LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016656.D
Acq On : 02 Oct 2021 05:10
Operator : CG/JU
Sample : M3829-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D1-20210917

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: BN016656.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	5	8	10	rBV	468264	643057	83.55%	17.030%
2	3.189	10	12	17	rVV	115587	403929	52.48%	10.697%
3	3.253	17	19	29	rVB	211451	769664	100.00%	20.383%
4	3.816	76	80	97	rVB	8829	39065	5.08%	1.035%
5	4.821	185	189	201	rVB	31085	76186	9.90%	2.018%
6	5.263	234	237	244	rVB	5073	14075	1.83%	0.373%
7	6.647	383	387	397	rVB	3470	9060	1.18%	0.240%
8	6.831	403	407	418	rVB3	3973	14807	1.92%	0.392%
9	7.264	450	454	460	rBV2	6151	14244	1.85%	0.377%
10	7.633	489	494	500	rBV2	47759	100814	13.10%	2.670%
11	7.864	515	519	527	rBV	12597	25703	3.34%	0.681%
12	8.168	549	552	560	rVV	7633	20928	2.72%	0.554%
13	8.306	563	567	569	rVB	11752	15819	2.06%	0.419%
14	8.784	601	605	610	rBV	19665	40022	5.20%	1.060%
15	10.191	713	716	725	rBV	28134	51015	6.63%	1.351%
16	10.407	729	733	736	rBV	97453	167307	21.74%	4.431%
17	12.003	919	931	943	rBV	38869	63298	8.22%	1.676%
18	12.886	1071	1074	1078	rBV	79134	132156	17.17%	3.500%
19	14.269	1180	1183	1186	rBV	126835	180292	23.42%	4.775%
20	15.766	1299	1301	1307	rVB2	11725	18632	2.42%	0.493%
21	17.018	1400	1403	1406	rBV	98603	148559	19.30%	3.934%
22	19.063	1689	1696	1716	rBV	122497	167808	21.80%	4.444%
23	19.679	1813	1820	1843	rBV	154412	198527	25.79%	5.258%
24	20.973	1974	1977	1981	rBV	4072	9842	1.28%	0.261%
25	21.164	1992	1995	1998	rBV	44718	54844	7.13%	1.452%
26	21.227	1998	2001	2011	rVB	128114	177465	23.06%	4.700%
27	23.419	2400	2408	2414	rBV	5456	8875	1.15%	0.235%
28	23.481	2414	2426	2462	rVB	94214	186543	24.24%	4.940%
29	24.084	2593	2602	2618	rVB	5778	11058	1.44%	0.293%
30	24.854	2817	2827	2846	rVB	5430	12416	1.61%	0.329%

