LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016658.D
Acq On : 02 Oct 2021 06:22
Operator : CG/JU
Sample : M3829-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D3-20210917

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: BN016658.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	502530	784027	100.00%	21.984%
2	3.253	17	19	29	rVB	160127	627942	80.09%	17.607%
3	3.364	29	31	47	rVB2	20767	56764	7.24%	1.592%
4	3.816	76	80	97	rVB	9714	40167	5.12%	1.126%
5	4.396	140	143	154	rVB2	3555	12342	1.57%	0.346%
6	4.821	185	189	203	rVB	44120	99288	12.66%	2.784%
7	5.263	234	237	245	rVB	5729	14856	1.89%	0.417%
8	6.296	345	349	357	rVB	11178	23607	3.01%	0.662%
9	6.646	383	387	401	rVB	3949	10431	1.33%	0.292%
10	6.821	403	406	418	rVB3	4189	15359	1.96%	0.431%
11	7.181	441	445	450	rVB2	2986	8361	1.07%	0.234%
12	7.264	451	454	460	rVB2	6633	14740	1.88%	0.413%
13	7.633	489	494	500	rVB	51423	106683	13.61%	2.991%
14	7.863	515	519	525	rBV	16211	32538	4.15%	0.912%
15	8.168	549	552	562	rVV	10096	27975	3.57%	0.784%
16	8.306	563	567	569	rVB	14080	18605	2.37%	0.522%
17	8.784	601	605	610	rBV	20471	42374	5.40%	1.188%
18	10.191	713	716	729	rBV	14513	29653	3.78%	0.831%
19	10.406	729	733	736	rBV	100600	178651	22.79%	5.009%
20	12.002	920	931	942	rBV	42185	68590	8.75%	1.923%
21	12.886	1071	1074	1078	rBV	85501	141079	17.99%	3.956%
22	14.268	1180	1183	1186	rBV	132198	191188	24.39%	5.361%
23	15.766	1299	1301	1308	rVB2	9680	15549	1.98%	0.436%
24	17.017	1400	1403	1406	rBV	100376	153948	19.64%	4.317%
25	19.063	1689	1696	1727	rBV	123601	170449	21.74%	4.779%
26	19.678	1813	1820	1851	rBV	114040	149519	19.07%	4.193%
27	21.163	1992	1995	1998	rBV	98068	118726	15.14%	3.329%
28	21.227	1998	2001	2011	rVB	129264	185516	23.66%	5.202%
29	23.419	2399	2408	2414	rBV	5817	9508	1.21%	0.267%
30	23.481	2414	2426	2465	rVB	97129	194495	24.81%	5.454%
31	24.083	2592	2602	2618	rBV2	5673	11212	1.43%	0.314%
32	24.850	2817	2826	2846	rVB	5286	12202	1.56%	0.342%

Sum of corrected areas: 3566344

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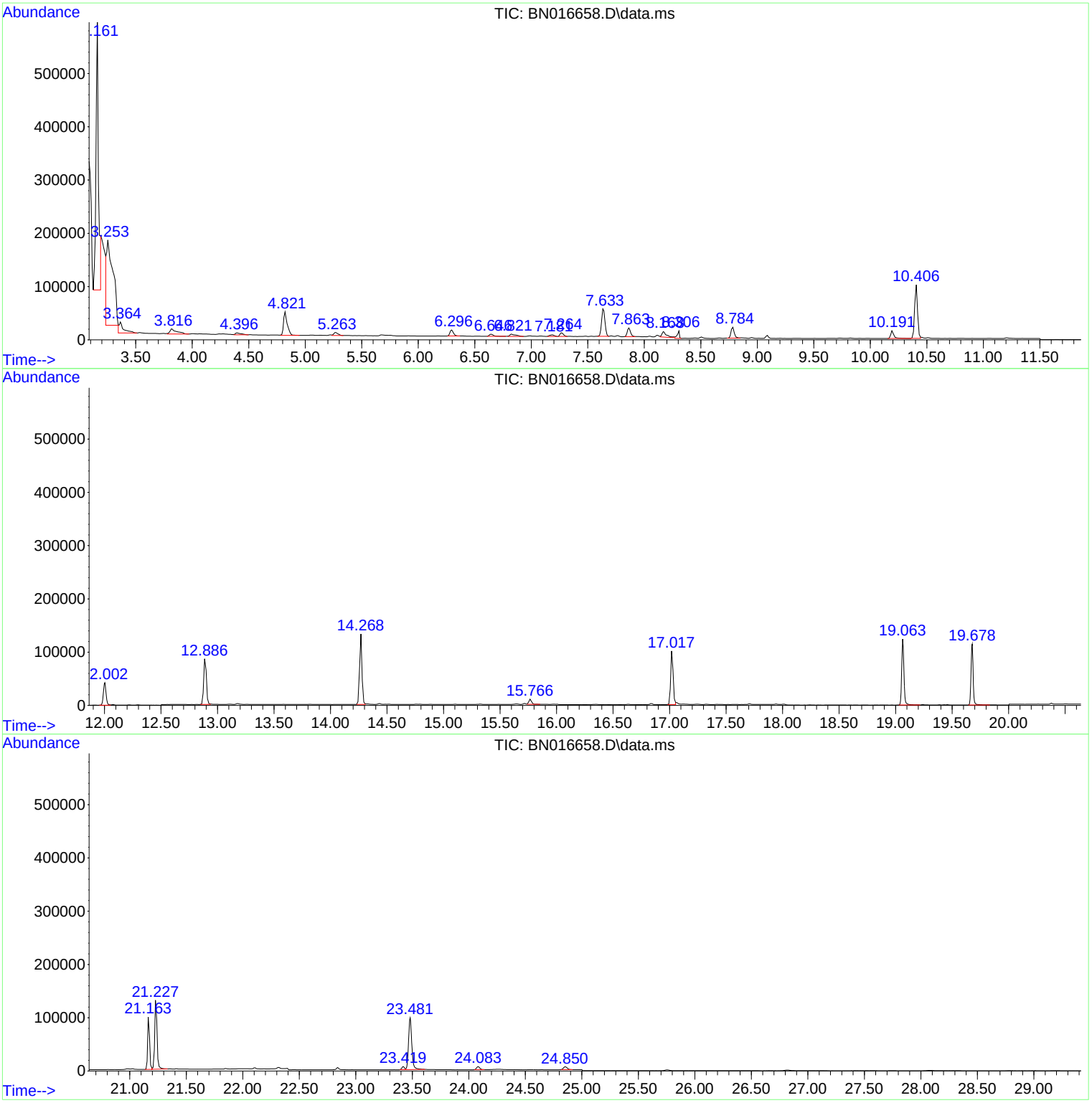
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE125D3-20210917

