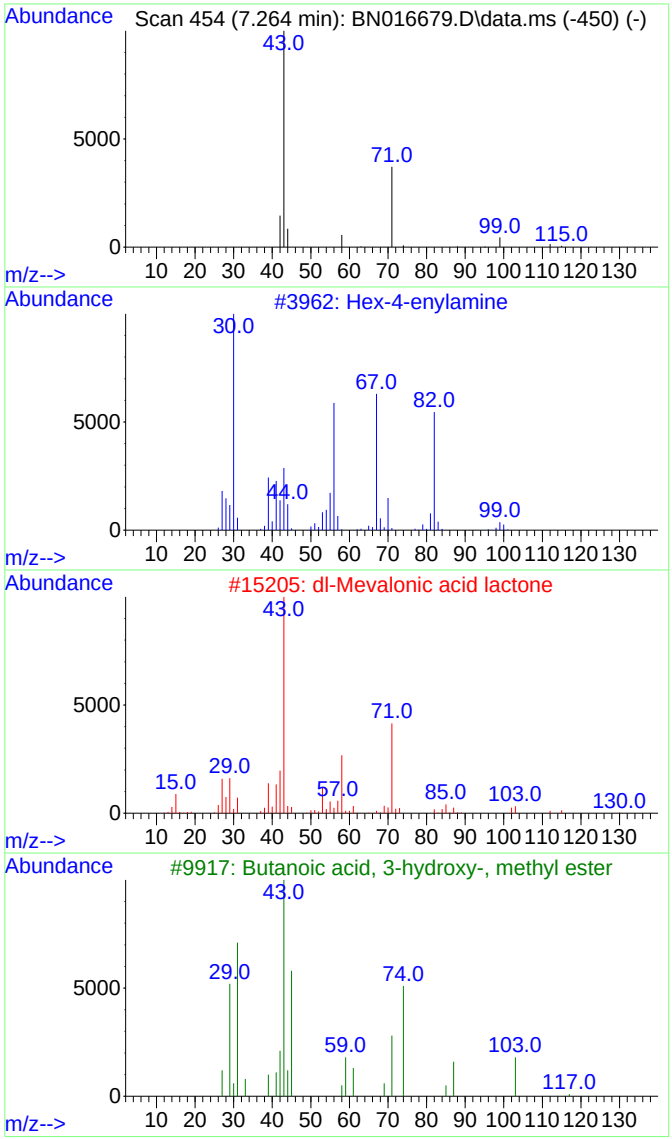
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

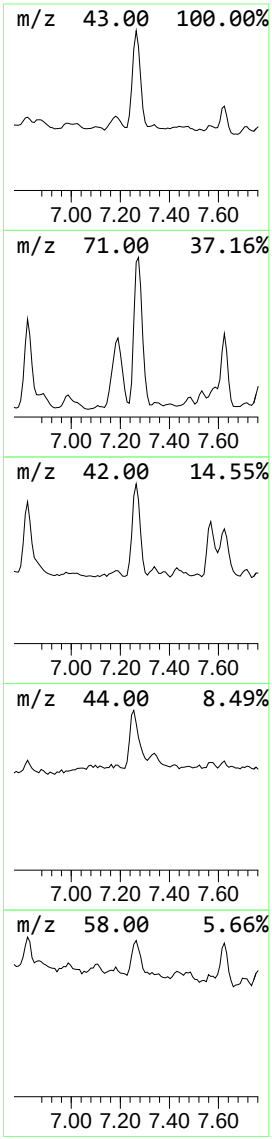
****

Peak Number 6 Hex-4-enylamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	17595	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	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	4
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4





