LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

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: BN016640.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.364	28	31	47	rVB	29890	96671	32.23%	3.421%
2	3.816	76	80	97	rVB	12730	50754	16.92%	1.796%
3	4.240	123	126	140	rVB	21240	66793	22.27%	2.363%
4	4.821	185	189	205	rVB	134812	299952	100.00%	10.613%
5	5.116	217	221	231	rVB2	4958	14645	4.88%	0.518%
6	5.273	234	238	247	rVB	7539	20211	6.74%	0.715%
7	6.296	345	349	354	rVV	9583	19242	6.42%	0.681%
8	6.370	354	357	367	rVB2	2339	6337	2.11%	0.224%
9	6.647	384	387	397	rVB	3439	7512	2.50%	0.266%
10	6.850	403	409	418	rVB2	7823	25015	8.34%	0.885%
11	7.265	450	454	460	rVB	6800	14988	5.00%	0.530%
12	7.643	490	495	500	rBV	46544	93531	31.18%	3.309%
13	7.707	500	502	506	rVB	2583	4087	1.36%	0.145%
14	7.864	516	519	526	rVB	3662	7375	2.46%	0.261%
15	8.306	565	567	569	rVB	5371	5074	1.69%	0.180%
16	8.785	601	605	611	rBV	30990	58743	19.58%	2.079%
17	10.191	713	716	722	rBV	31479	53982	18.00%	1.910%
18	10.407	729	733	737	rBV	99625	173821	57.95%	6.150%
19	11.205	794	796	802	rBV2	3205	8117	2.71%	0.287%
20	12.003	921	931	943	rBV	48990	79641	26.55%	2.818%
21	12.899	1071	1075	1078	rBV	89471	165356	55.13%	5.851%
22	14.269	1180	1183	1186	rBV	130533	193439	64.49%	6.845%
23	14.434	1193	1196	1198	rBV	4797	6839	2.28%	0.242%
24	15.766	1299	1301	1308	rVB2	14032	22611	7.54%	0.800%
25	17.018	1400	1403	1410	rBV	92324	158248	52.76%	5.599%
26	17.943	1477	1479	1483	rBV2	2492	5649	1.88%	0.200%
27	19.063	1689	1696	1707	rBV	135036	186436	62.16%	6.597%
28	19.212	1711	1726	1728	rBV2	10383	33421	11.14%	1.183%
29	19.679	1813	1820	1841	rVB	124700	162573	54.20%	5.752%
30	20.017	1884	1887	1904	rBV	15558	81214	27.08%	2.874%
31	20.760	1948	1957	1972	rBV	38436	212541	70.86%	7.520%
32	20.973	1974	1977	1980	rVV	5262	8414	2.81%	0.298%
33	21.164	1992	1995	1998	rBV	35162	44431	14.81%	1.572%
34	21.228	1998	2001	2011	rVB	128453	189662	63.23%	6.711%
35	22.109	2081	2084	2087	rBV	3388	4990	1.66%	0.177%
36	22.396	2109	2111	2112	rVB	7799	9636	3.21%	0.341%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

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	2233	2239	2249	rVB	4313	6478	2.16%	0.229%
38	23.420	2400	2408	2414	rBV	5831	9201	3.07%	0.326%
39	23.481	2415	2426	2464	rVB	92044	180553	60.19%	6.389%
40	24.084	2594	2602	2617	rVB2	6669	12449	4.15%	0.440%
41	24.854	2818	2827	2848	rVB2	6458	14726	4.91%	0.521%
42	25.754	3078	3090	3107	rVB	2054	5515	1.84%	0.195%
43	26.822	3386	3402	3422	rBV2	1611	5318	1.77%	0.188%

Sum of corrected areas: 2826191

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
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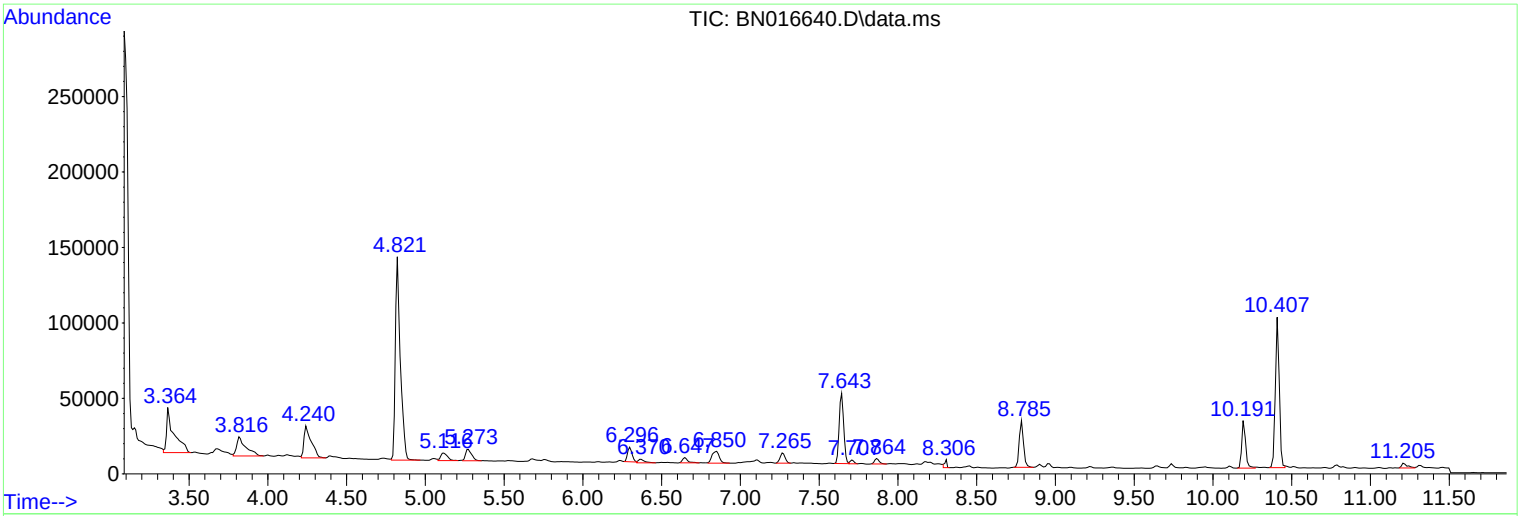
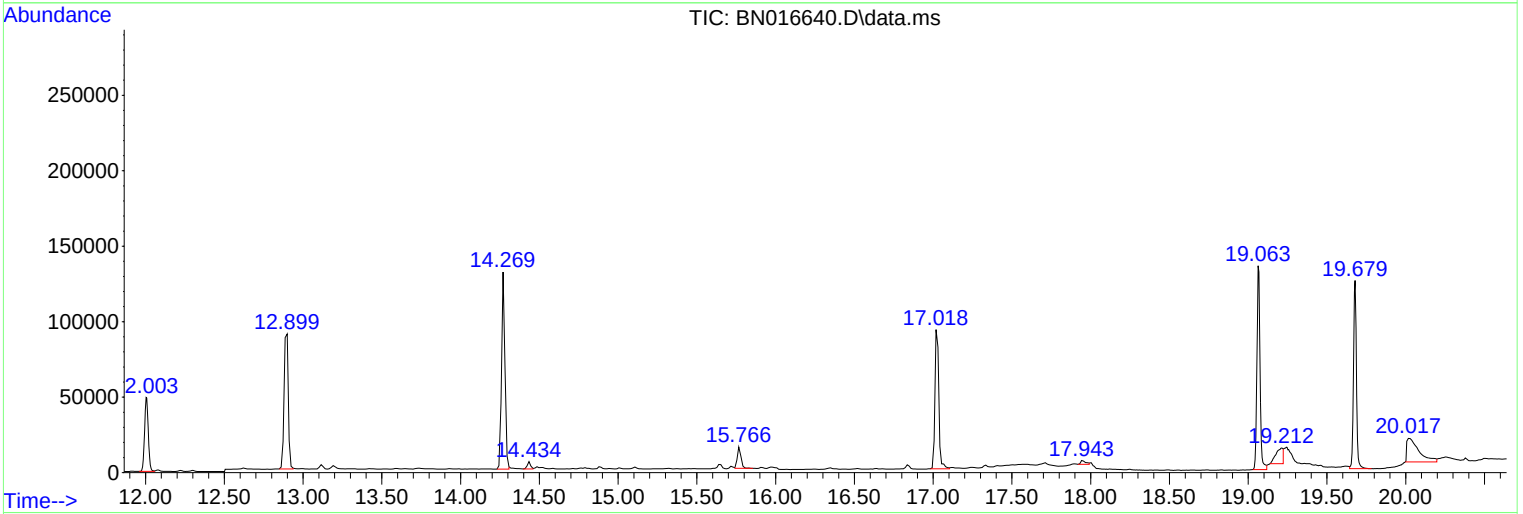
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

