

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016682.D
 Acq On : 02 Oct 2021 21:57
 Operator : CG/JU
 Sample : M3829-03
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE114D2-20210916

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: BN016682.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	194322	281404	95.89%	9.050%
2	3.253	17	19	29	rVB	93771	293470	100.00%	9.438%
3	3.364	29	31	42	rVB	48352	86153	29.36%	2.771%
4	3.816	77	80	97	rVB	8385	33790	11.51%	1.087%
5	4.821	185	189	203	rVB	54509	123186	41.98%	3.962%
6	5.263	234	237	245	rVB	5686	14139	4.82%	0.455%
7	5.678	279	282	288	rBV2	1498	4572	1.56%	0.147%
8	6.296	345	349	355	rBV	14633	32063	10.93%	1.031%
9	6.637	383	386	395	rVB3	4476	11077	3.77%	0.356%
10	6.822	403	406	419	rVB3	4351	17232	5.87%	0.554%
11	7.181	441	445	449	rBV2	2858	7401	2.52%	0.238%
12	7.264	449	454	460	rVB3	7611	19195	6.54%	0.617%
13	7.633	490	494	500	rVB	55804	115541	39.37%	3.716%
14	7.864	515	519	526	rBV	16127	32412	11.04%	1.042%
15	8.112	543	546	549	rBV	2744	6064	2.07%	0.195%
16	8.168	549	552	561	rVV	10446	29902	10.19%	0.962%
17	8.306	563	567	569	rVB	12995	17184	5.86%	0.553%
18	8.784	601	605	610	rBV	22835	46284	15.77%	1.488%
19	9.088	626	629	632	rBV	6387	10811	3.68%	0.348%
20	10.191	713	716	724	rBV	114659	193051	65.78%	6.208%
21	10.407	729	733	739	rVB	112049	193704	66.00%	6.229%
22	11.205	790	796	803	rBV4	3445	11435	3.90%	0.368%
23	12.003	921	931	942	rBV	44279	71443	24.34%	2.298%
24	12.886	1071	1074	1078	rBV	90652	148542	50.62%	4.777%
25	13.177	1094	1097	1103	rBV2	4508	8695	2.96%	0.280%
26	14.269	1180	1183	1186	rBV	143659	204165	69.57%	6.566%
27	14.434	1193	1196	1198	rBV	6055	9269	3.16%	0.298%
28	15.715	1294	1297	1299	rBV	8026	11746	4.00%	0.378%
29	15.766	1299	1301	1311	rVB2	12528	21847	7.44%	0.703%
30	17.017	1400	1403	1410	rBV	104974	167716	57.15%	5.394%
31	19.063	1688	1696	1715	rBV	124840	175577	59.83%	5.646%
32	19.678	1813	1820	1843	rBV	169314	212767	72.50%	6.842%
33	21.164	1993	1995	1998	rBV	30177	39870	13.59%	1.282%
34	21.227	1998	2001	2011	rVB	120672	190529	64.92%	6.127%
35	22.311	2100	2103	2108	rBV	4984	10929	3.72%	0.351%
36	22.841	2232	2239	2259	rVB	3981	6430	2.19%	0.207%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016682.D
 Acq On : 02 Oct 2021 21:57
 Operator : CG/JU
 Sample : M3829-03
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE114D2-20210916

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	23.423	2400	2409	2415	rBV	5627	9845	3.35%	0.317%
38	23.481	2415	2426	2460	rVB	97599	201045	68.51%	6.465%
39	24.087	2593	2603	2624	rBV	6149	12115	4.13%	0.390%
40	24.853	2817	2827	2844	rBV	5787	13423	4.57%	0.432%
41	25.757	3073	3091	3110	rBV	1902	5478	1.87%	0.176%
42	26.818	3385	3401	3424	rBV	1406	4993	1.70%	0.161%
43	28.081	3747	3770	3796	rBV2	760	3023	1.03%	0.097%