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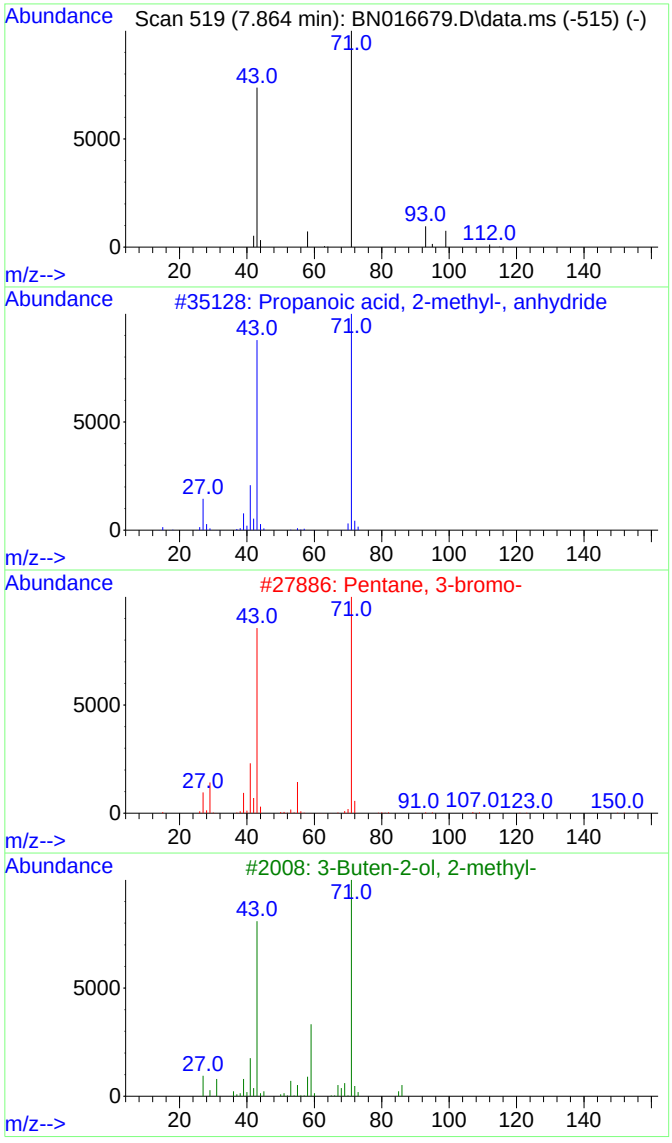
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

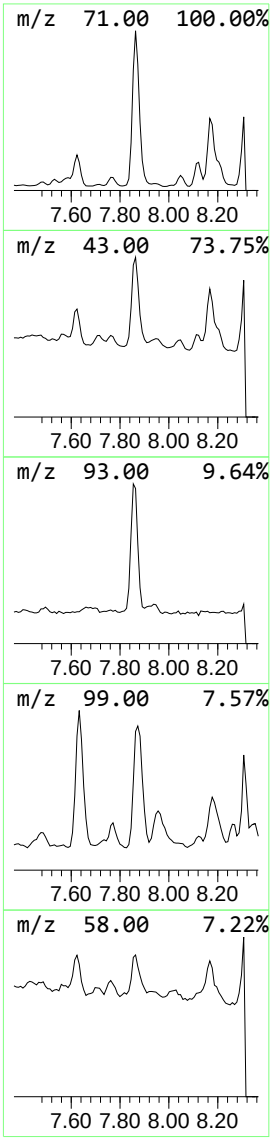
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.07 ng	18367	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	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-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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Data File : BN016679.D
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Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