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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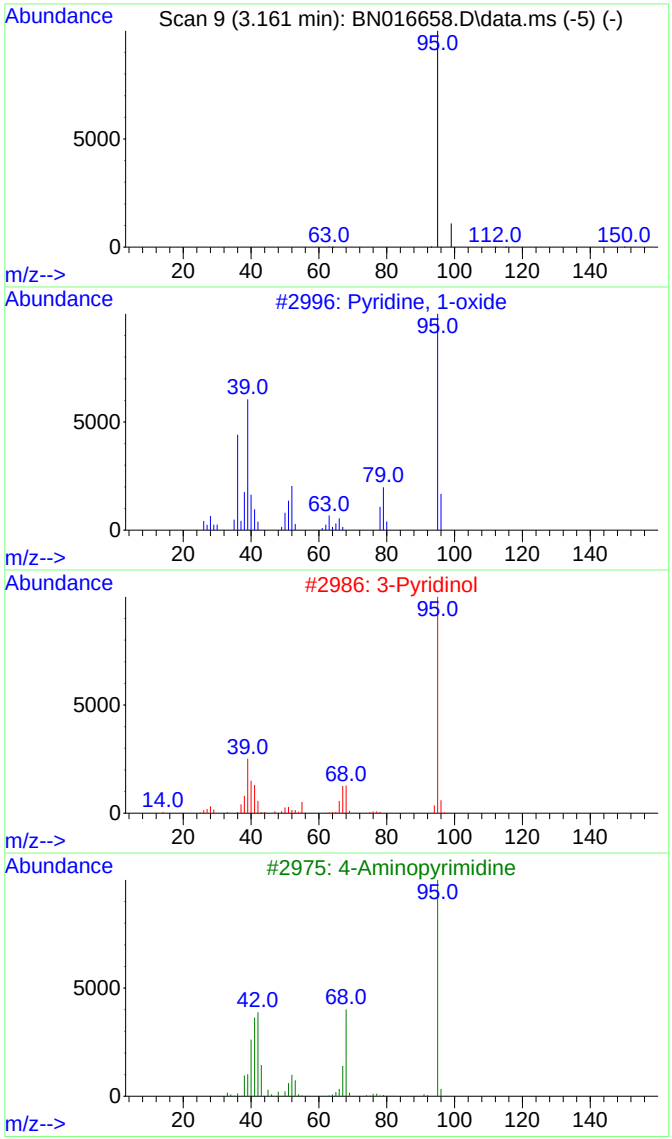
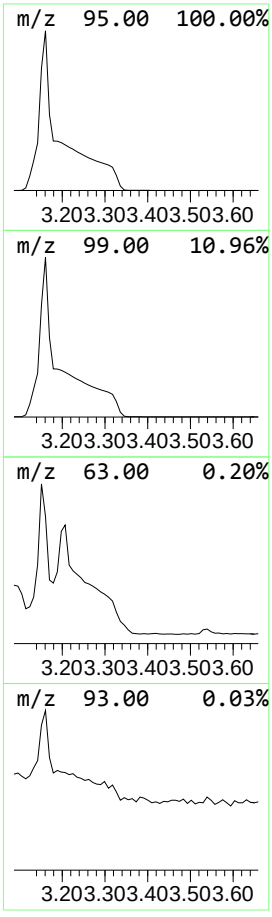
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	2.94 ng	784027	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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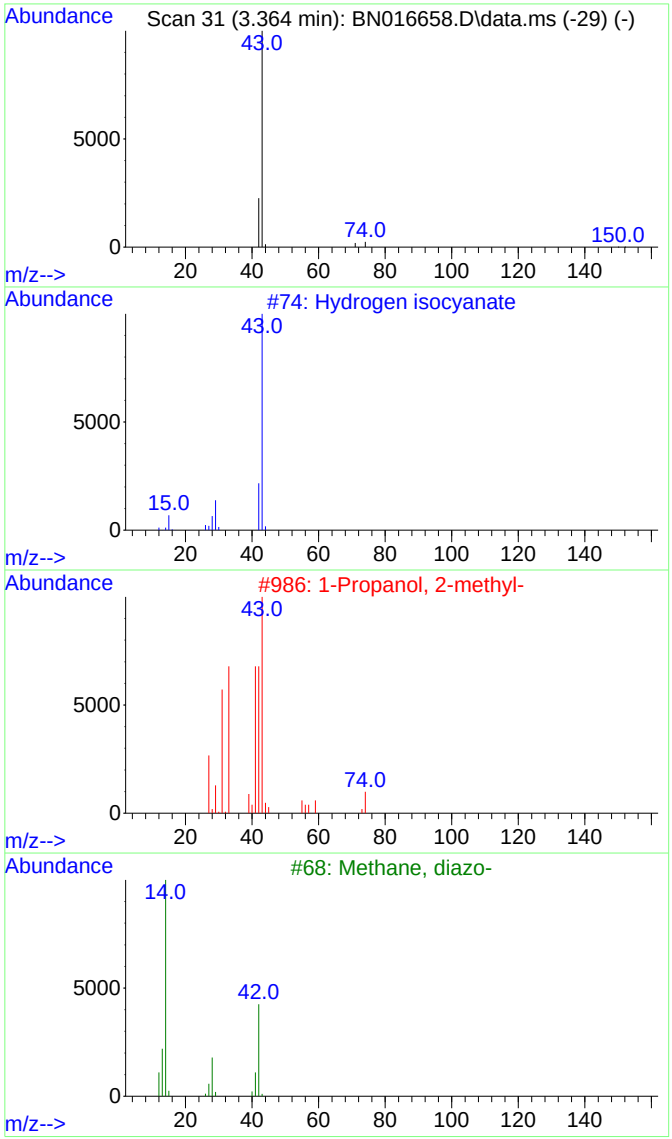
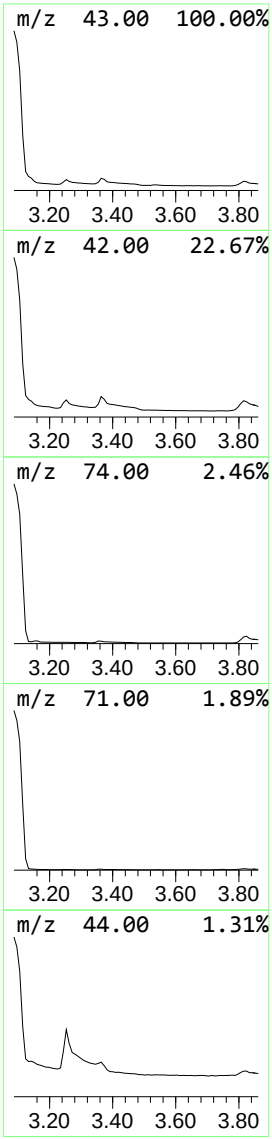
Peak Number 2 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.21 ng	56764	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-Propanol, 2-methyl-	74	C4H10O	000078-83-1	3
3	Methane, diazo-	42	CH2N2	000334-88-3	2
4	Diazirine	42	CH2N2	1000305-84-1	2
5	Propene	42	C3H6	000115-07-1	1