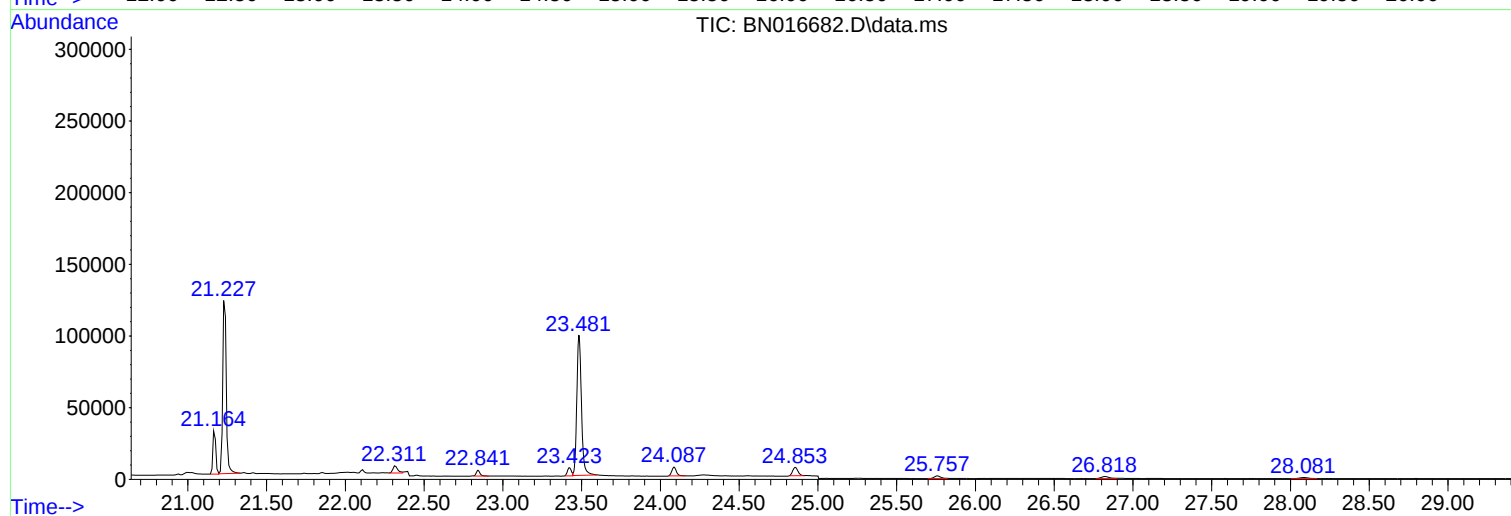
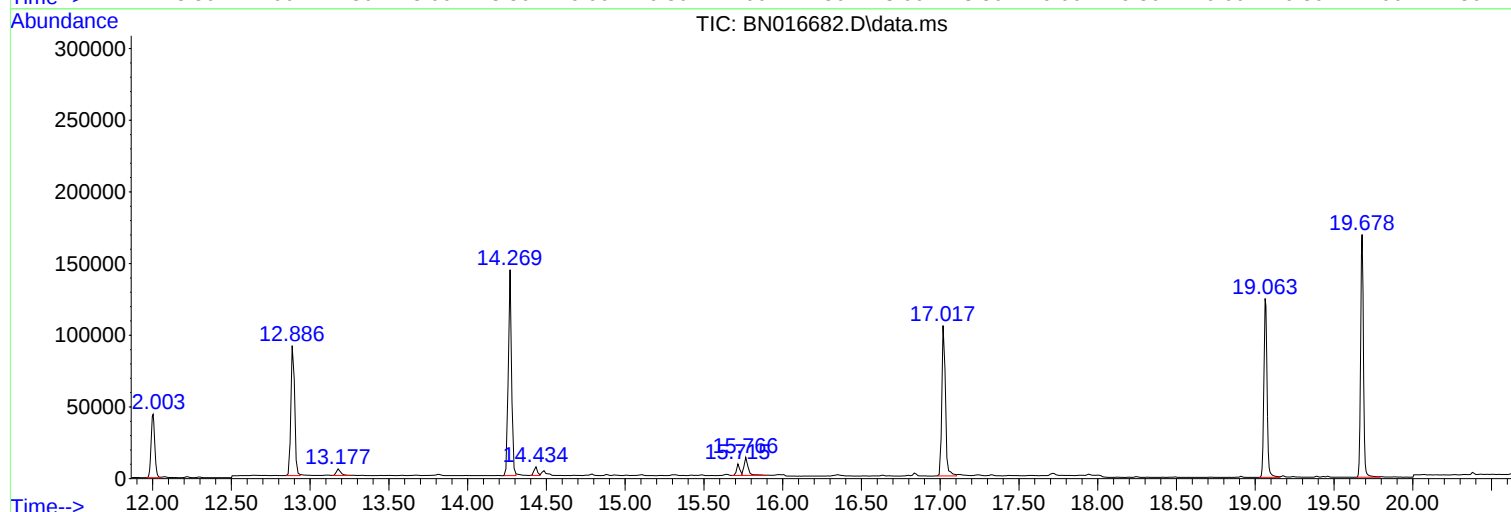
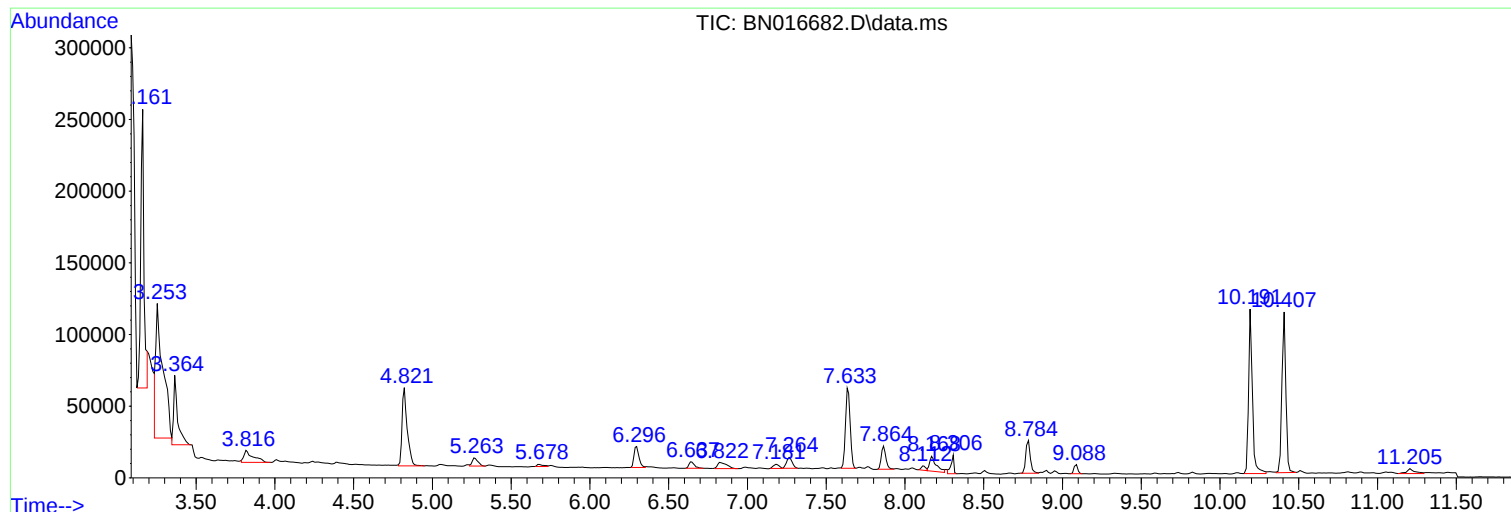
Sum of corrected areas: 3109517

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

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 : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