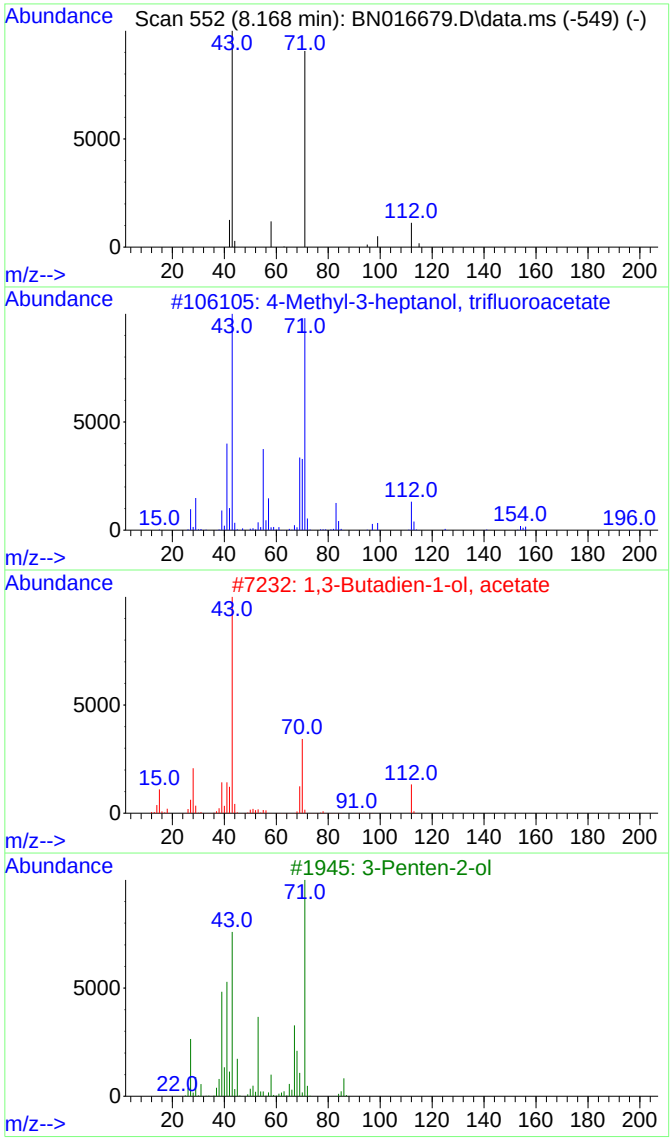
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

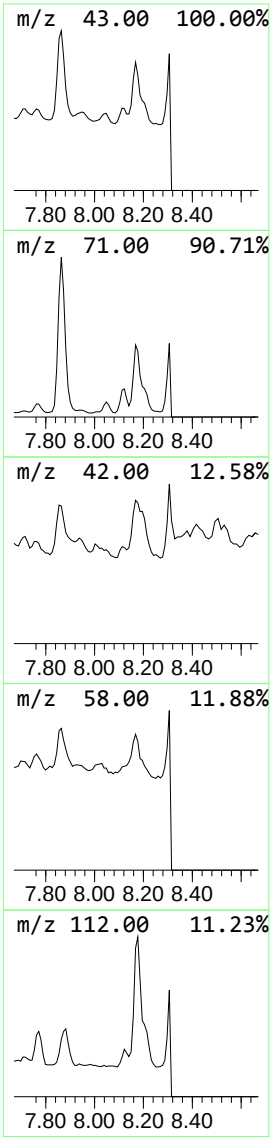
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Methyl-3-heptanol, triflu... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.06 ng	16428	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	43
2	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3	3-Penten-2-ol	86	C5H10O	001569-50-2	9
4	Decane, 4-methyl-	156	C11H24	002847-72-5	9
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	9





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Data File : BN016679.D
Acq On : 02 Oct 2021 20:09
Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