Sum of corrected areas: 3776010

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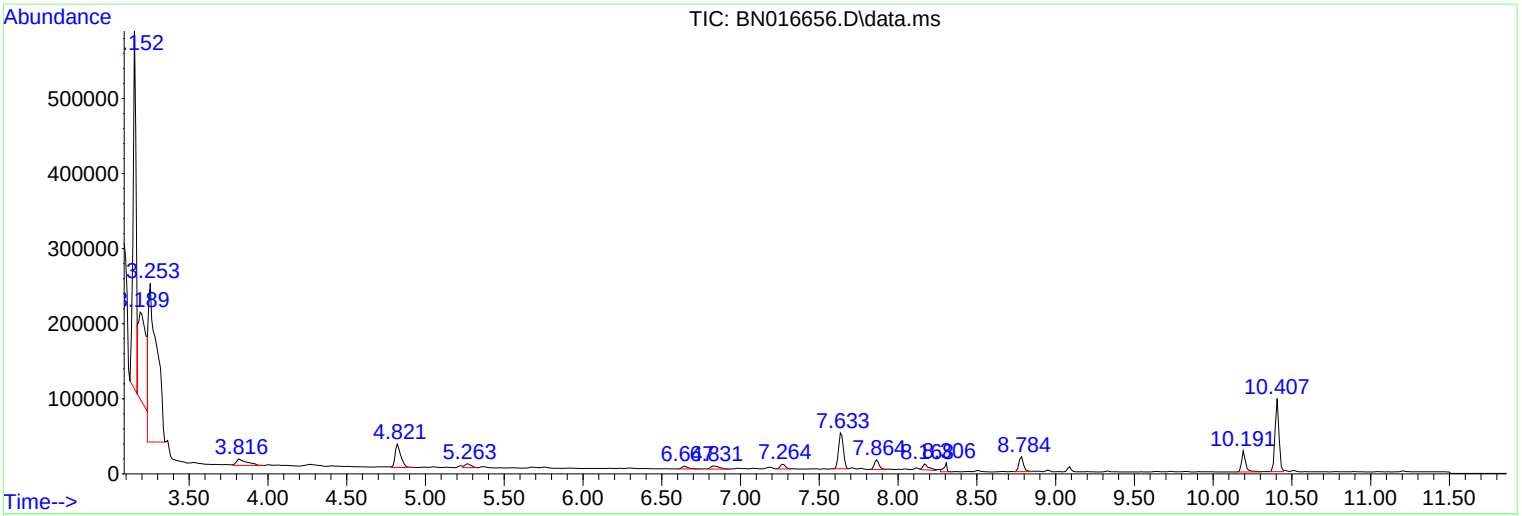
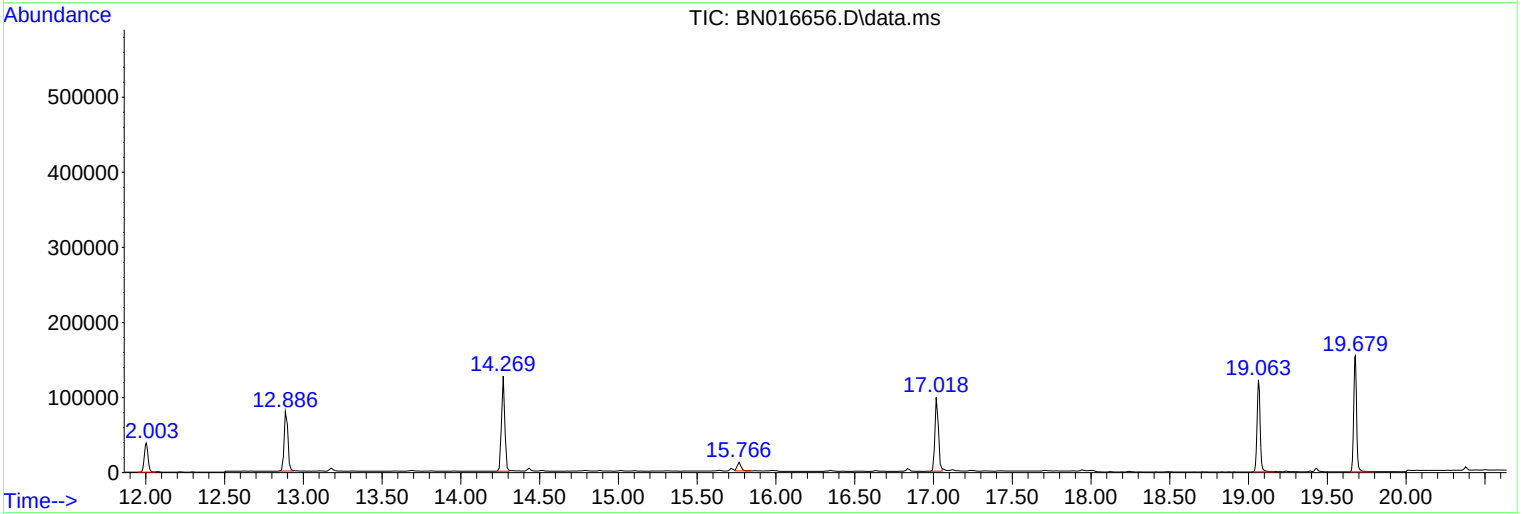
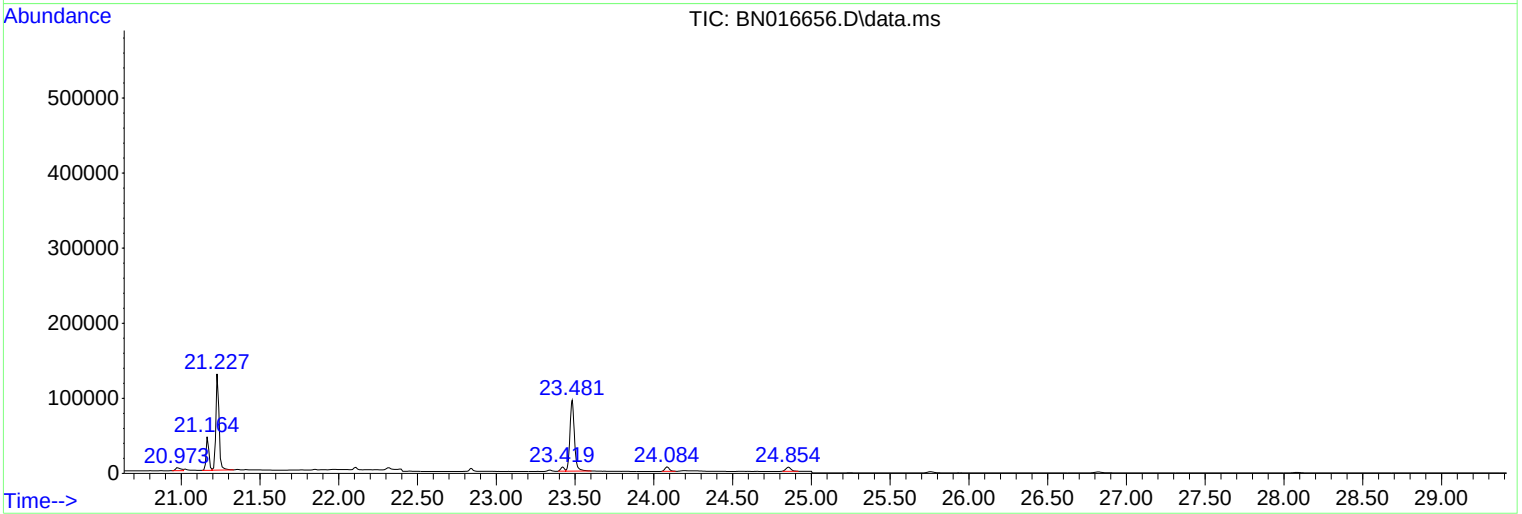
ClientSampleId :
RE125D1-20210917