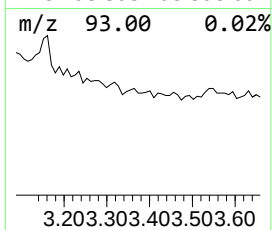
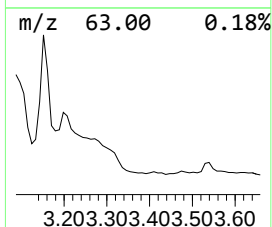
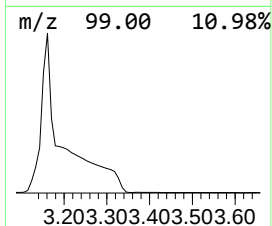
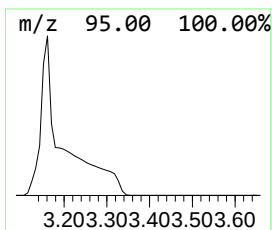
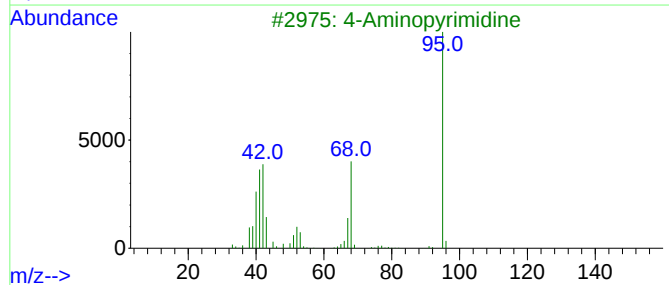
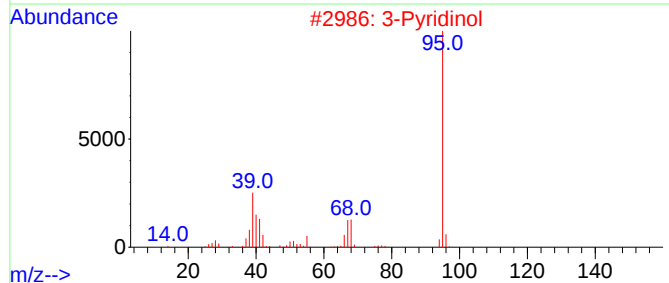
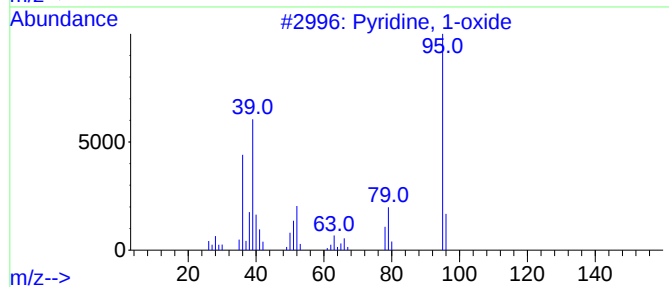
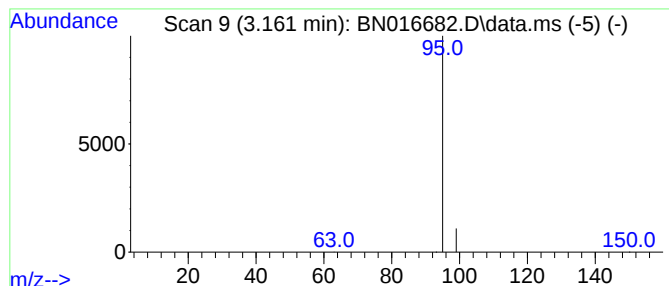
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	0.97 ng	281404	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)aminoacrylonitrile	95	C4H5N3	167320-31-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

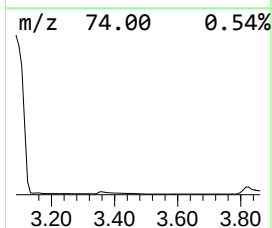
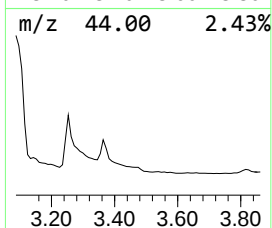
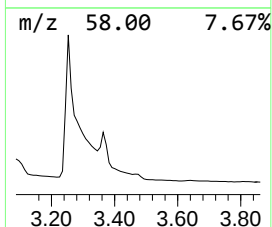
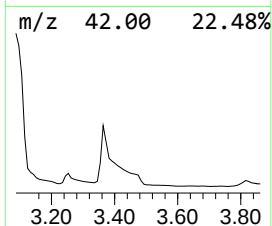
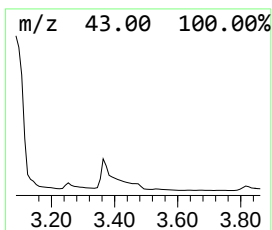
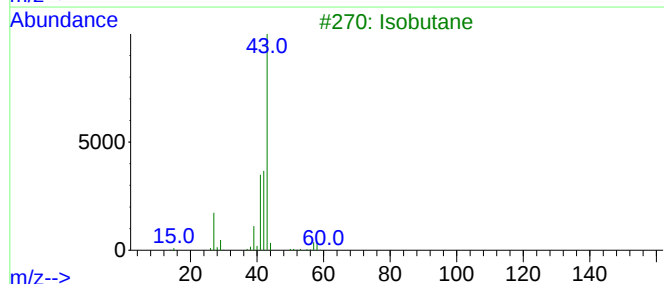
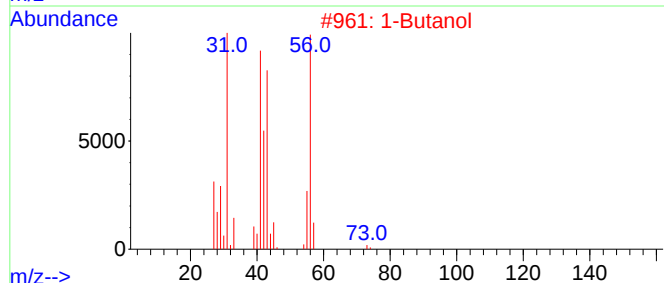
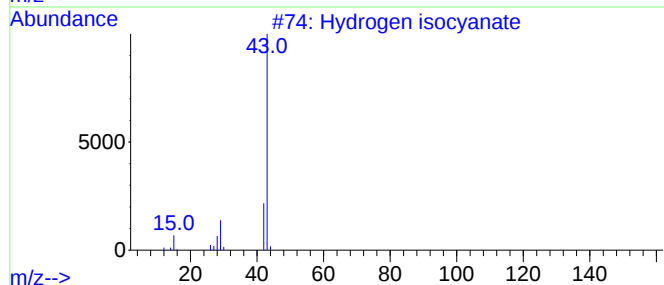
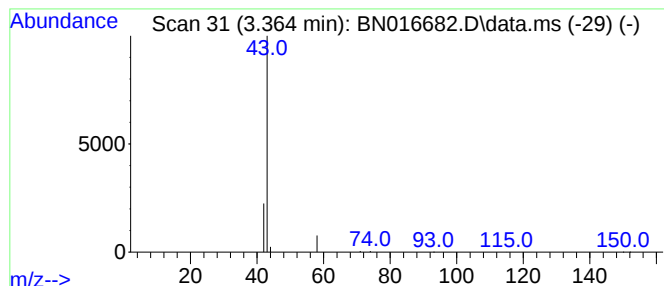
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hydrogen isocyanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.30 ng	86153	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-Butanol	74	C4H10O	000071-36-3	3
3			Isobutane	58	C4H10	000075-28-5	3
4			Hydrogen azide	43	HN3	007782-79-8	2
5			Butane	58	C4H10	000106-97-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

