

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleID :
 MW201D-20210919

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: BN016643.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	11	rBV	252466	397108	51.72%	10.692%
2	3.253	17	19	42	rVB	198707	767769	100.00%	20.672%
3	3.502	43	46	59	rVB	5944	25363	3.30%	0.683%
4	3.816	76	80	97	rVB	11543	48563	6.33%	1.308%
5	4.406	141	144	166	rVB	10306	42771	5.57%	1.152%
6	4.821	185	189	205	rVB	41697	96825	12.61%	2.607%
7	5.273	234	238	244	rVB2	7501	18929	2.47%	0.510%
8	5.365	245	248	260	rVB	3429	10380	1.35%	0.279%
9	6.647	383	387	397	rBV	6948	15593	2.03%	0.420%
10	6.849	403	409	418	rVB2	9491	29666	3.86%	0.799%
11	7.264	449	454	460	rVB3	7787	21979	2.86%	0.592%
12	7.642	490	495	500	rBV	45785	94016	12.25%	2.531%
13	7.864	515	519	525	rBV	9961	21013	2.74%	0.566%
14	8.177	549	553	559	rVB2	5151	13559	1.77%	0.365%
15	8.306	564	567	569	rVB	9488	10900	1.42%	0.293%
16	8.784	602	605	610	rBV	29218	54775	7.13%	1.475%
17	8.949	616	618	621	rVB	5255	8638	1.13%	0.233%
18	9.089	626	629	633	rVB	5506	8280	1.08%	0.223%
19	10.204	713	717	720	rBV	159619	293172	38.18%	7.894%
20	10.407	730	733	736	rBV	95685	162898	21.22%	4.386%
21	11.205	794	796	802	rBV	4087	8087	1.05%	0.218%
22	12.007	919	932	943	rBV	45756	74683	9.73%	2.011%
23	12.898	1071	1075	1078	rBV2	87416	166485	21.68%	4.483%
24	13.114	1089	1092	1095	rBV	5135	8160	1.06%	0.220%
25	13.178	1095	1097	1106	rVB2	10383	21482	2.80%	0.578%
26	14.269	1180	1183	1193	rBV	123162	189620	24.70%	5.106%
27	14.434	1193	1196	1199	rBV	9772	14332	1.87%	0.386%
28	15.284	1260	1263	1269	rBV	7103	11609	1.51%	0.313%
29	15.715	1295	1297	1299	rBV	12242	18893	2.46%	0.509%
30	15.766	1299	1301	1305	rVB2	14084	23390	3.05%	0.630%
31	15.969	1315	1317	1322	rVB3	3386	8618	1.12%	0.232%
32	16.835	1386	1388	1392	rVB	6213	9848	1.28%	0.265%
33	17.018	1400	1403	1409	rBV	89995	157878	20.56%	4.251%
34	17.955	1477	1480	1482	rBV	3638	7748	1.01%	0.209%
35	19.063	1688	1696	1714	rBV	134891	188225	24.52%	5.068%
36	19.678	1813	1820	1837	rBV	128054	158597	20.66%	4.270%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016643.D
Acq On : 01 Oct 2021 19:34
Operator : CG/JU
Sample : M3833-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D-20210919

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	20.972	1975	1977	1980	rBV	10018	15511	2.02%	0.418%
38	21.026	1980	1982	1992	rVB	5650	8327	1.08%	0.224%
39	21.164	1992	1995	1998	rBV	42787	54259	7.07%	1.461%
40	21.227	1998	2001	2010	rVB	129449	185387	24.15%	4.992%
41	22.109	2081	2084	2088	rVB	5641	7760	1.01%	0.209%
42	23.419	2401	2408	2415	rBV	6019	9026	1.18%	0.243%
43	23.481	2415	2426	2458	rVB	101812	195848	25.51%	5.273%
44	24.087	2594	2603	2617	rVB	6743	12793	1.67%	0.344%
45	24.857	2818	2828	2847	rVB	6613	15248	1.99%	0.411%