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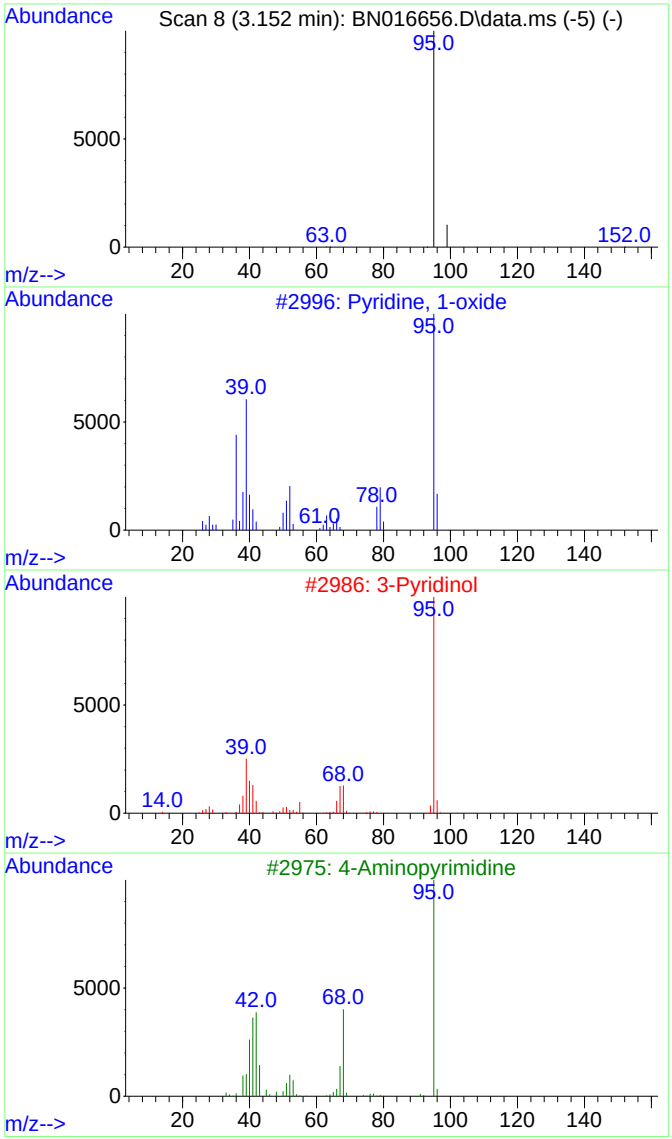
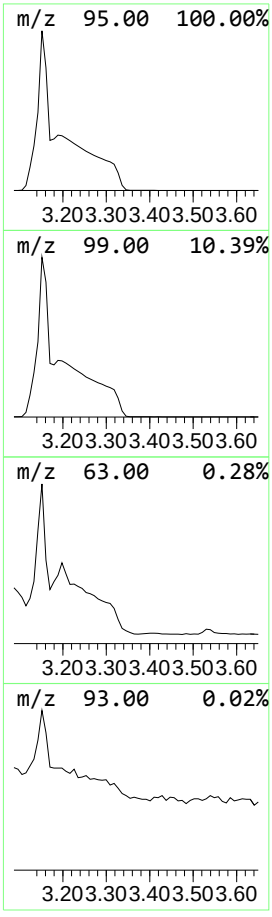
****
Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	2.55 ng	643057	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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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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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

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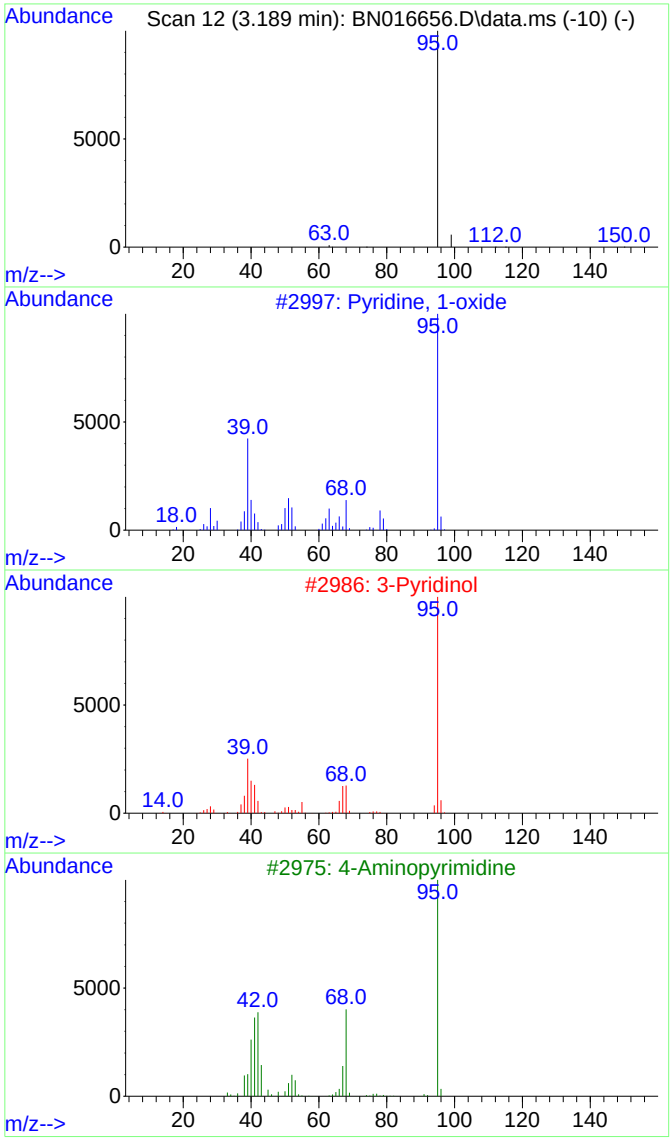
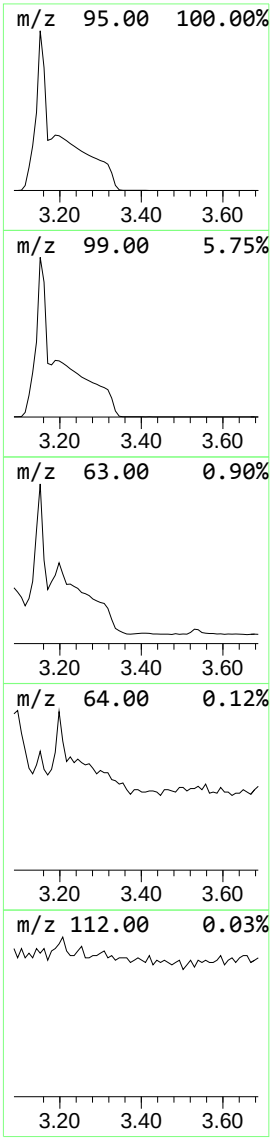
****