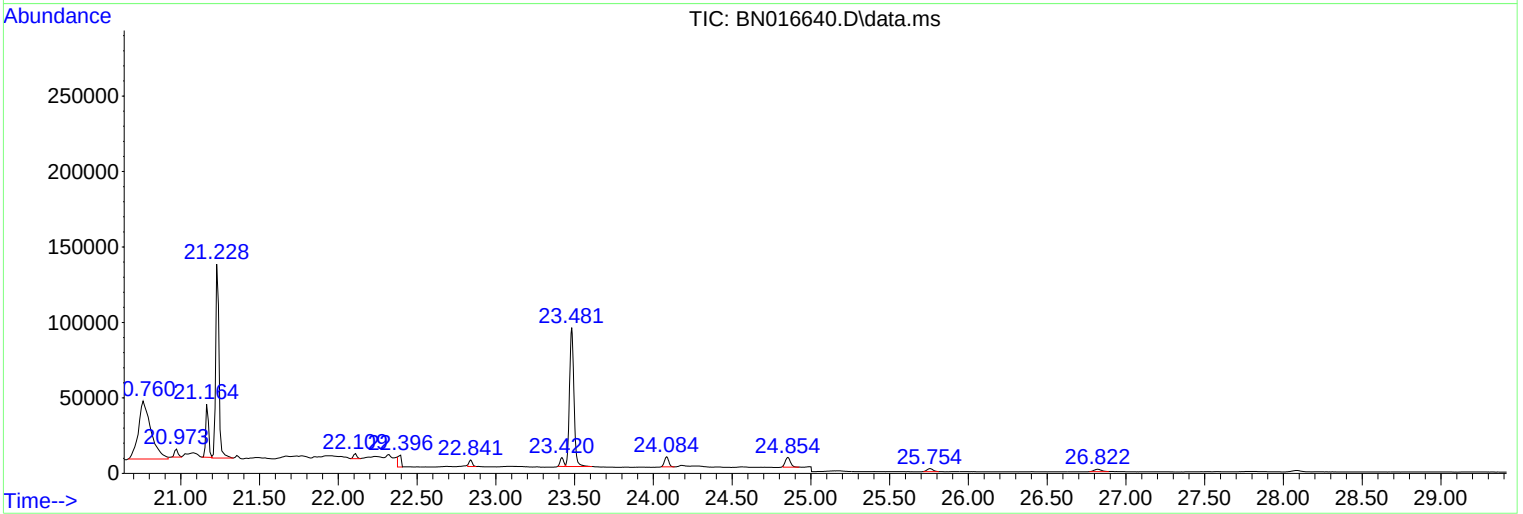
Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

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 : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

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

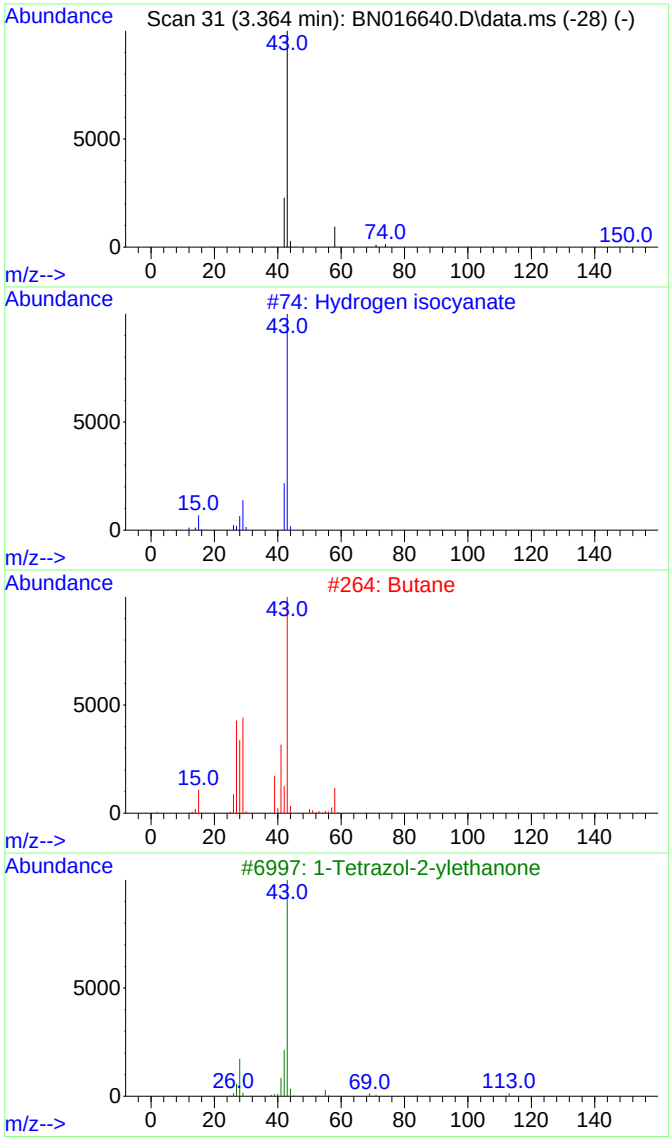
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