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Instrument : BNA_N
ClientSampleId : RE125D3-20210917

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TIC Library : C:\Database\NIST20.L
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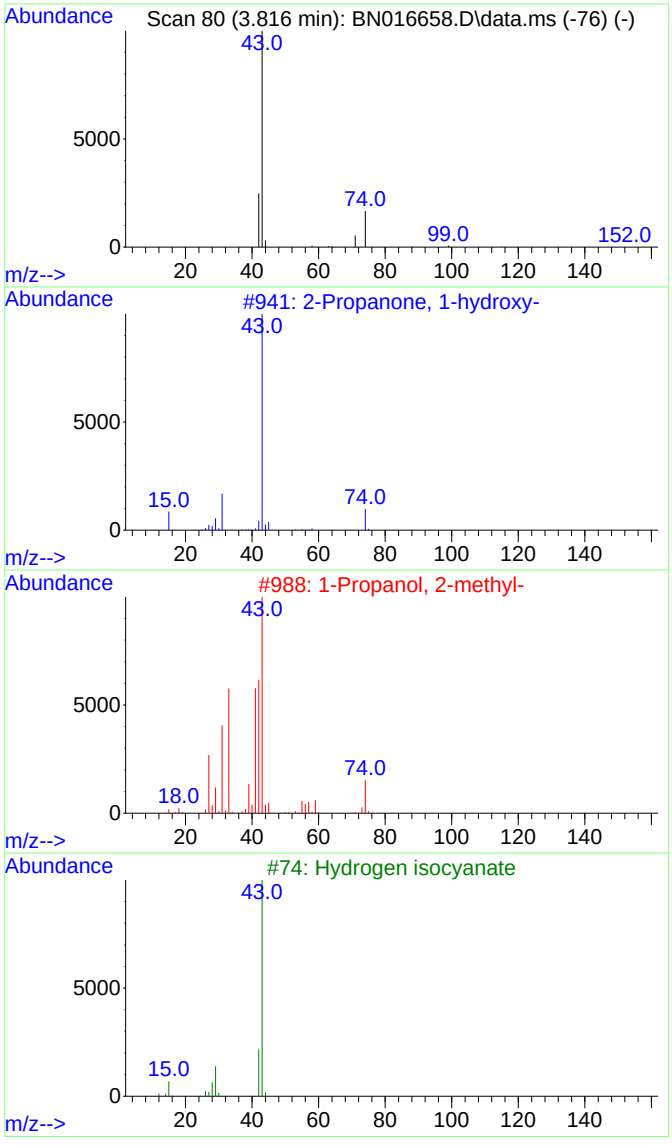
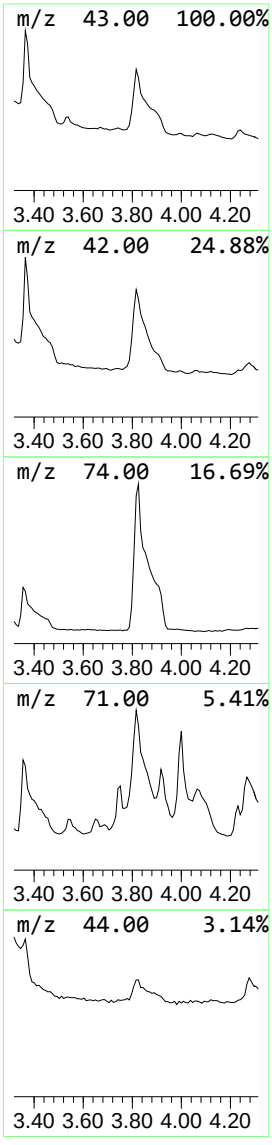
****
Peak Number 3 2-Propanone, 1-hydroxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.15 ng	40167	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	5
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3