Peak Number 2 Pyridine, 1-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	1.60 ng	403929	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	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	4-Pyridazinamine	95	C4H5N3	020744-39-2	2





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Sample : M3829-04
Misc :
ALS Vial : 24 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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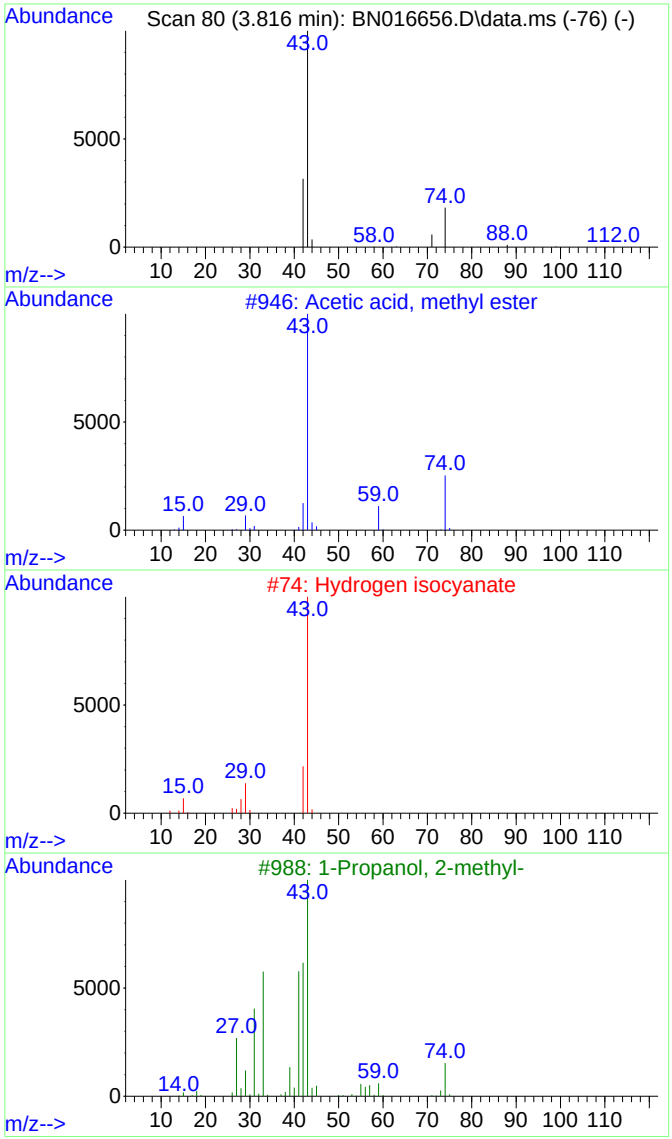
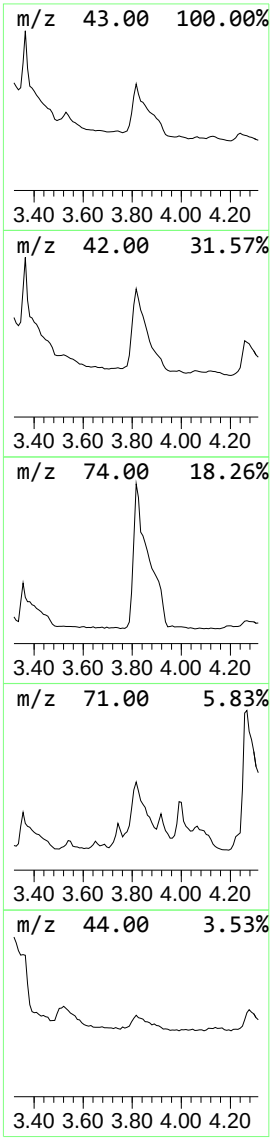
****
Peak Number 3 Acetic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.15 ng	39065	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	5
2	Hydrogen isocyanate	43	CHNO	000075-13-8	4
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3





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Misc :
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Instrument :
BNA_N
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RE125D1-20210917