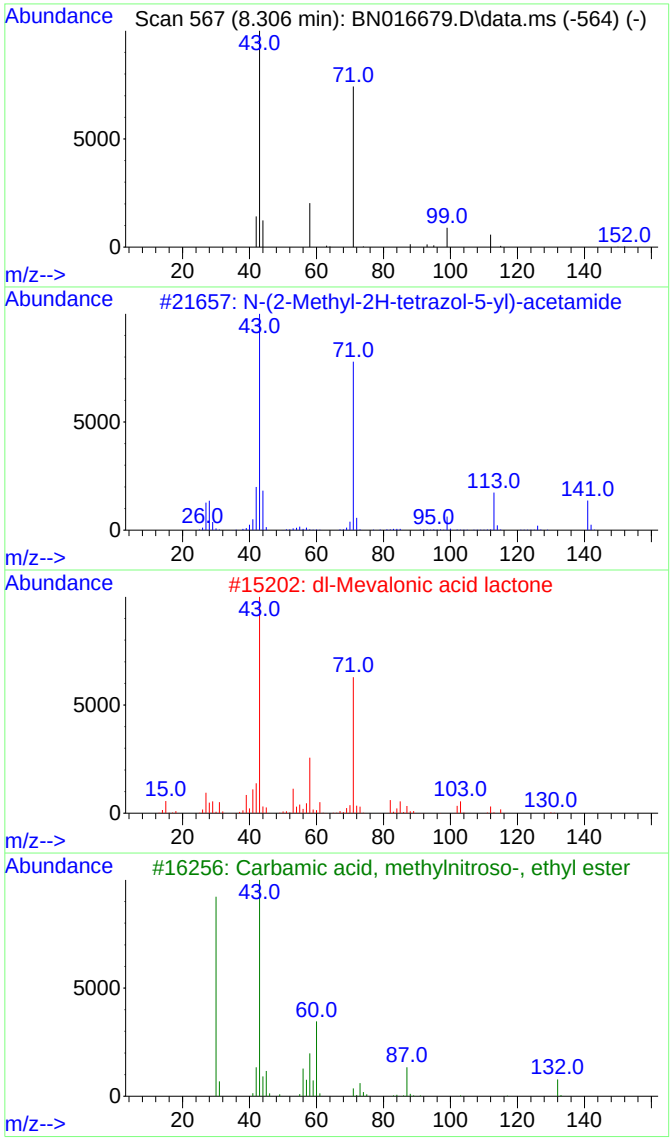
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

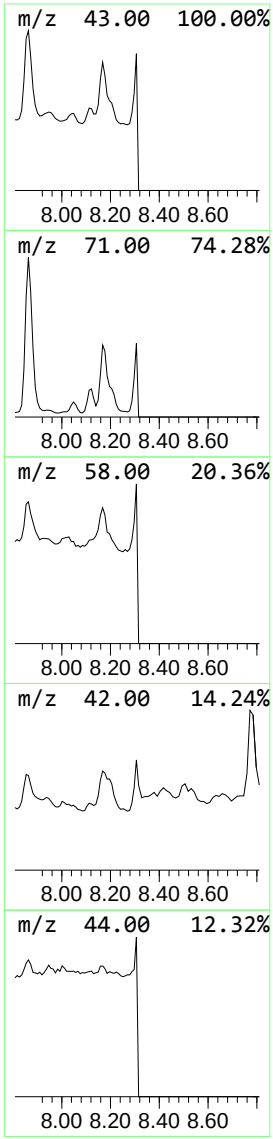
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 N-(2-Methyl-2H-tetrazol-5-y... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.04 ng	11088	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(2-Methyl-2H-tetrazol-5-yl)-ac...	141	C4H7N5O	006154-06-9	39
2	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	9
3	Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9
4	Butane	58	C4H10	000106-97-8	5
5	Acetone	58	C3H6O	000067-64-1	5