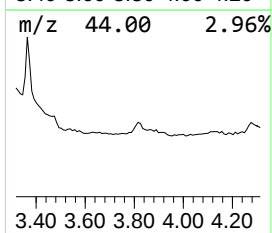
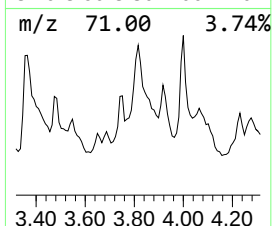
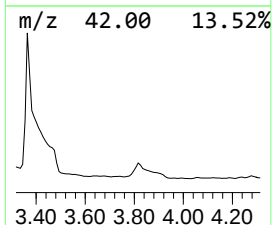
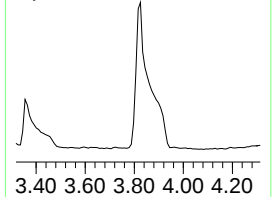
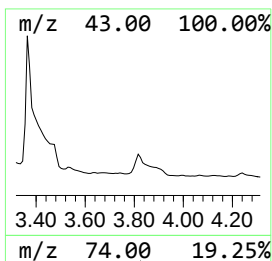
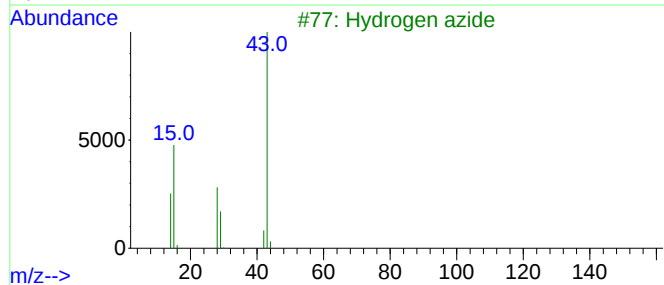
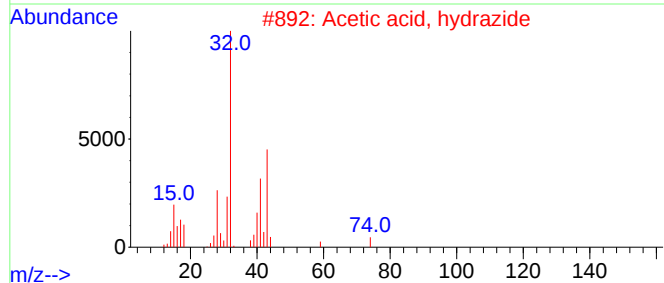
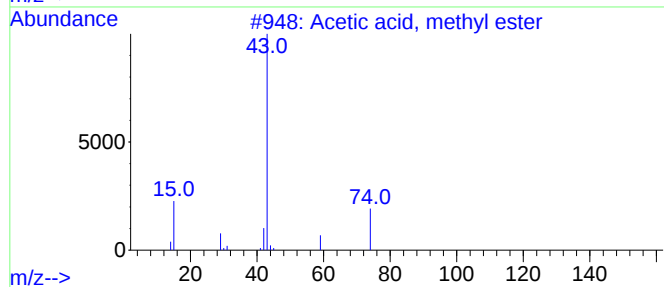
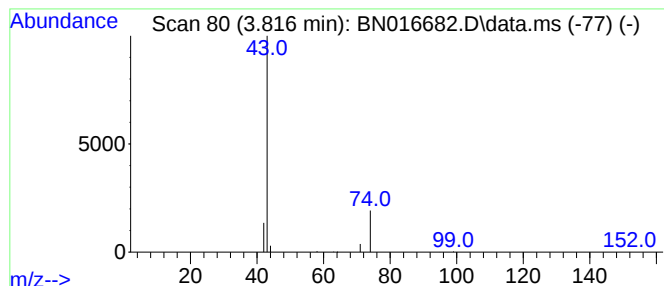
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.12 ng	33790	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	9
2			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	5
3			Hydrogen azide	43	HN3	007782-79-8	4
4			O-Methylisourea	74	C2H6N2O	002440-60-0	4
5			2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

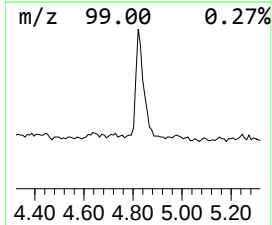
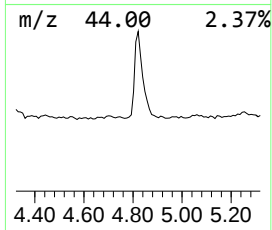
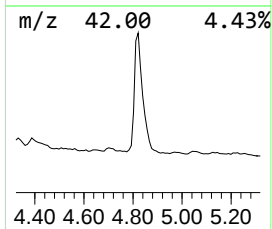
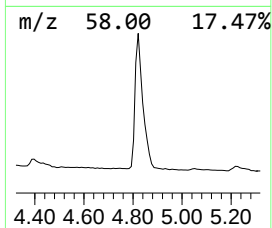
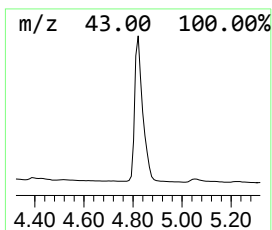
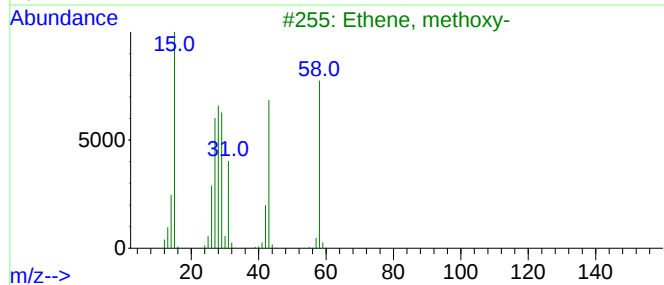
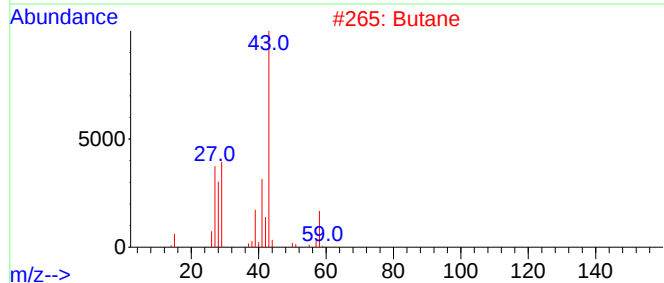
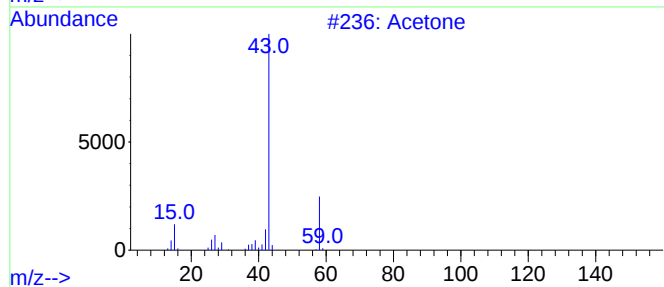
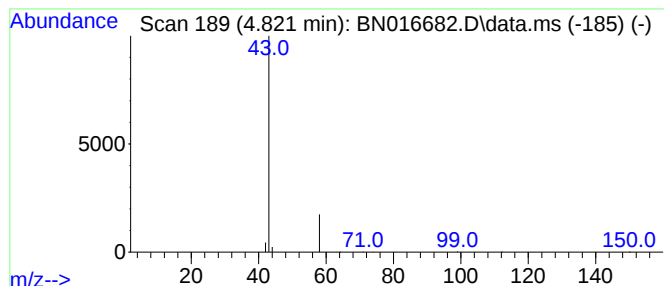
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Acetone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.43 ng	123186	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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