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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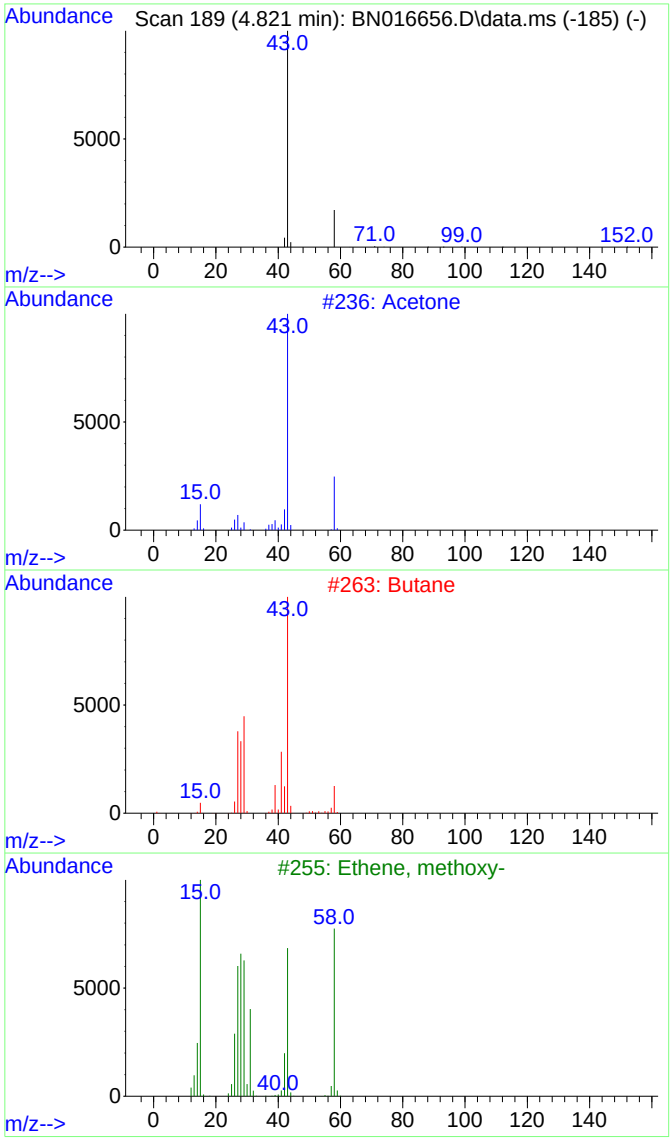
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

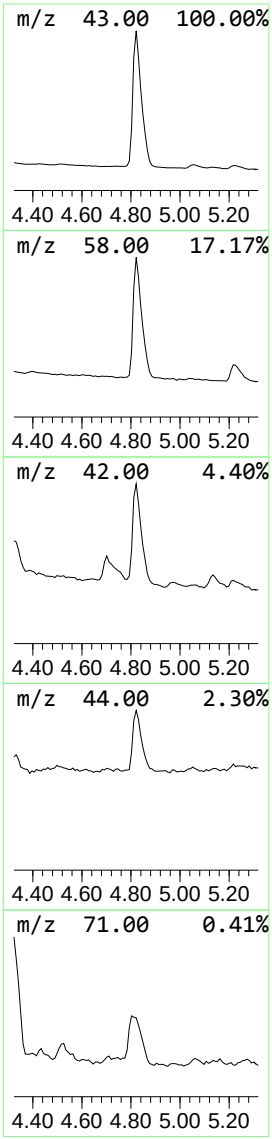
****

Peak Number 4 Acetone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.30 ng	76186	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone	58	C3H6O	000067-64-1	4
2	Butane	58	C4H10	000106-97-8	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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Sample : M3829-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE125D1-20210917

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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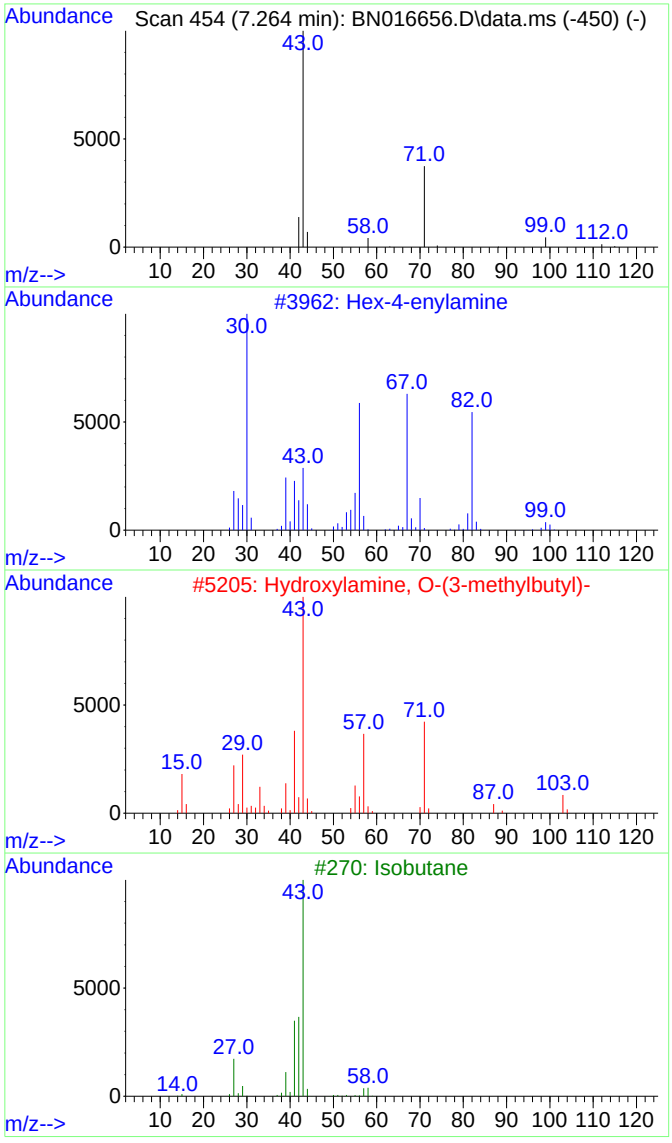
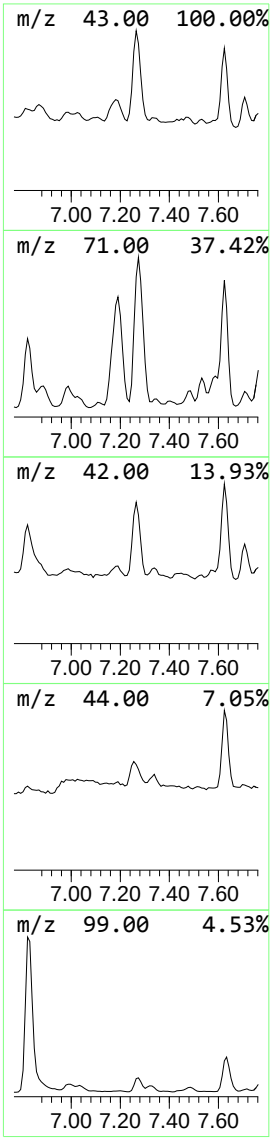
****