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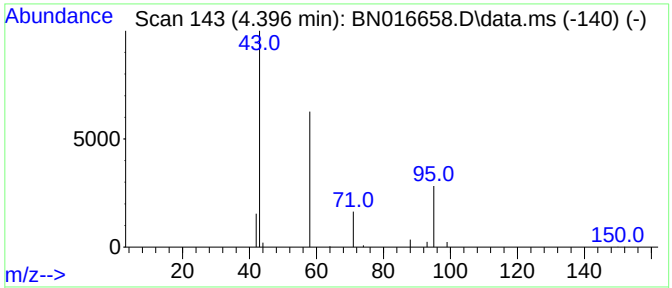
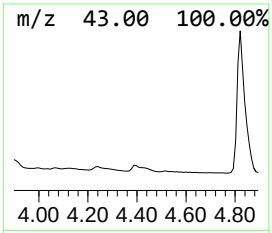
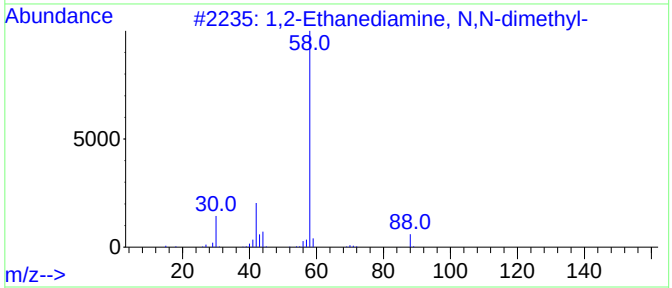
****
Peak Number 4 1,2-Ethanediamine, N,N-dime... Concentration Rank 11

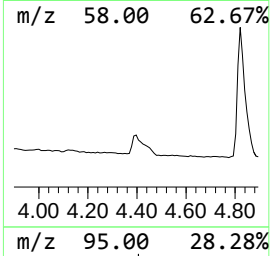
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.396	0.05 ng	12342	1,4-Dichlorobenzene-d4	7.642

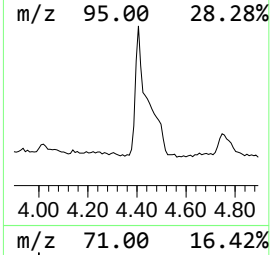
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediamine, N,N-dimethyl-	88	C4H12N2	000108-00-9	7
2	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5
3	Acetone	58	C3H6O	000067-64-1	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	4
5	Ethene, methoxy-	58	C3H6O	000107-25-5	4

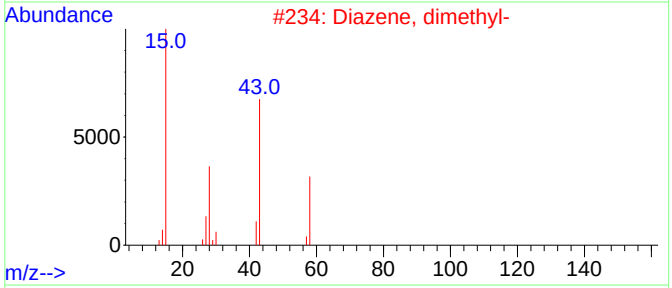


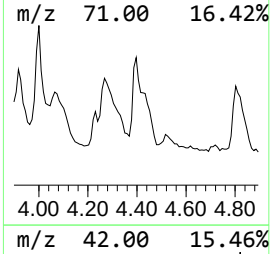


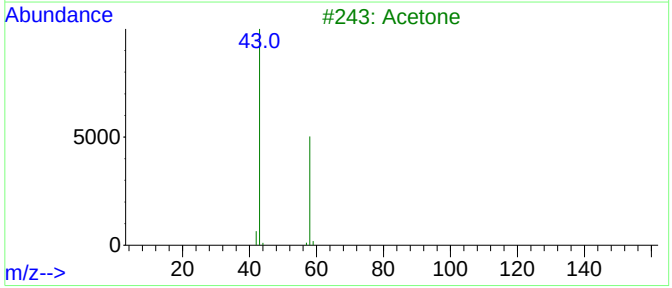


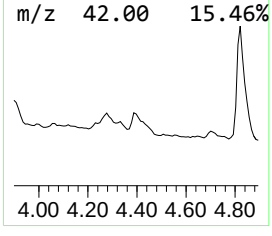












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TIC Library : C:\Database\NIST20.L
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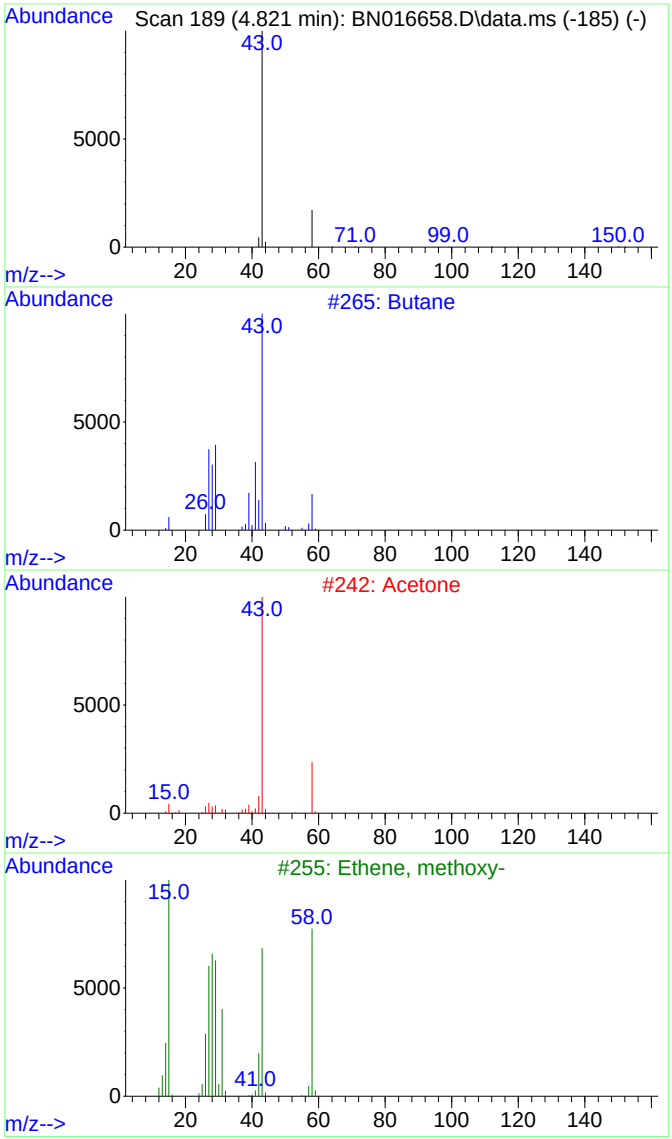
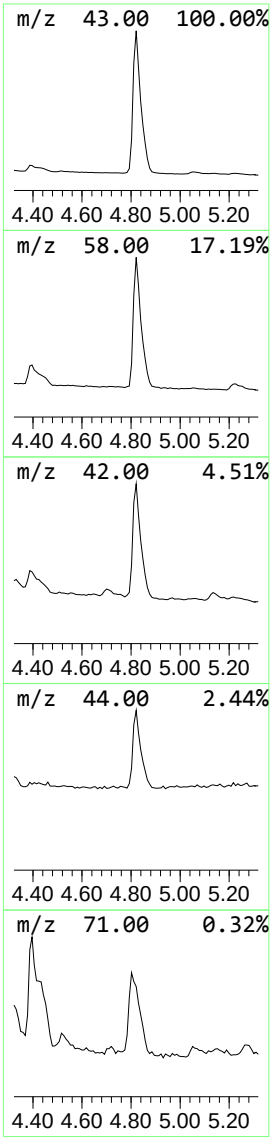
****