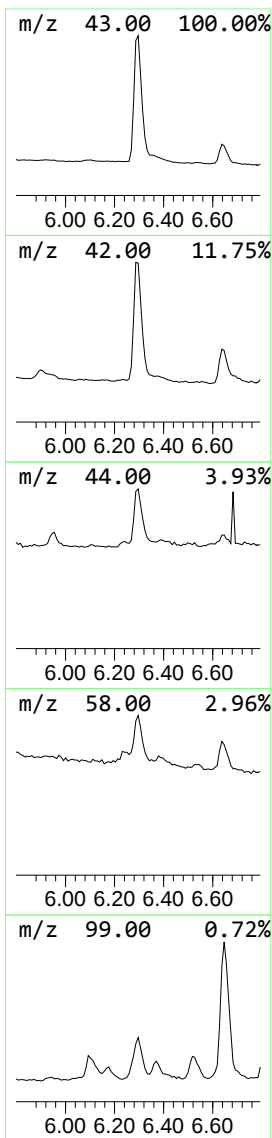
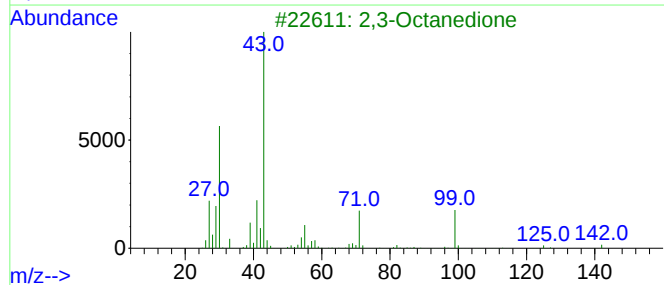
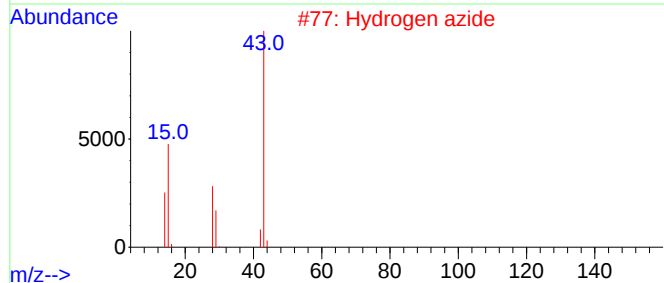
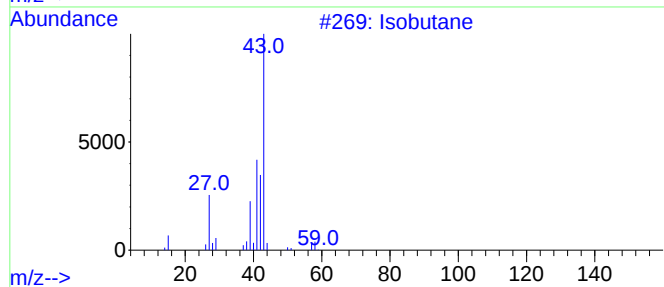
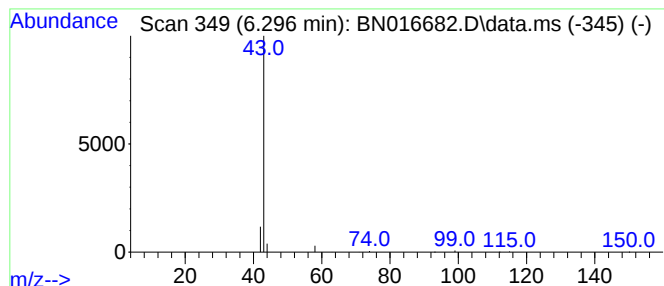
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.11 ng	32063	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-Octanedione	142	C8H14O2	000585-25-1	2
4			1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-66-3	2
5			Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