Peak Number 5 Hex-4-enylamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	14244	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	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	4
3	Isobutane	58	C4H10	000075-28-5	4
4	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
5	1-Butanol	74	C4H10O	000071-36-3	3





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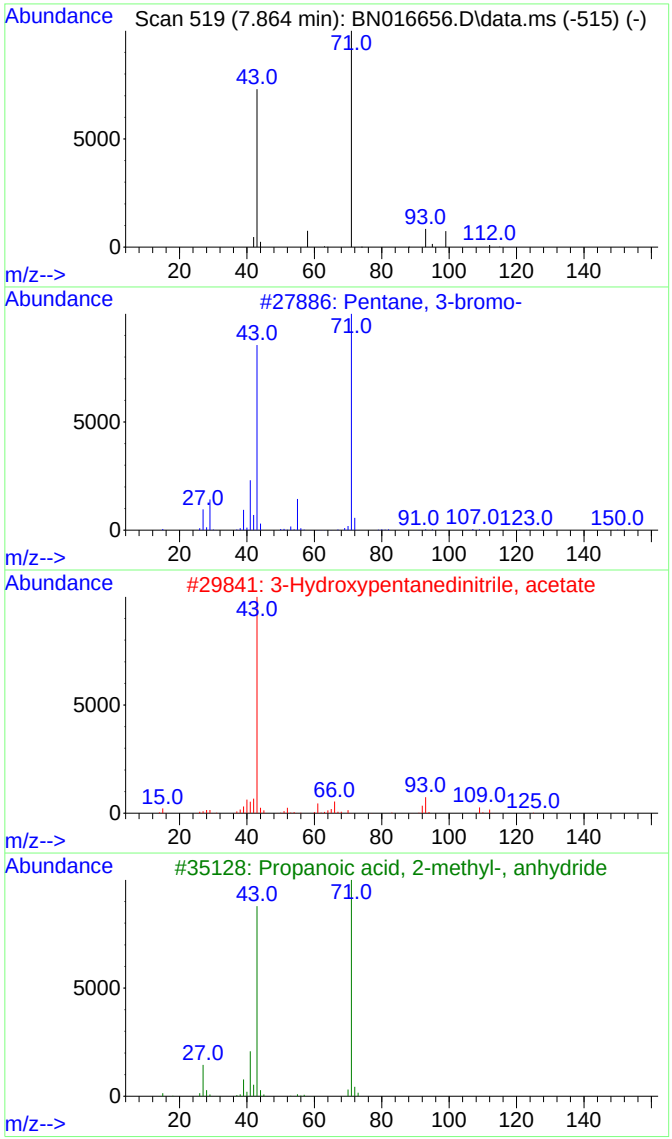
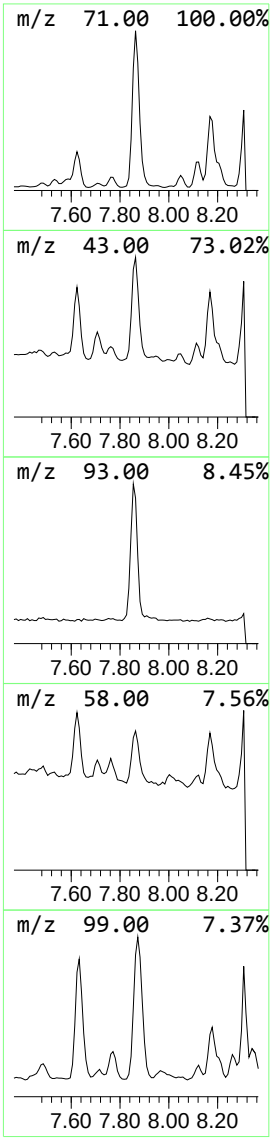
****