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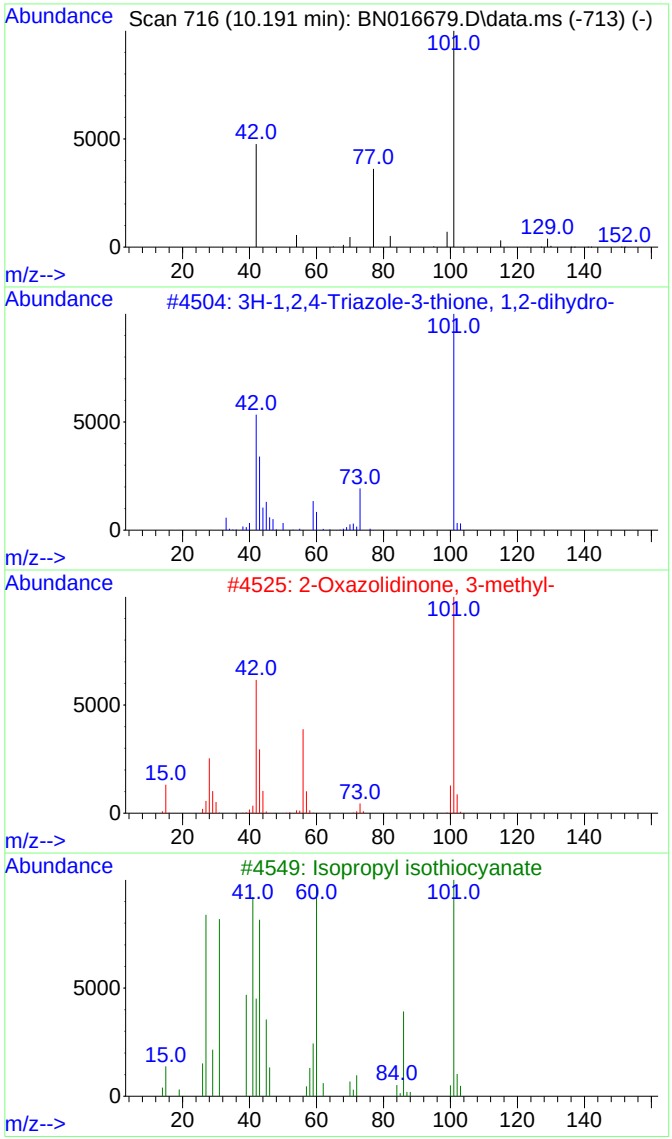
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

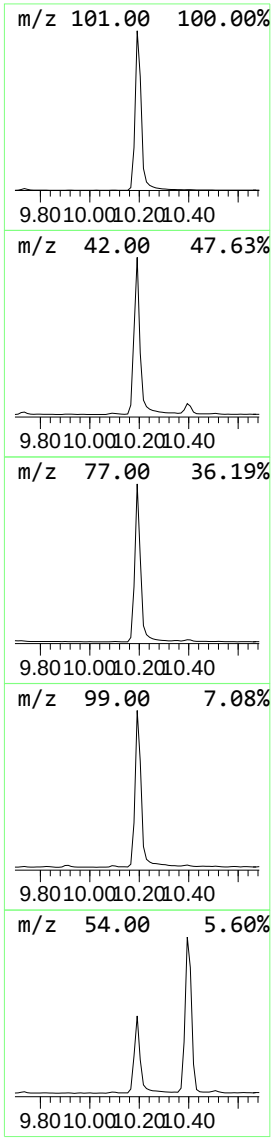
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3H-1,2,4-Triazole-3-thione,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.42 ng	204161	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	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





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Operator : CG/JU
Sample : M3829-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D1-20210918