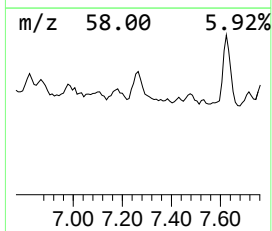
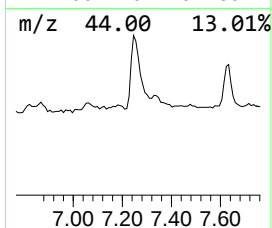
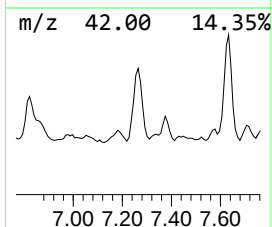
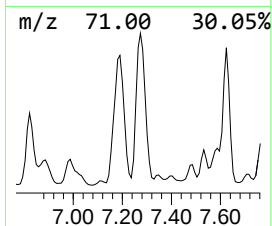
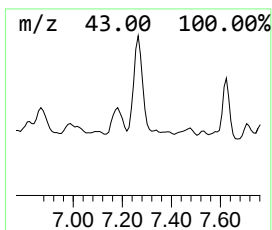
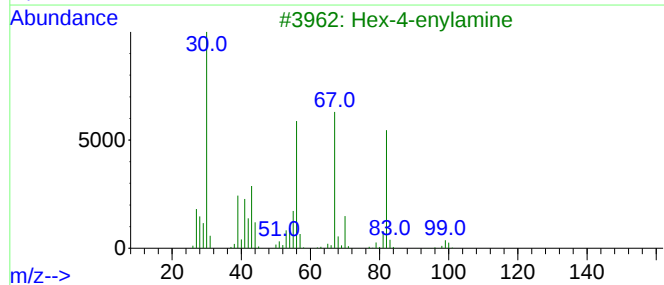
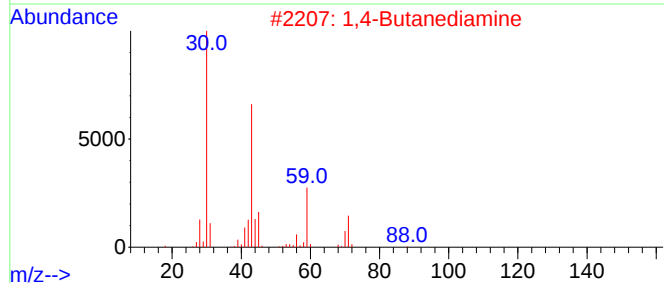
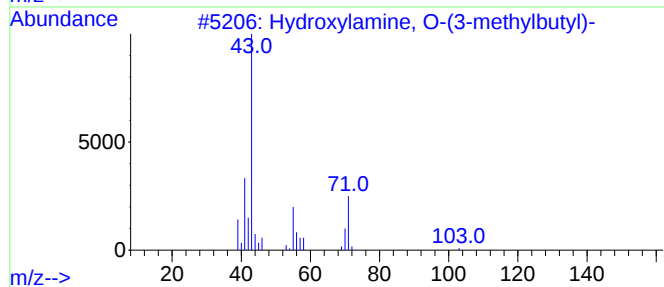
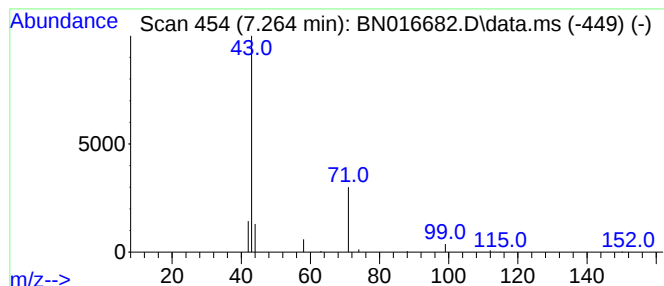
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hydroxylamine, O-(3-methylb... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.07 ng	19195	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
2		1,4-Butanediamine	88	C4H12N2	000110-60-1	5
3		Hex-4-enylamine	99	C6H13N	055108-01-5	5
4		N-Acetyethylenediamine	102	C4H10N2O	001001-53-2	4
5		Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

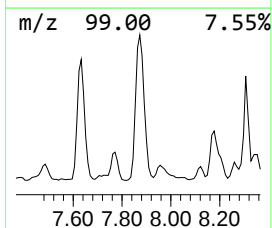
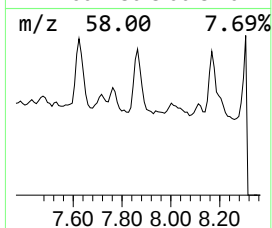
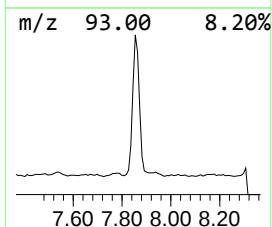
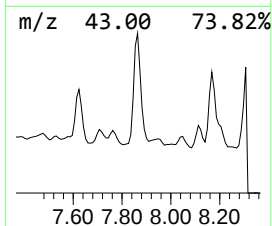
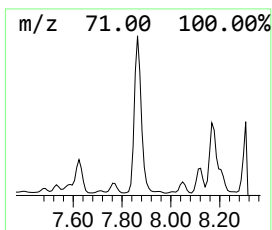
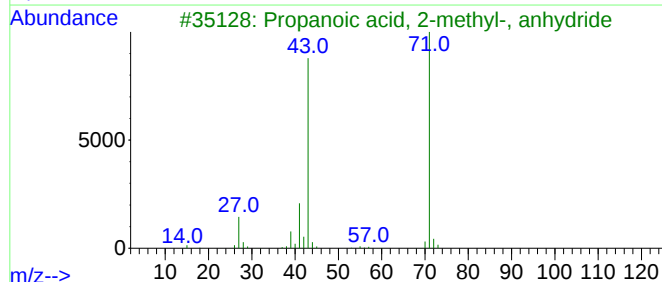
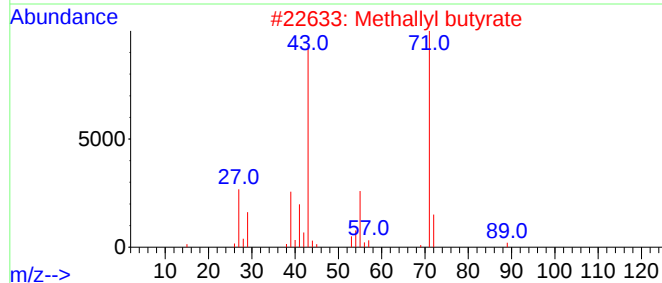
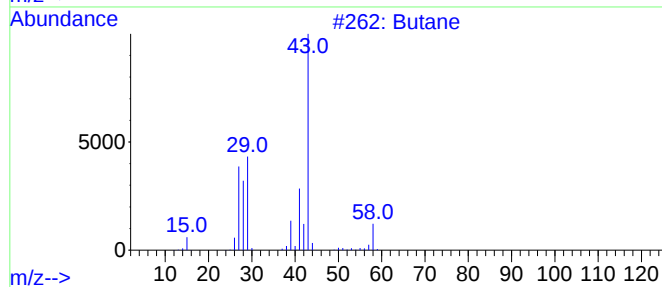
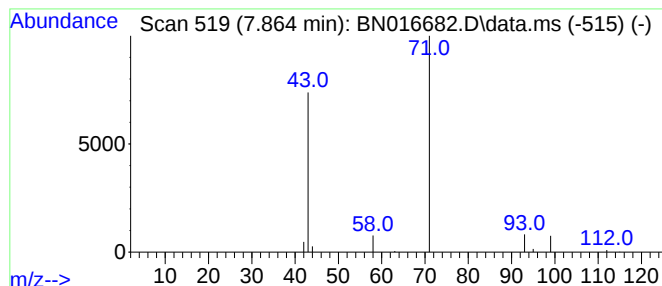
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.11 ng	32412	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Methallyl butyrate	142	C8H14O2	1000428-83-8	4
3			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
4			Hydrogen azide	43	HN3	007782-79-8	4
5			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