Peak Number 6 Pentane, 3-bromo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.10 ng	25703	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4
2	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
3	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
5	Methallyl butyrate	142	C8H14O2	1000428-83-8	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
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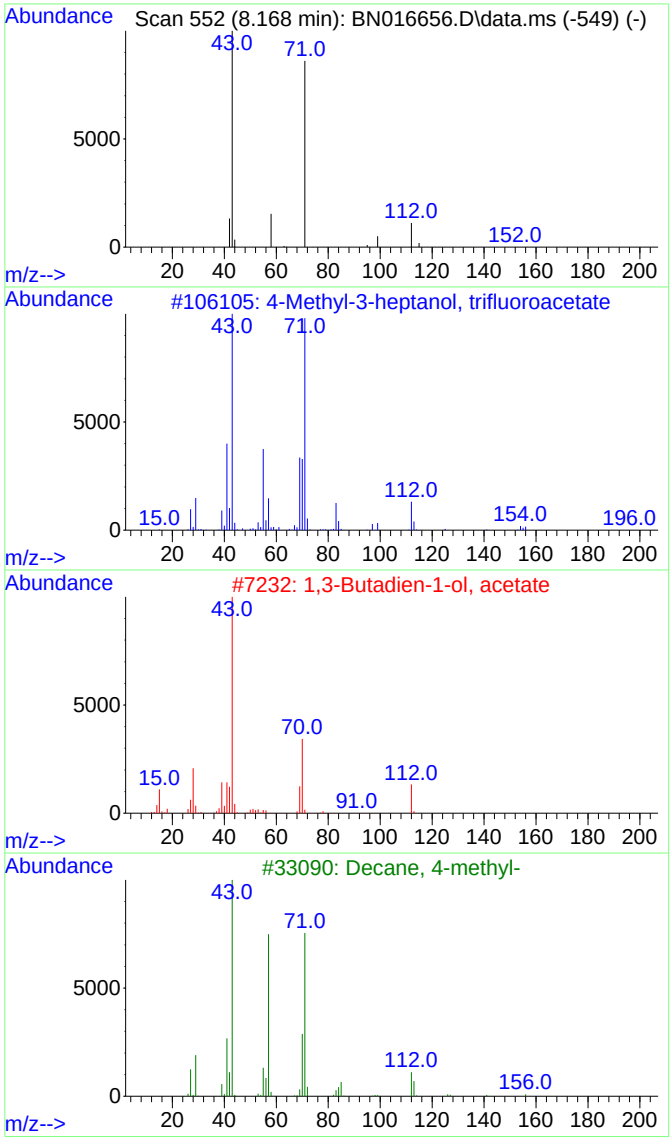
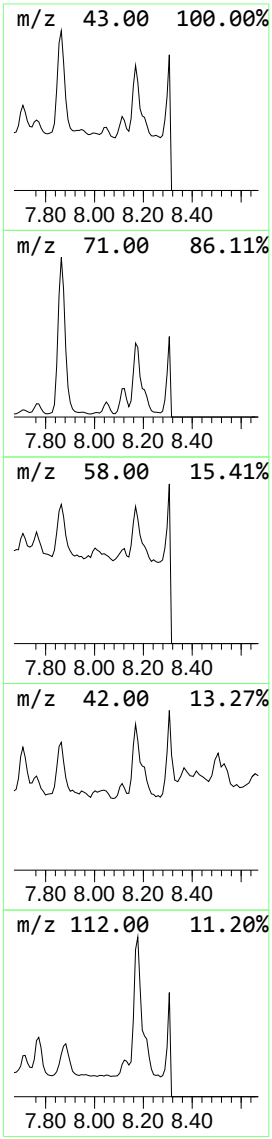
****
Peak Number 7 4-Methyl-3-heptanol, triflu... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.08 ng	20928	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	Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	9





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TIC Library : C:\Database\NIST20.L
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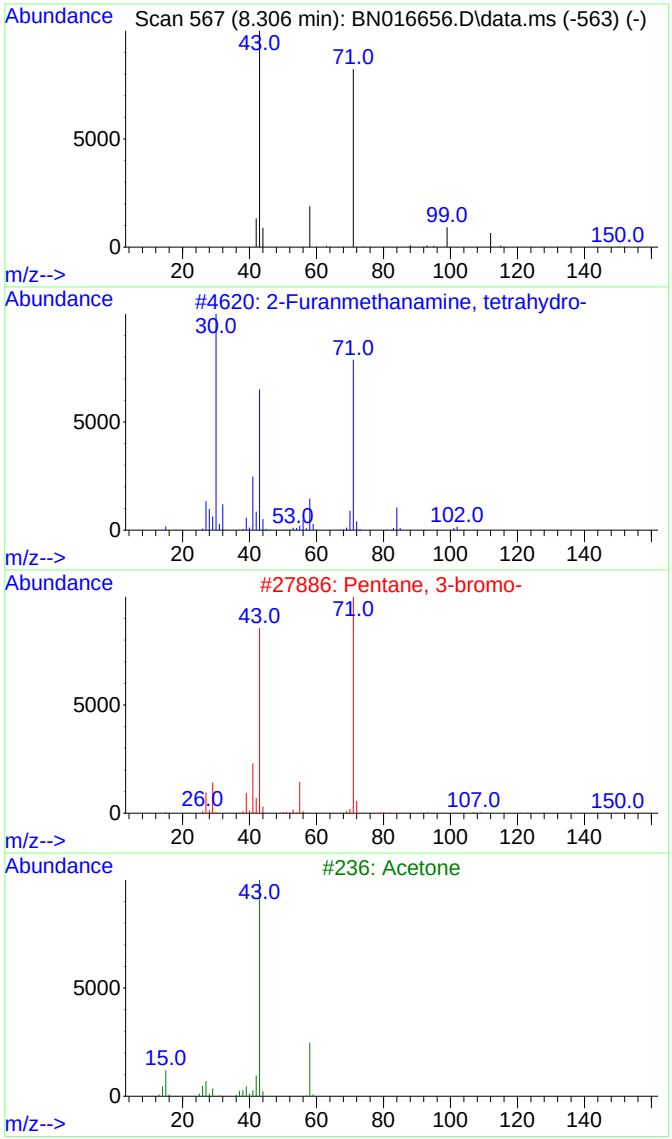
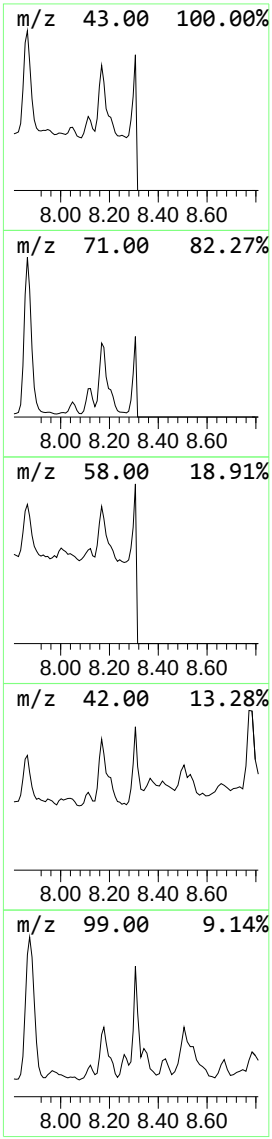
****
Peak Number 8 2-Furanmethanamine, tetrahy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.06 ng	15819	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9
2	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	7
3	Acetone	58	C3H6O	000067-64-1	5
4	Butane	58	C4H10	000106-97-8	5
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4