Peak Number 5 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.37 ng	99288	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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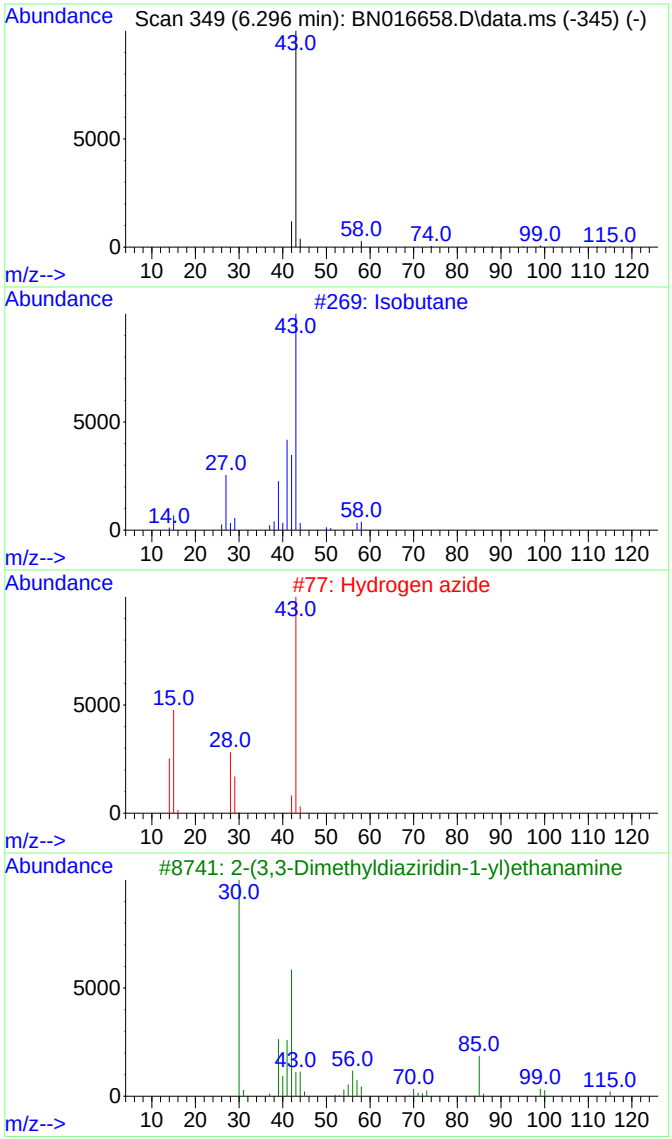
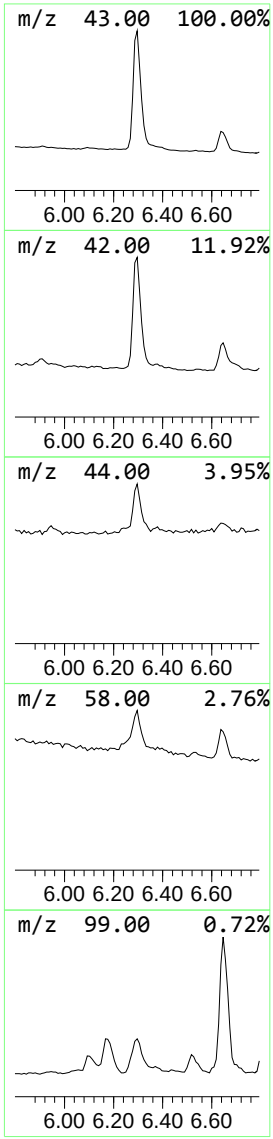
Peak Number 6 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.09 ng	23607	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	4
2	Hydrogen azide	43	HN3	007782-79-8	4
3	2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	3
4	2,3-Octanedione	142	C8H14O2	000585-25-1	2
5	1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-66-3	2