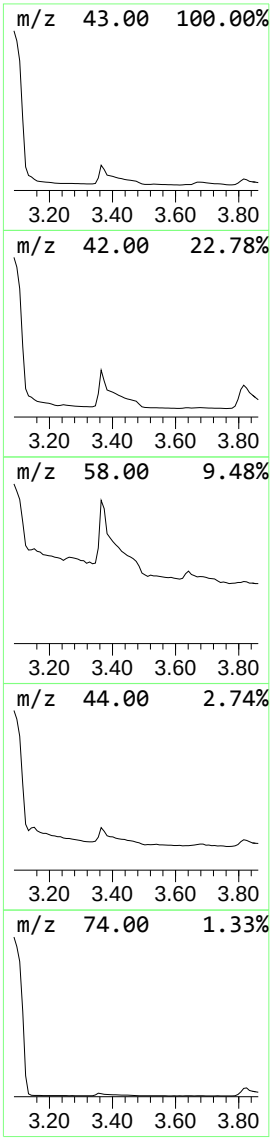
****

Peak Number 1 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.41 ng	96671	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-Tetrazol-2-ylethanone	112	C3H4N4O	051410-11-8	2
4	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	2
5	Hydrogen azide	43	HN3	007782-79-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

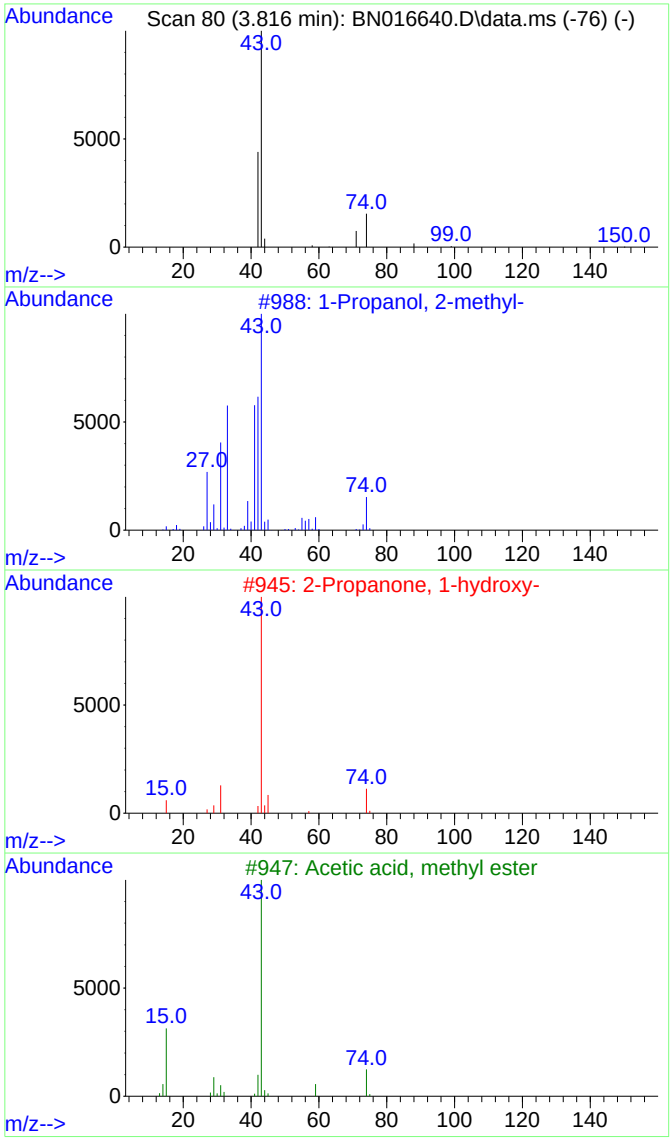
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

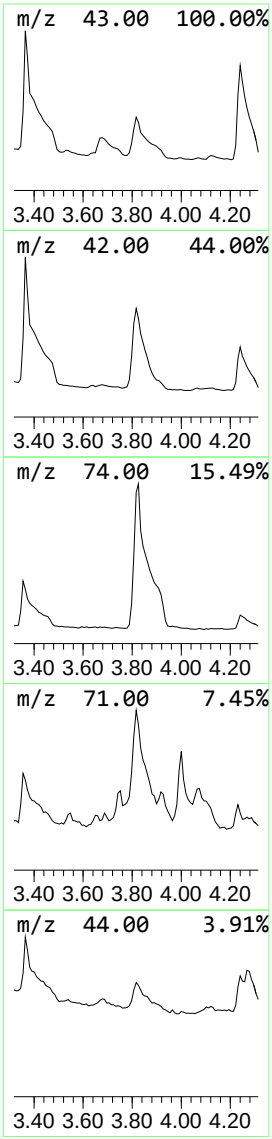
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.22 ng	50754	1,4-Dichlorobenzene-d4	7.643

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	1,4-Butanediamine	88	C4H12N2	000110-60-1	3
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

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

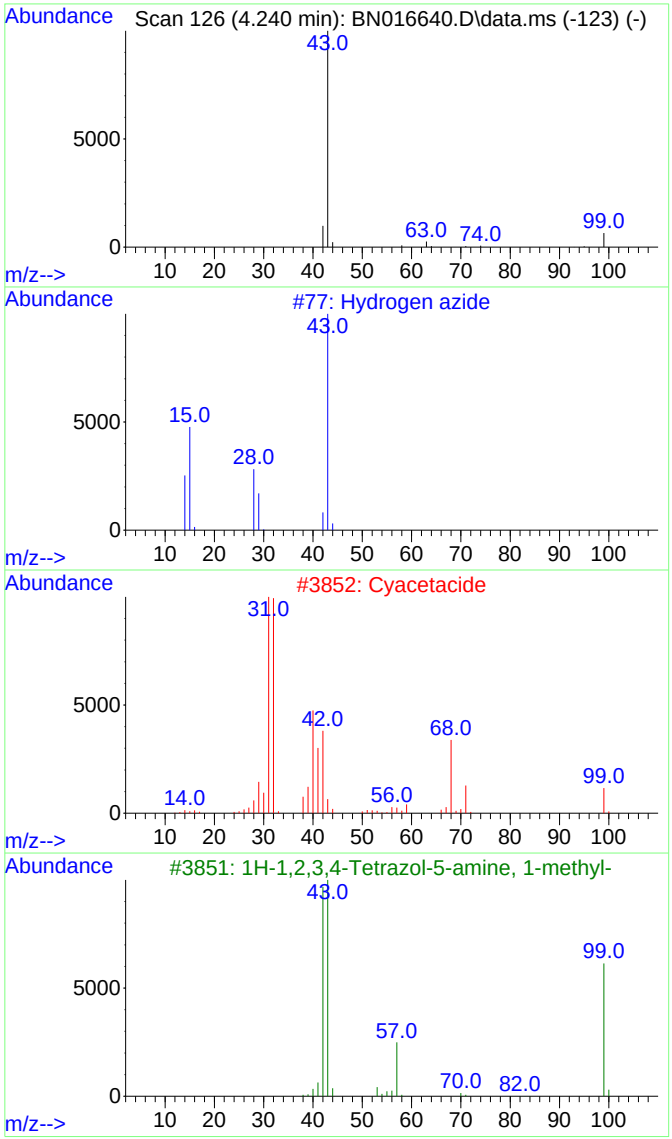
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