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TIC Library : C:\Database\NIST20.L
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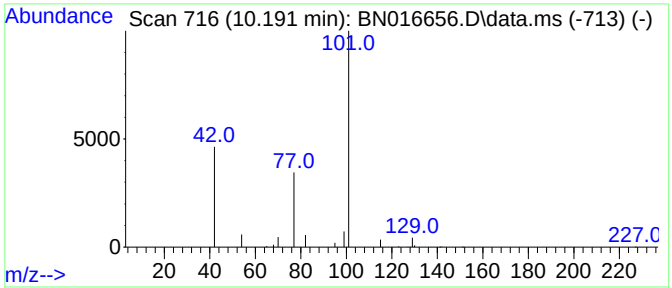
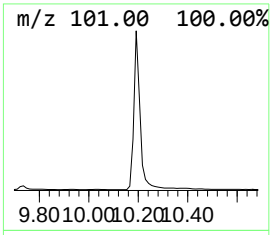
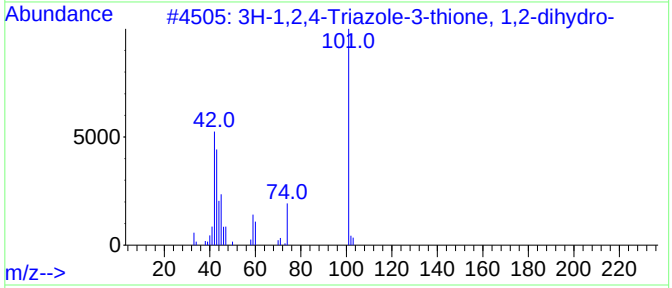
****
Peak Number 9 3H-1,2,4-Triazole-3-thione,... Concentration Rank 5

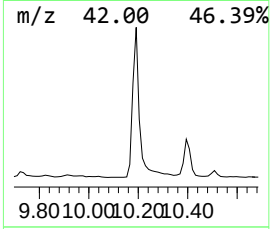
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.12 ng	51015	Naphthalene-d8	10.407

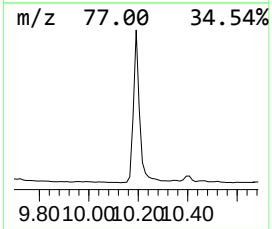
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5	3-Aminopropionitrile	70	C3H6N2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

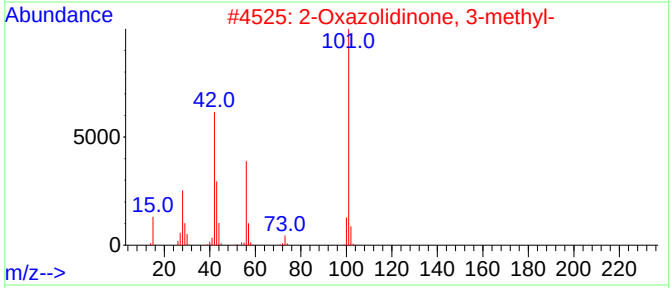


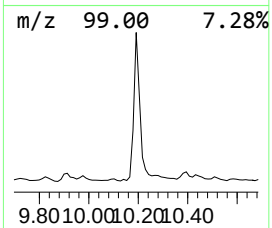


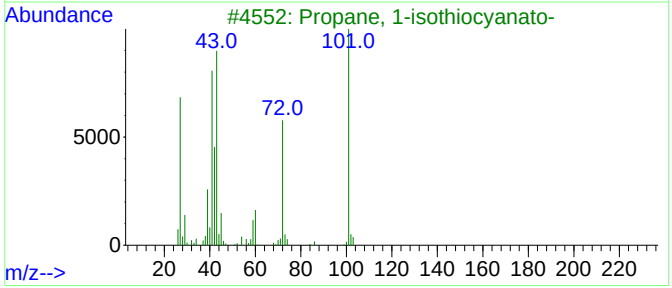


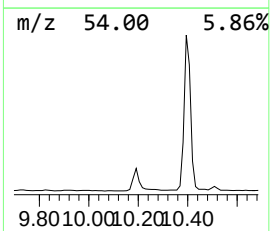












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016656.D
Acq On : 02 Oct 2021 05:10
Operator : CG/JU
Sample : M3829-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE125D1-20210917

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyridine, 1-oxide	3.152	2.6	ng	643057	1	7.642	100814	0.4
Pyridine, 1-oxide	3.189	1.6	ng	403929	1	7.642	100814	0.4
Acetic acid, me...	3.816	0.2	ng	39065	1	7.642	100814	0.4
Acetone	4.821	0.3	ng	76186	1	7.642	100814	0.4
Hex-4-enylamine	7.264	0.1	ng	14244	1	7.642	100814	0.4
Pentane, 3-bromo-	7.864	0.1	ng	25703	1	7.642	100814	0.4
4-Methyl-3-hept...	8.168	0.1	ng	20928	1	7.642	100814	0.4
2-Furanmethanam...	8.306	0.1	ng	15819	1	7.642	100814	0.4
3H-1,2,4-Triazo...	10.191	0.1	ng	51015	2	10.407	167307	0.4