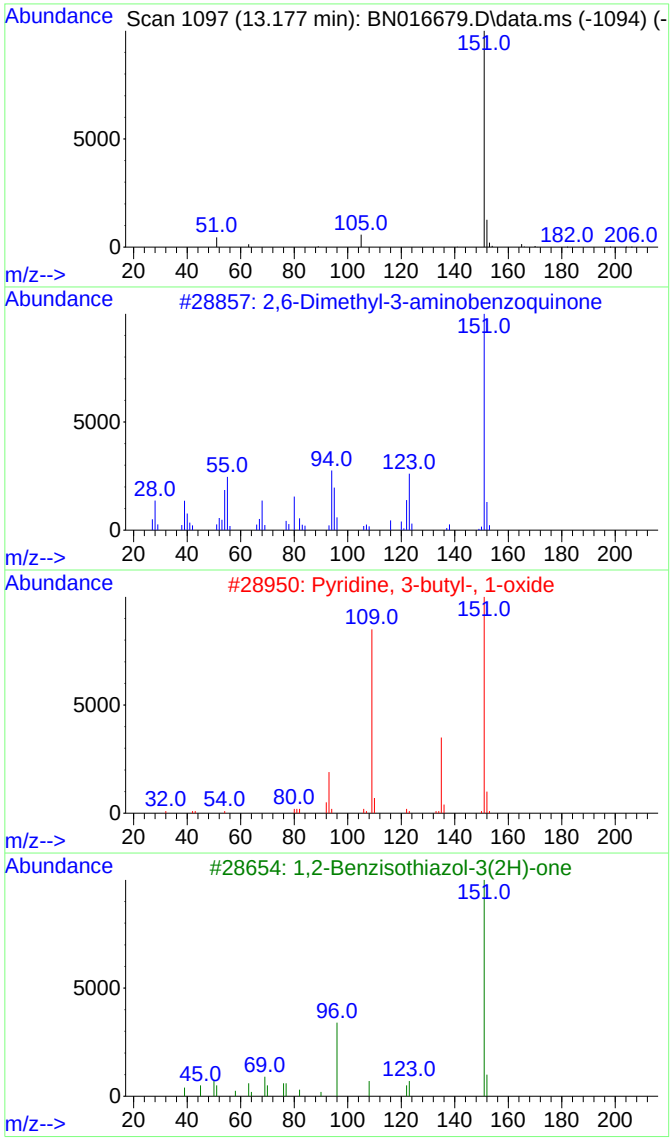
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

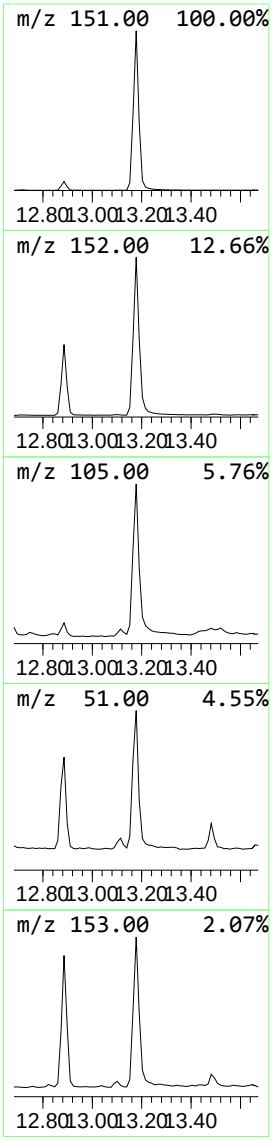
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.21 ng	109322	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
5	Carbamic acid, phenyl-, methyl e...	151	C8H9NO2	002603-10-3	7





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	3.152	0.1	ng	22364	1	7.642	108630	0.4
Hydrogen isocya...	3.364	0.4	ng	120890	1	7.642	108630	0.4
1-Propanol, 2-m...	3.816	0.1	ng	38313	1	7.642	108630	0.4
Ethene, (methyl...	3.908	0.3	ng	93959	1	7.642	108630	0.4
Butane	4.821	0.3	ng	81987	1	7.642	108630	0.4
Hex-4-enylamine	7.264	0.1	ng	17595	1	7.642	108630	0.4
Propanoic acid,...	7.864	0.1	ng	18367	1	7.642	108630	0.4
4-Methyl-3-hept...	8.168	0.1	ng	16428	1	7.642	108630	0.4
N-(2-Methyl-2H-...	8.306	0.0	ng	11088	1	7.642	108630	0.4
3H-1,2,4-Triazo...	10.191	0.4	ng	204161	2	10.406	192679	0.4
2,6-Dimethyl-3-...	13.178	0.2	ng	109322	3	14.269	213038	0.4