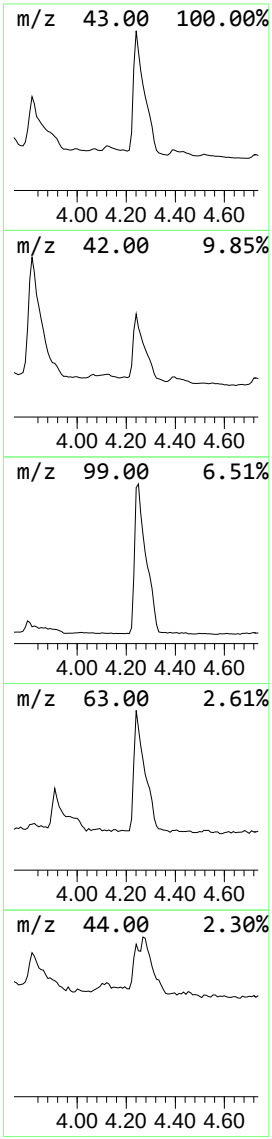
****

Peak Number 3 Hydrogen azide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	0.29 ng	66793	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	Cyacetacide	99	C3H5N3O	000140-87-4	3
3	1H-1,2,3,4-Tetrazol-5-amine, 1-m...	99	C2H5N5	005422-44-6	3
4	Hydrogen isocyanate	43	CHNO	000075-13-8	2
5	4-Methyl-pent-3-enylamine	99	C6H13N	013296-28-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

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

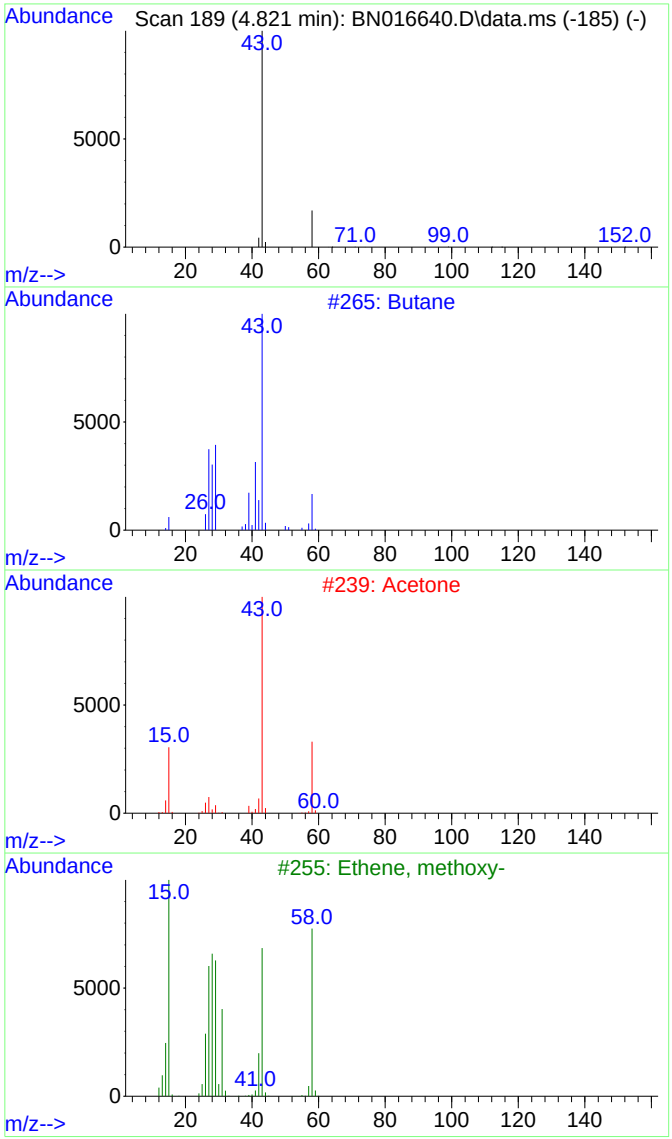
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

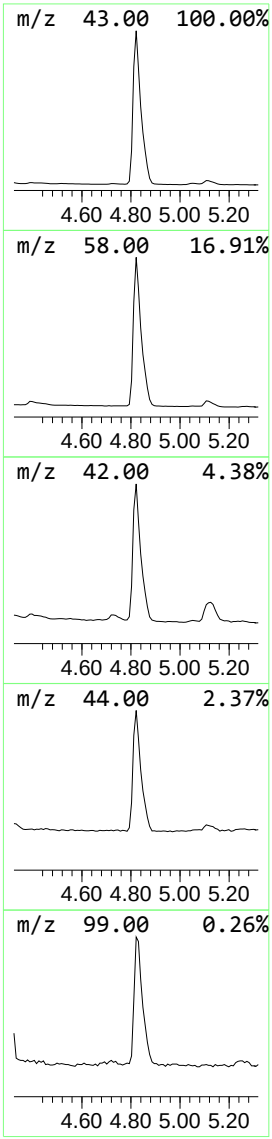
****

Peak Number 4 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	1.28 ng	299952	1,4-Dichlorobenzene-d4	7.643

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 : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