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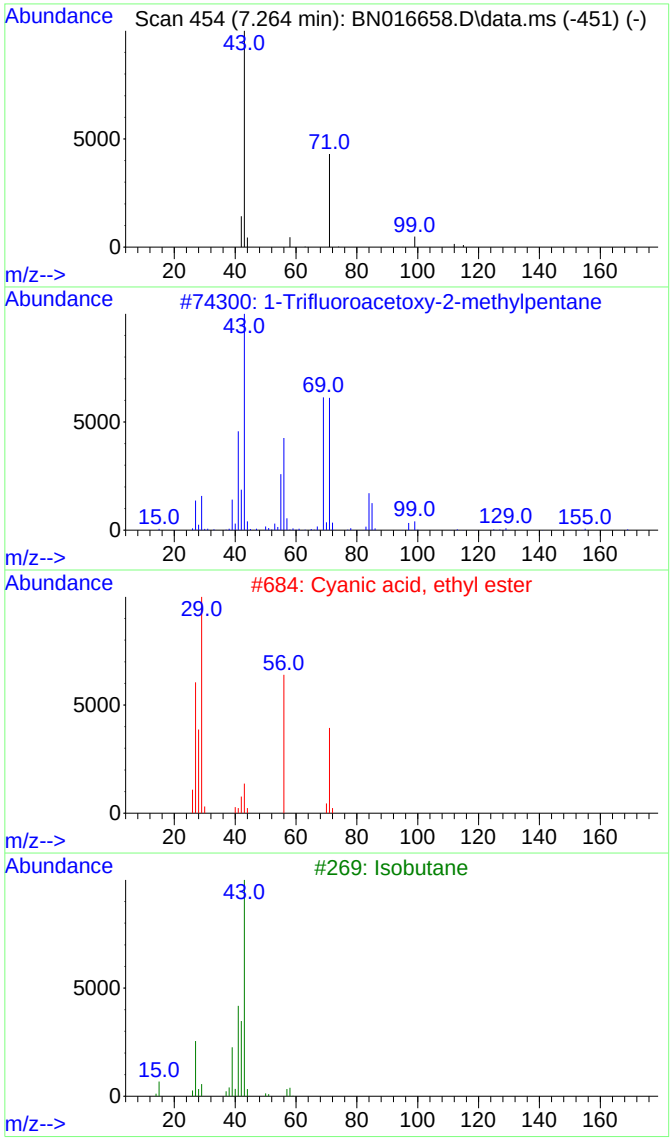
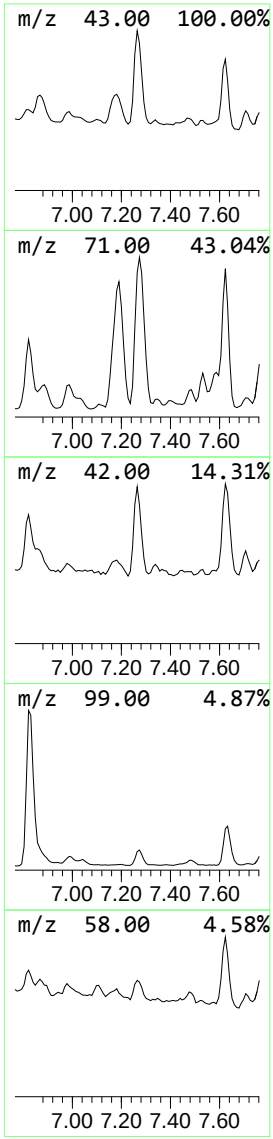
****
Peak Number 7 1-Trifluoroacetoxy-2-methyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	14740	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	9
2	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
3	Isobutane	58	C4H10	000075-28-5	4
4	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	4





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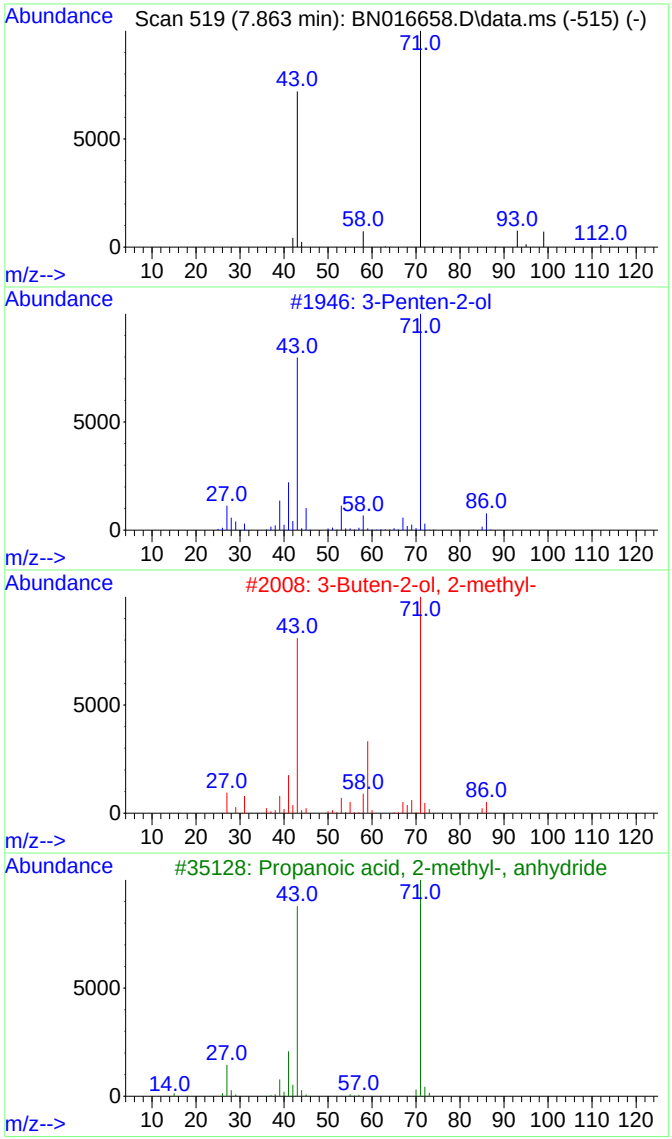
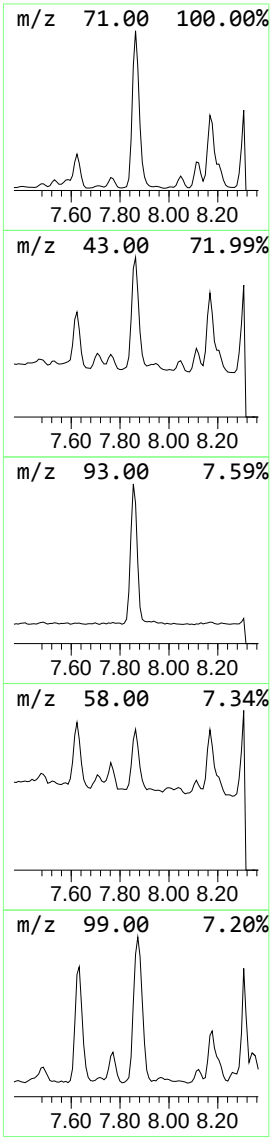
Peak Number 8 3-Penten-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	0.12 ng	32538	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	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-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016658.D
Acq On : 02 Oct 2021 06:22
Operator : CG/JU
Sample : M3829-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE125D3-20210917