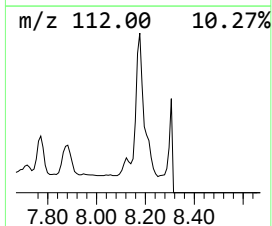
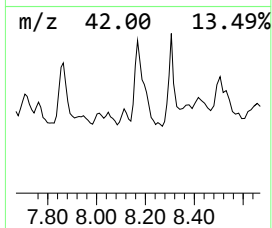
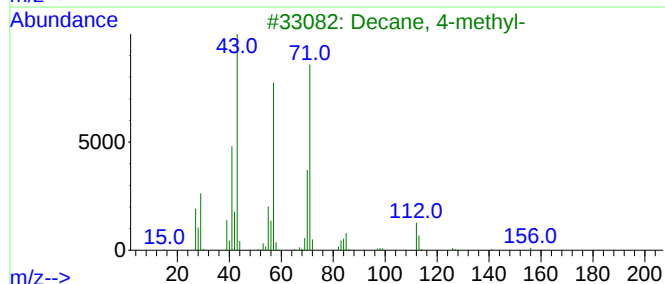
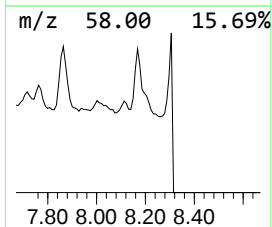
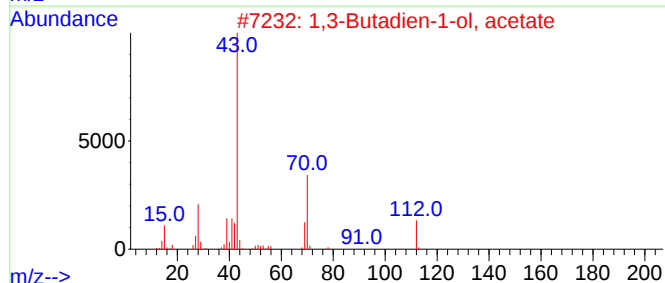
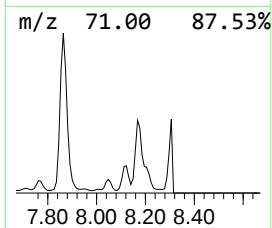
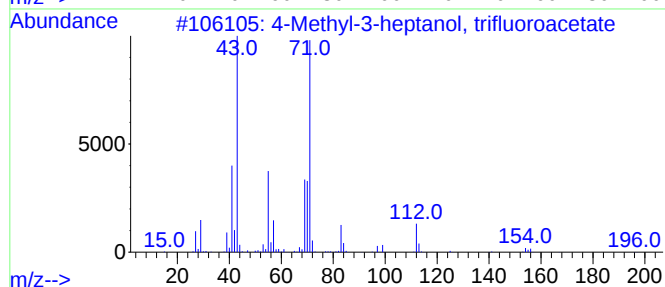
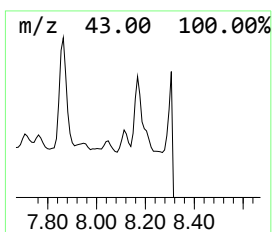
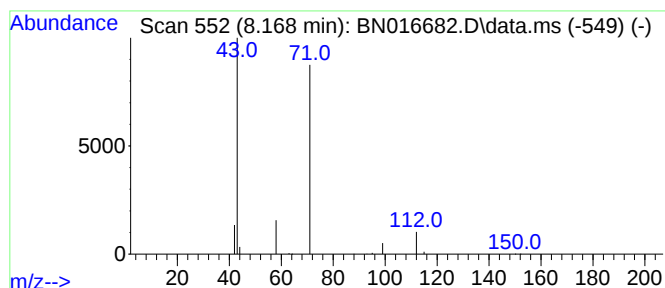
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.10 ng	29902	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			Butane	58	C4H10	000106-97-8	7
5			Trifluoroacetamide	112	C2H3F3N2	000354-37-0	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

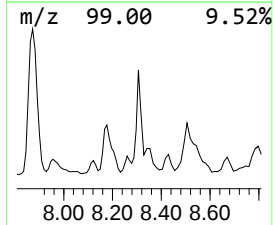
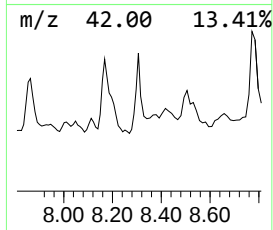
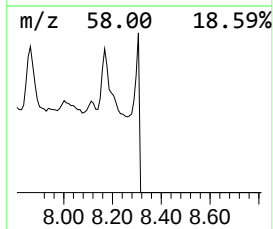
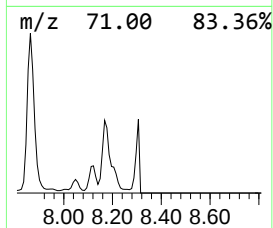
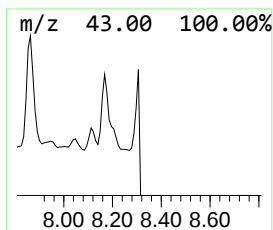
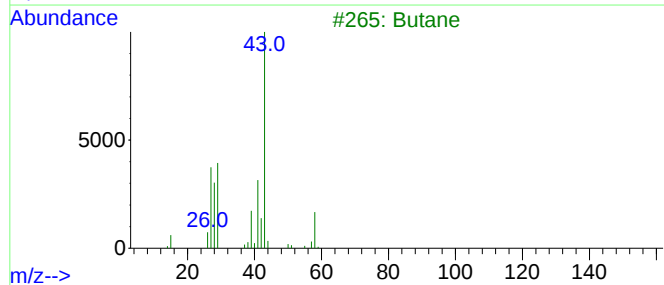
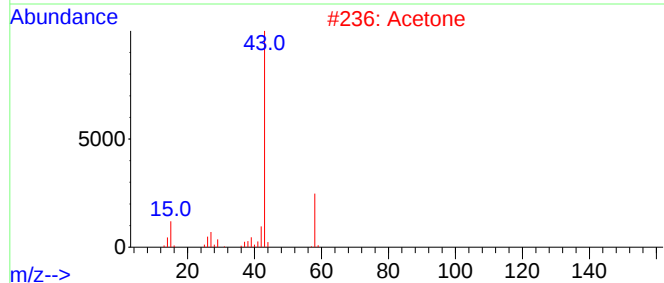
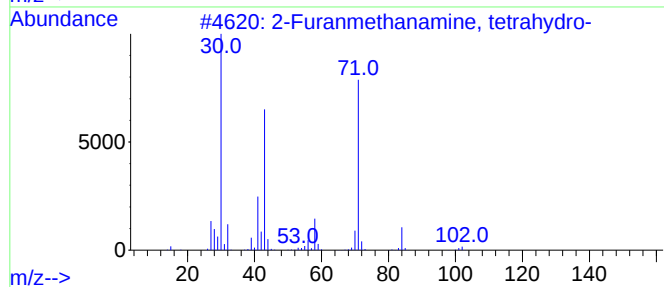
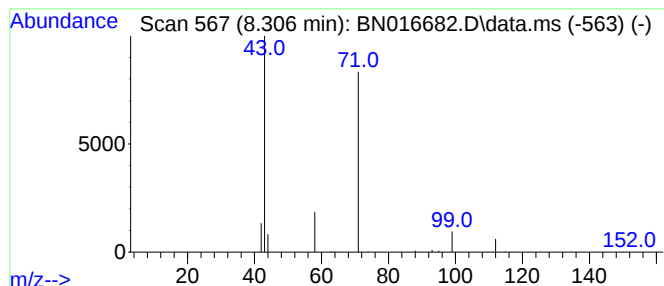
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Furanmethanamine, tetrahy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.06 ng	17184	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		Acetone	58	C3H6O	000067-64-1	5
3		Butane	58	C4H10	000106-97-8	5
4		Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	4
5		Hexamethylenimine	99	C6H13N	000111-49-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