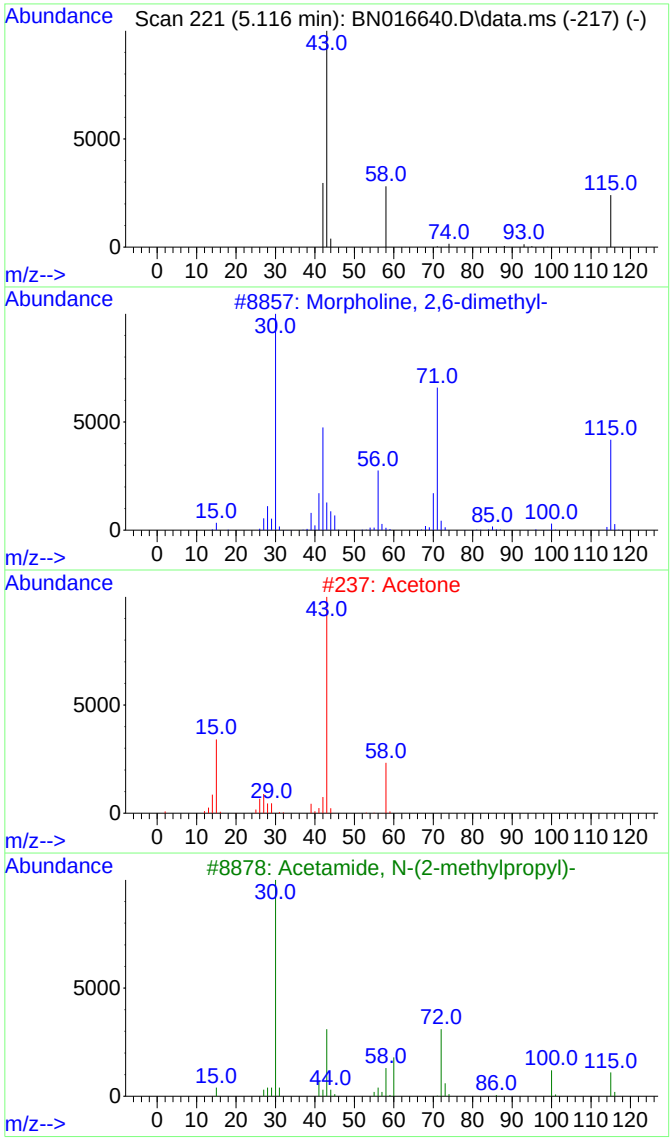
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

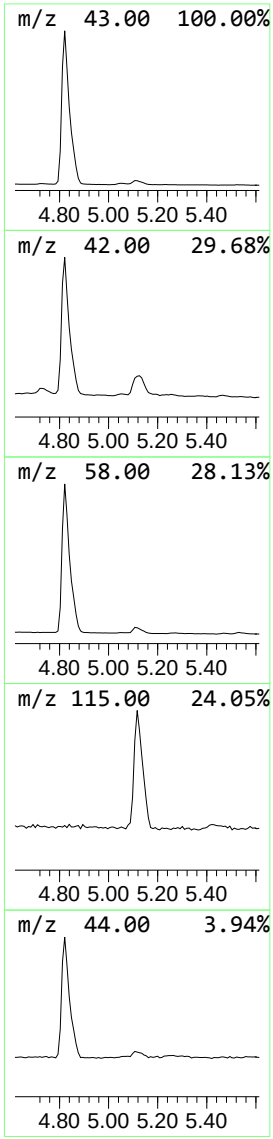
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Morpholine, 2,6-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	0.06 ng	14645	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	5
2	Acetone	58	C3H6O	000067-64-1	4
3	Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	4
4	Cyclopropanesulfonamide, acetate	163	C5H9NO3S	1010507-55-0	4
5	1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-65-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

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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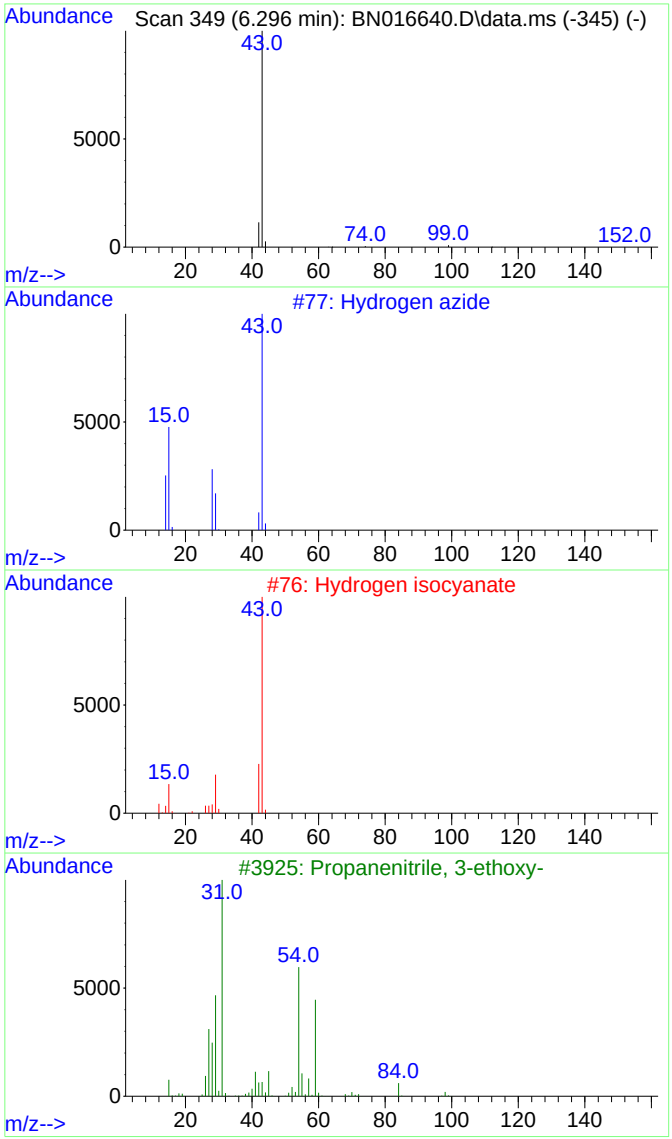
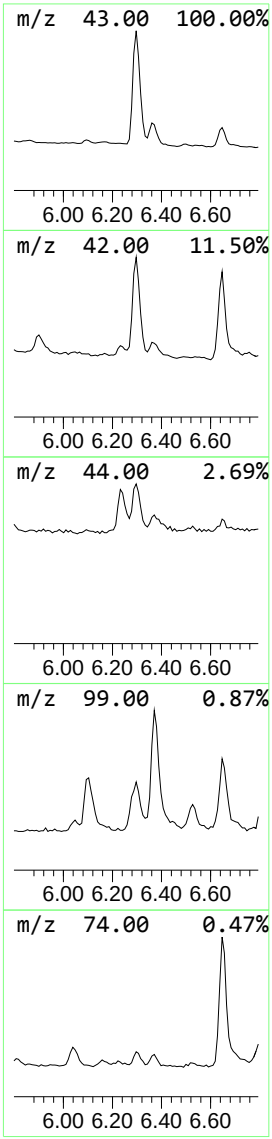
Peak Number 6 Hydrogen azide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.08 ng	19242	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	Hydrogen isocyanate	43	CHNO	000075-13-8	2
3	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	2
4	Hex-5-enylamine	99	C6H13N	034825-70-2	2
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