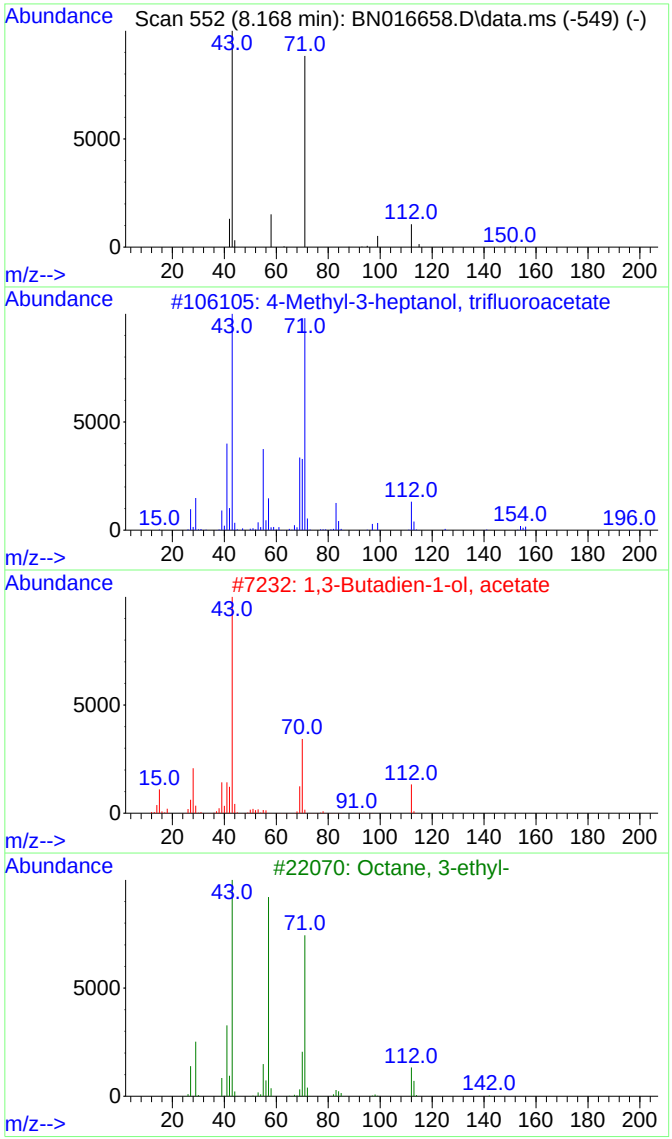
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

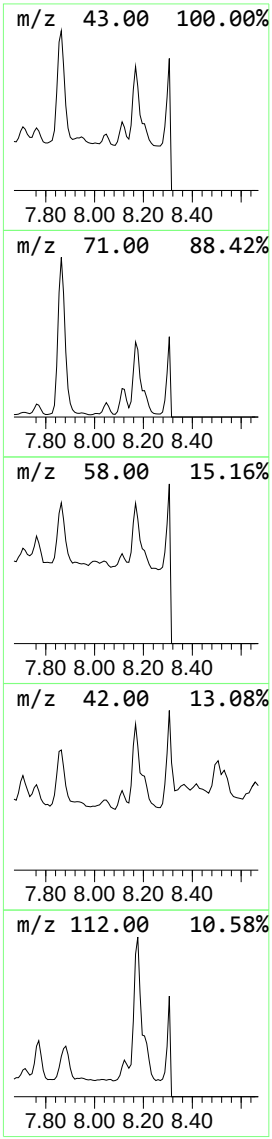
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Methyl-3-heptanol, triflu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.10 ng	27975	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	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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ClientSampleId :
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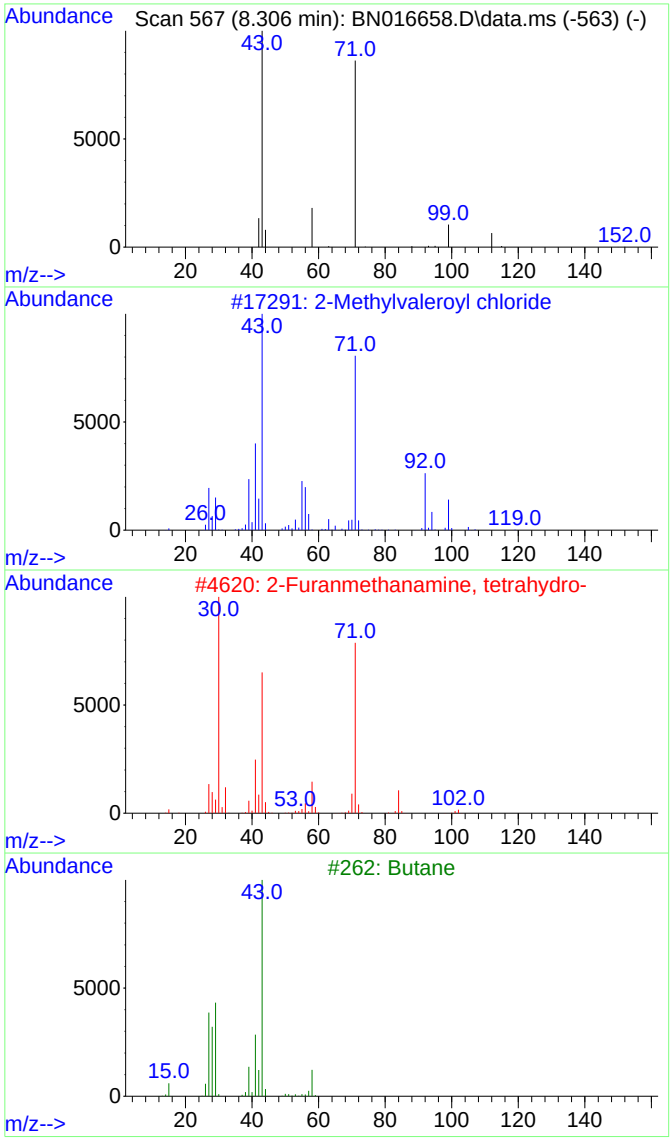
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