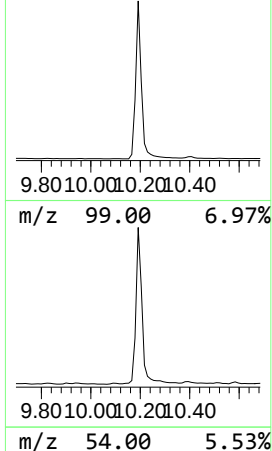
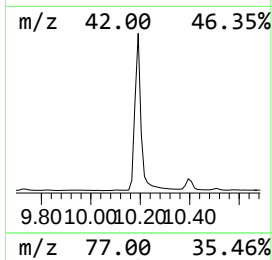
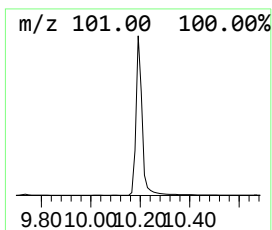
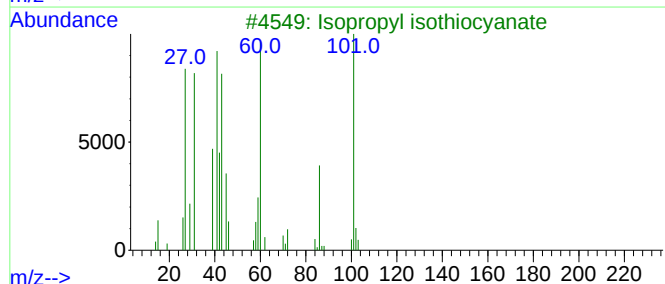
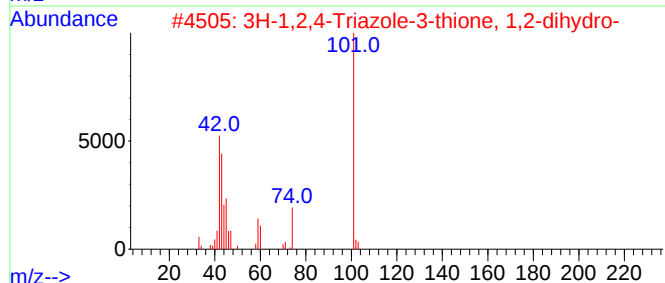
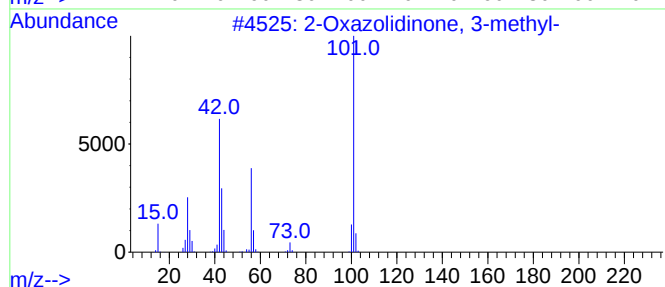
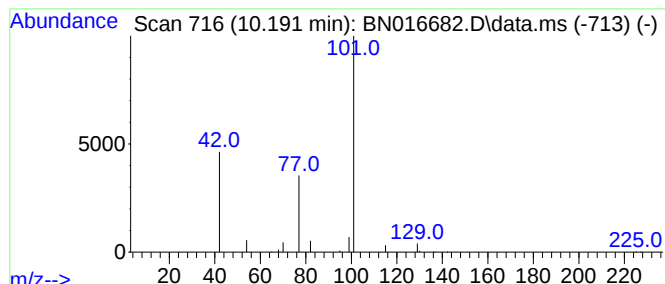
Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

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-Oxazolidinone, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.191	0.40 ng	193051	Naphthalene-d8		10.406	
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	2-Pyrrolidinethione		101	C4H7NS	002295-35-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016682.D
Acq On : 02 Oct 2021 21:57
Operator : CG/JU
Sample : M3829-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE114D2-20210916

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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.161	1.0	ng	281404	1	7.642	115541	0.4
Hydrogen isocya...	3.364	0.3	ng	86153	1	7.642	115541	0.4
Acetic acid, me...	3.816	0.1	ng	33790	1	7.642	115541	0.4
Acetone	4.821	0.4	ng	123186	1	7.642	115541	0.4
Isobutane	6.296	0.1	ng	32063	1	7.642	115541	0.4
Hydroxylamine, ...	7.264	0.1	ng	19195	1	7.642	115541	0.4
Butane	7.864	0.1	ng	32412	1	7.642	115541	0.4
4-Methyl-3-hept...	8.168	0.1	ng	29902	1	7.642	115541	0.4
2-Furanmethanam...	8.306	0.1	ng	17184	1	7.642	115541	0.4
2-Oxazolidinone...	10.191	0.4	ng	193051	2	10.406	193704	0.4