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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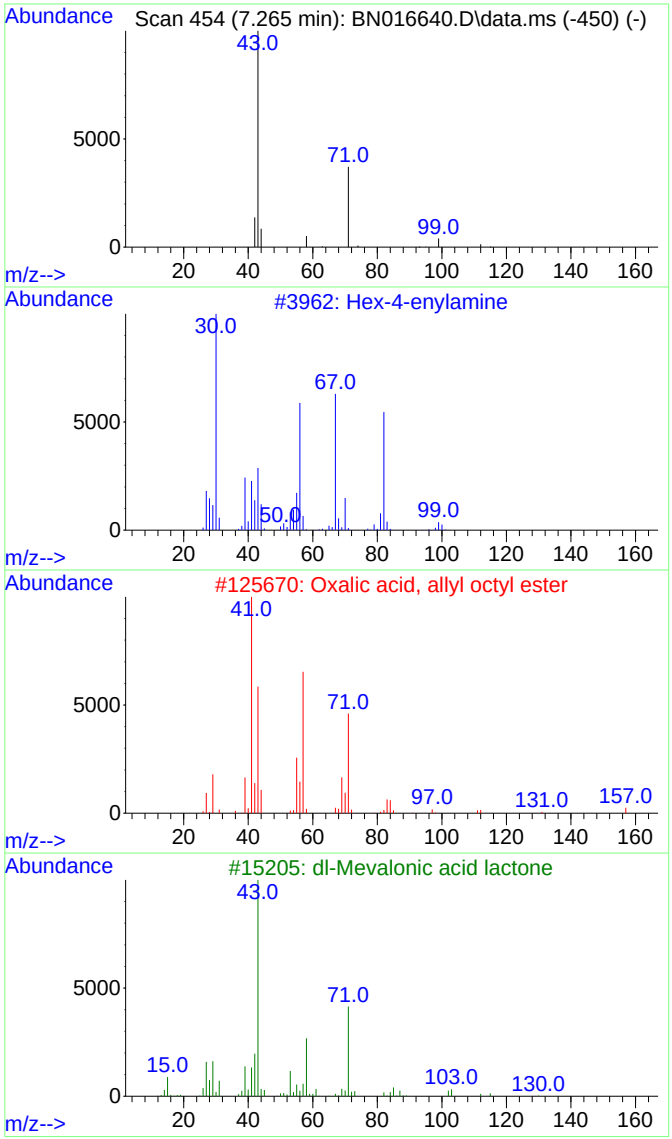
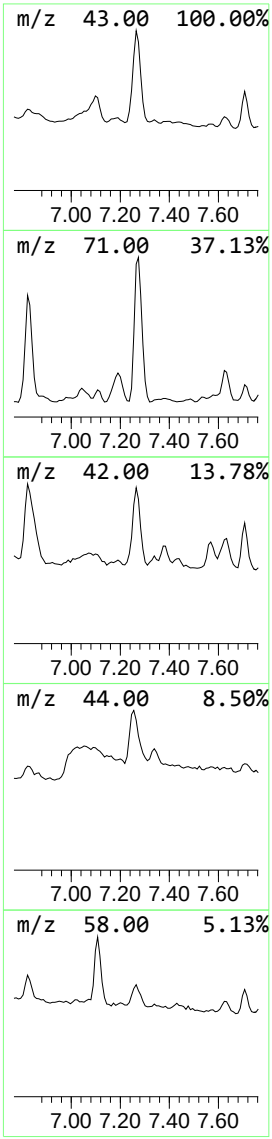
Peak Number 7 Hex-4-enylamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.265	0.06 ng	14988	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	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
3	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	4
5	1-Butanol	74	C4H10O	000071-36-3	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

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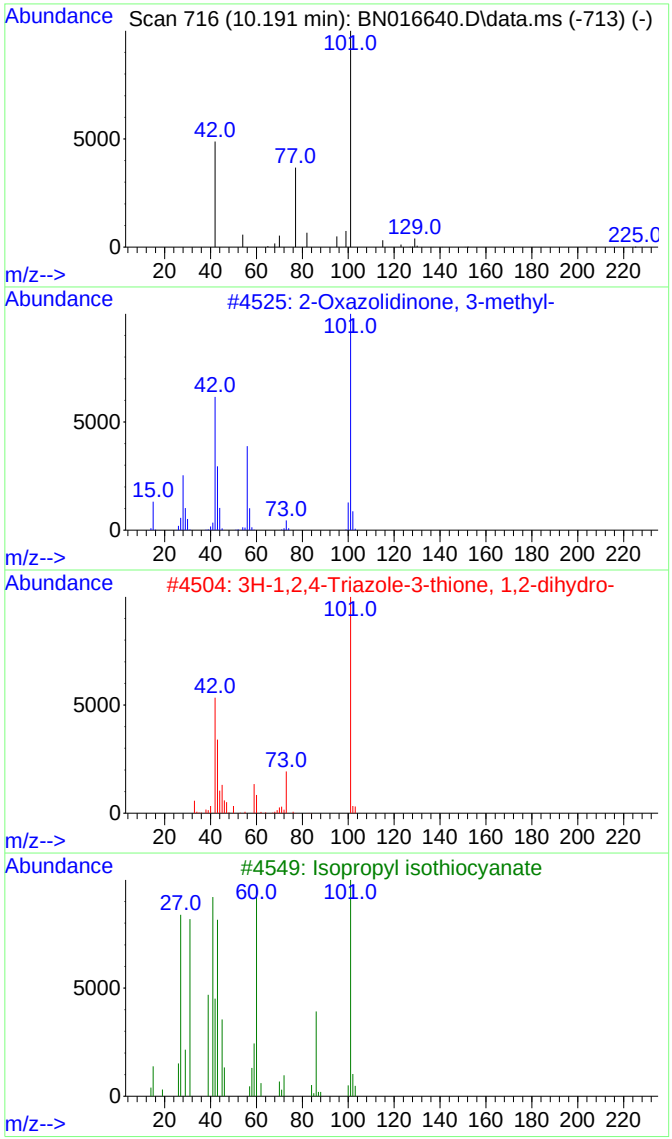
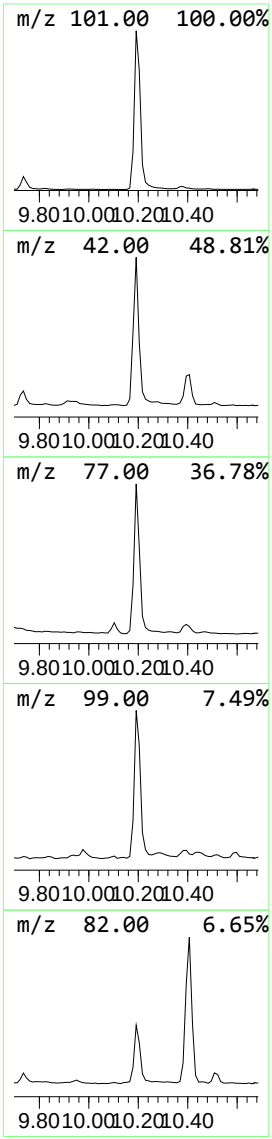
Peak Number 8 2-Oxazolidinone, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.12 ng	53982	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