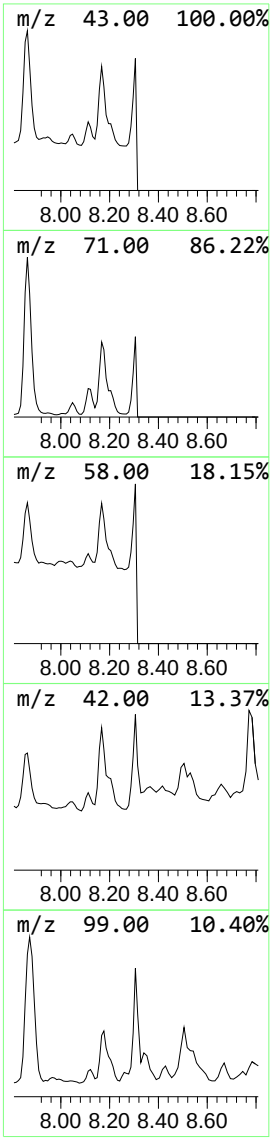
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Methylvaleroyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.07 ng	18605	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylvaleroyl chloride	134	C6H11ClO	005238-27-7	9
2	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9
3	Butane	58	C4H10	000106-97-8	5
4	Acetone	58	C3H6O	000067-64-1	5
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4





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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D3-20210917

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

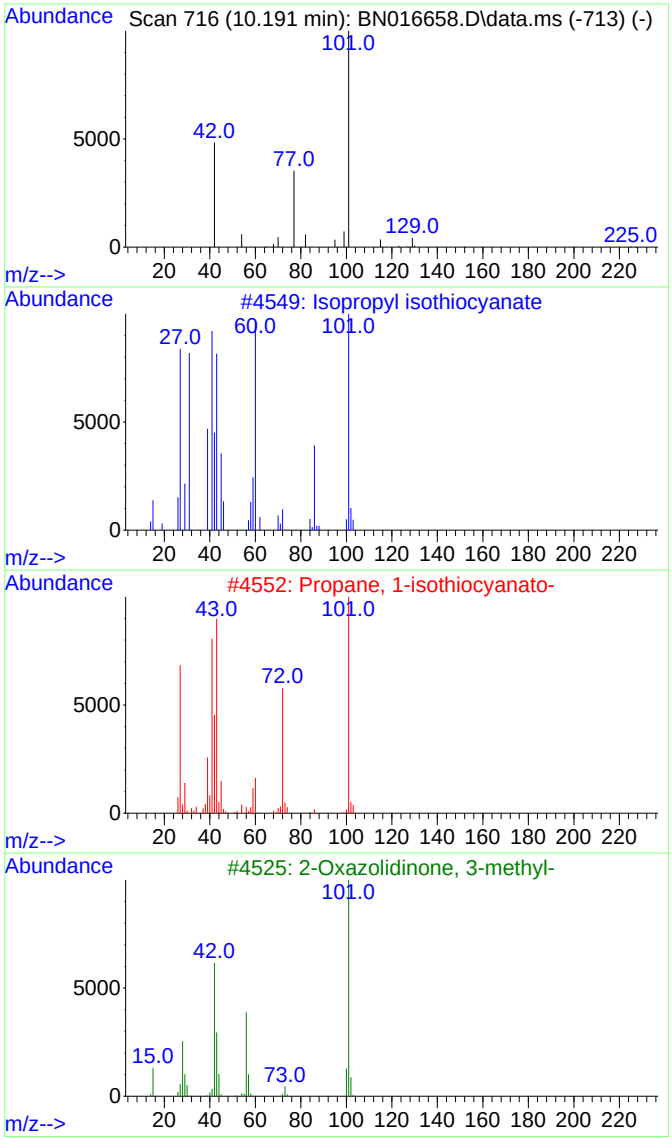
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

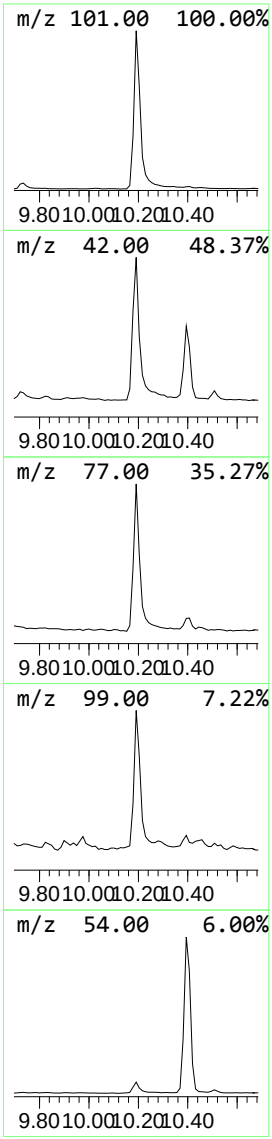
****

Peak Number 11 Isopropyl isothiocyanate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.07 ng	29653	Naphthalene-d8	10.406

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





Tentatively Identified Compound (LSC) summary

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Instrument : 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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	2.9	ng	784027	1	7.642	106683	0.4
Hydrogen isocya...	3.364	0.2	ng	56764	1	7.642	106683	0.4
2-Propanone, 1-...	3.816	0.2	ng	40167	1	7.642	106683	0.4
1,2-Ethanediami...	4.396	0.0	ng	12342	1	7.642	106683	0.4
Butane	4.821	0.4	ng	99288	1	7.642	106683	0.4
Isobutane	6.296	0.1	ng	23607	1	7.642	106683	0.4
1-Trifluoroacet...	7.264	0.1	ng	14740	1	7.642	106683	0.4
3-Penten-2-ol	7.863	0.1	ng	32538	1	7.642	106683	0.4
4-Methyl-3-hept...	8.168	0.1	ng	27975	1	7.642	106683	0.4
2-Methylvaleroy...	8.306	0.1	ng	18605	1	7.642	106683	0.4
Isopropyl isoth...	10.191	0.1	ng	29653	2	10.406	178651	0.4