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Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

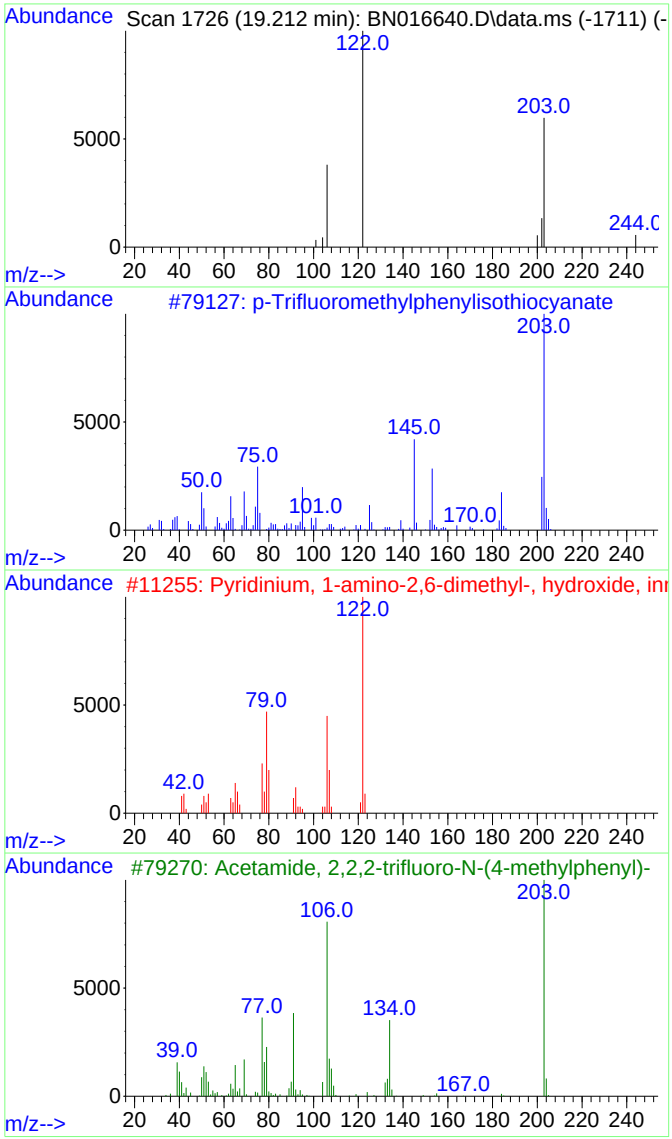
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

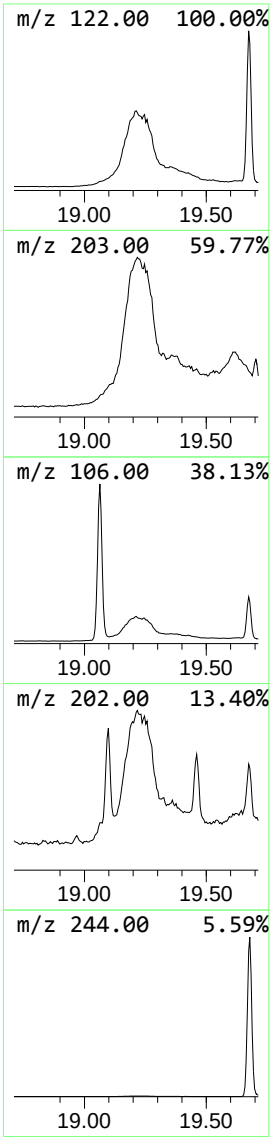
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 p-Trifluoromethylphenylisot... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.212	0.07 ng	33421	Chrysene-d12	21.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Trifluoromethylphenylisothiocy...	203	C8H4F3NS	001645-65-4	9
2	Pyridinium, 1-amino-2,6-dimethyl...	122	C7H10N2	051135-76-3	9
3	Acetamide, 2,2,2-trifluoro-N-(4-...	203	C9H8F3NO	1000351-68-4	7
4	3-Amino-4,6-dimethylthieno[2,3-b...	203	C10H9N3S	052505-57-4	7
5	9-Cyanophenanthrene	203	C15H9N	002510-55-6	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

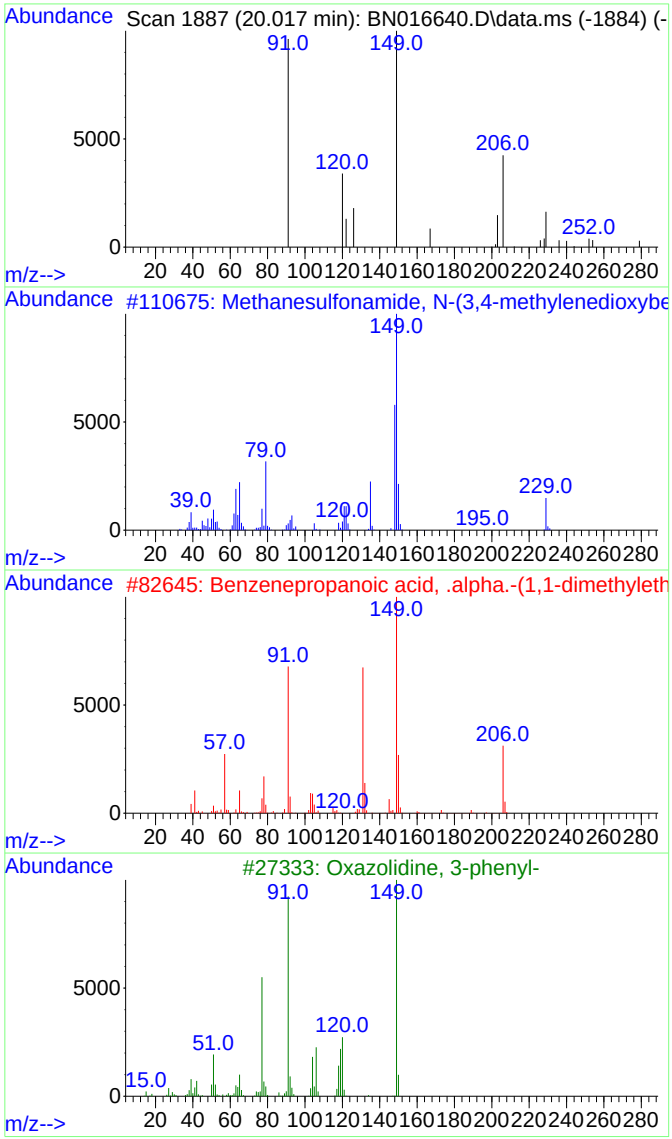
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

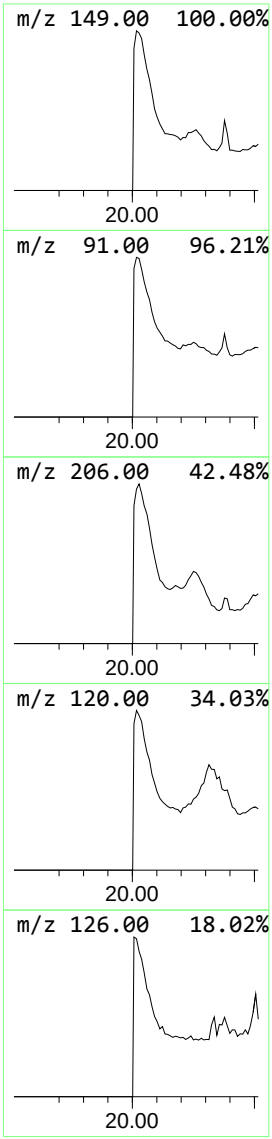
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Methanesulfonamide, N-(3,4-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.017	0.17 ng	81214	Chrysene-d12	21.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanesulfonamide, N-(3,4-methy...	229	C9H11NO4S	184041-99-4	9
2	Benzenepropanoic acid, .alpha.-(...	206	C13H18O2	053483-12-8	9
3	Oxazolidine, 3-phenyl-	149	C9H11NO	020503-92-8	9
4	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	9
5	Benzaldehyde, 4-methyl-, O-methy...	149	C9H11NO	033499-39-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE122D3-20210920

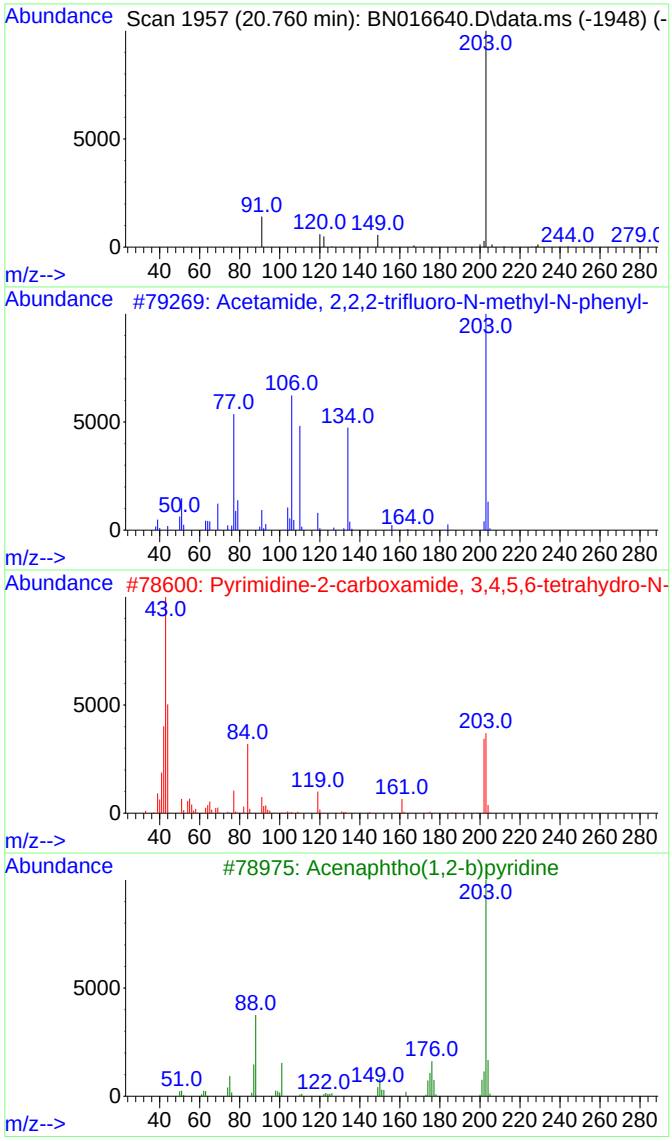
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

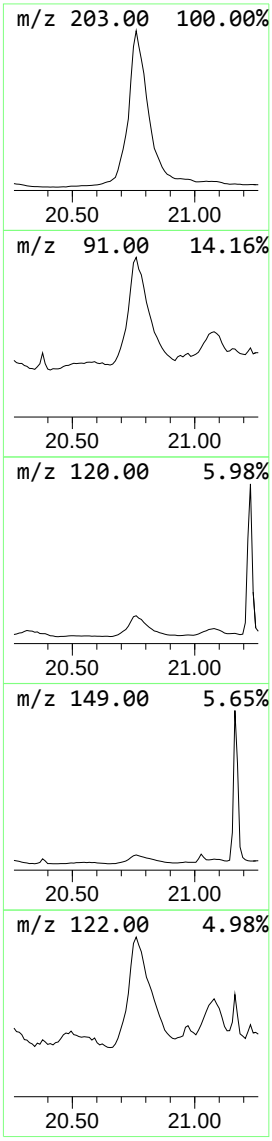
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Acetamide, 2,2,2-trifluoro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.760	0.45 ng	212541	Chrysene-d12	21.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2,2,2-trifluoro-N-met...	203	C9H8F3NO	000345-81-3	7
2	Pyrimidine-2-carboxamide, 3,4,5,...	203	C11H13N3O	156309-07-8	5
3	Acenaphtho(1,2-b)pyridine	203	C15H9N	000206-49-5	4
4	2,3-Dichlorophenyl isothiocyanate	203	C7H3Cl2NS	006590-97-2	4
5	Glutarimide, N-(3-methylphenyl)-	203	C12H13NO2	1000360-92-6	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016640.D
Acq On : 01 Oct 2021 17:45
Operator : CG/JU
Sample : M3833-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE122D3-20210920

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
Hydrogen isocya...	3.364	0.4	ng	96671	1	7.643	93531	0.4
1-Propanol, 2-m...	3.816	0.2	ng	50754	1	7.643	93531	0.4
Hydrogen azide	4.240	0.3	ng	66793	1	7.643	93531	0.4
Butane	4.821	1.3	ng	299952	1	7.643	93531	0.4
Morpholine, 2,6...	5.116	0.1	ng	14645	1	7.643	93531	0.4
Hydrogen azide	6.296	0.1	ng	19242	1	7.643	93531	0.4
Hex-4-enylamine	7.265	0.1	ng	14988	1	7.643	93531	0.4
2-Oxazolidinone...	10.191	0.1	ng	53982	2	10.407	173821	0.4
p-Trifluorometh...	19.212	0.1	ng	33421	5	21.228	189662	0.4
Methanesulfonam...	20.017	0.2	ng	81214	5	21.228	189662	0.4
Acetamide, 2,2,...	20.760	0.4	ng	212541	5	21.228	189662	0.4