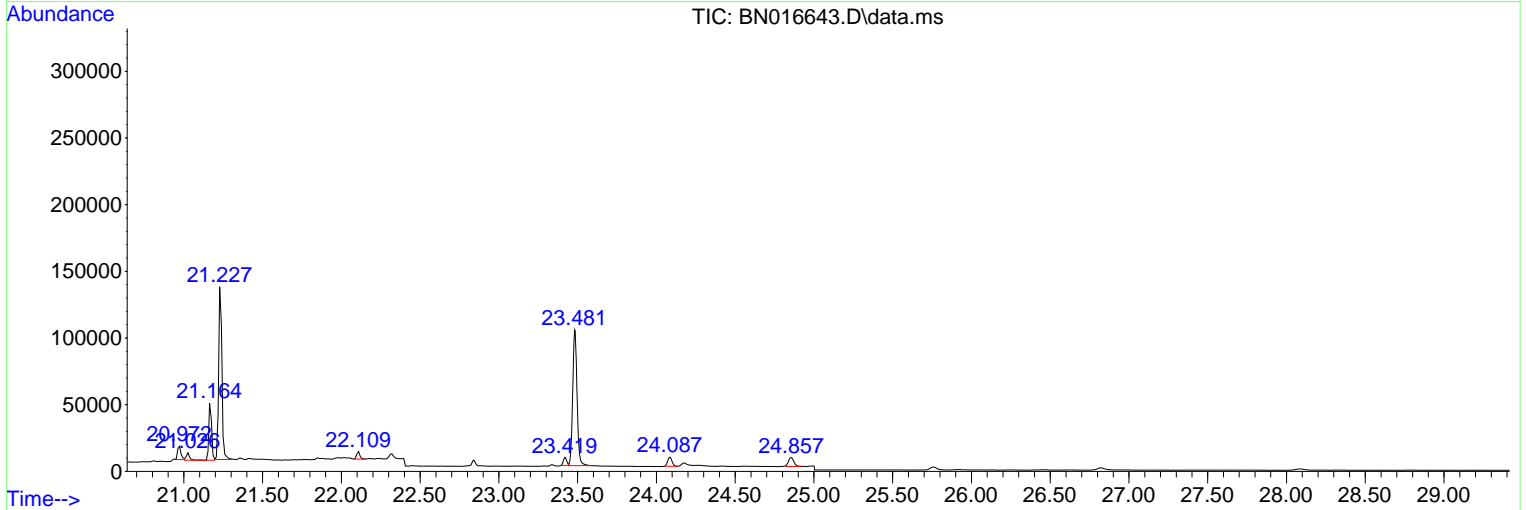
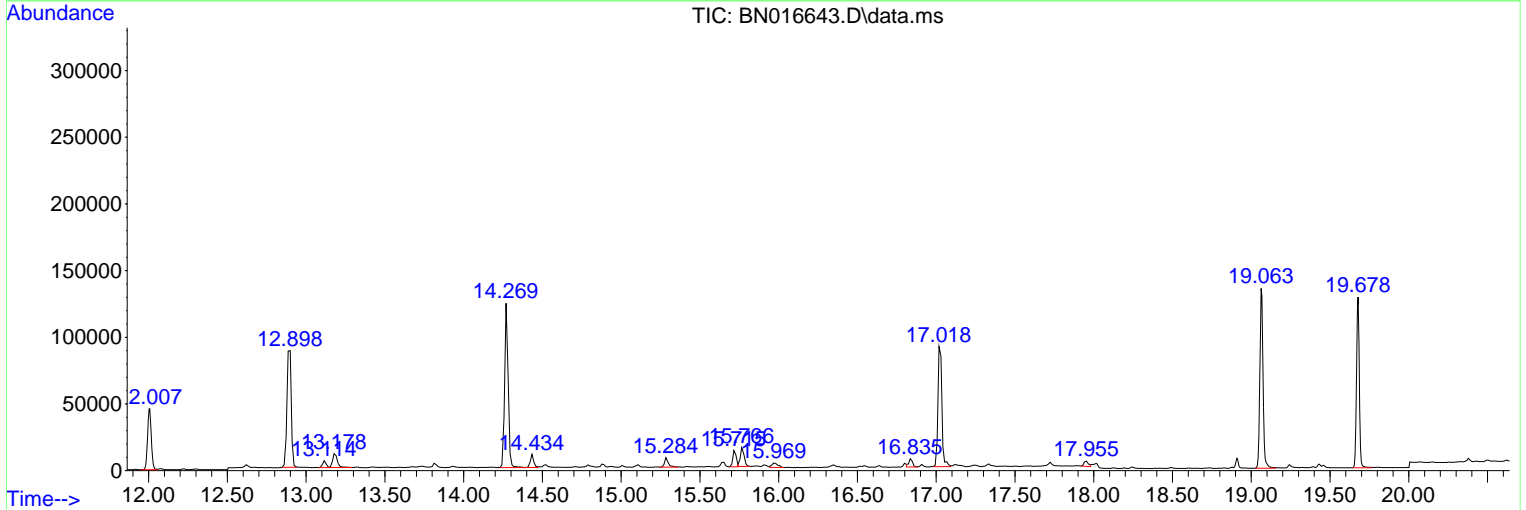
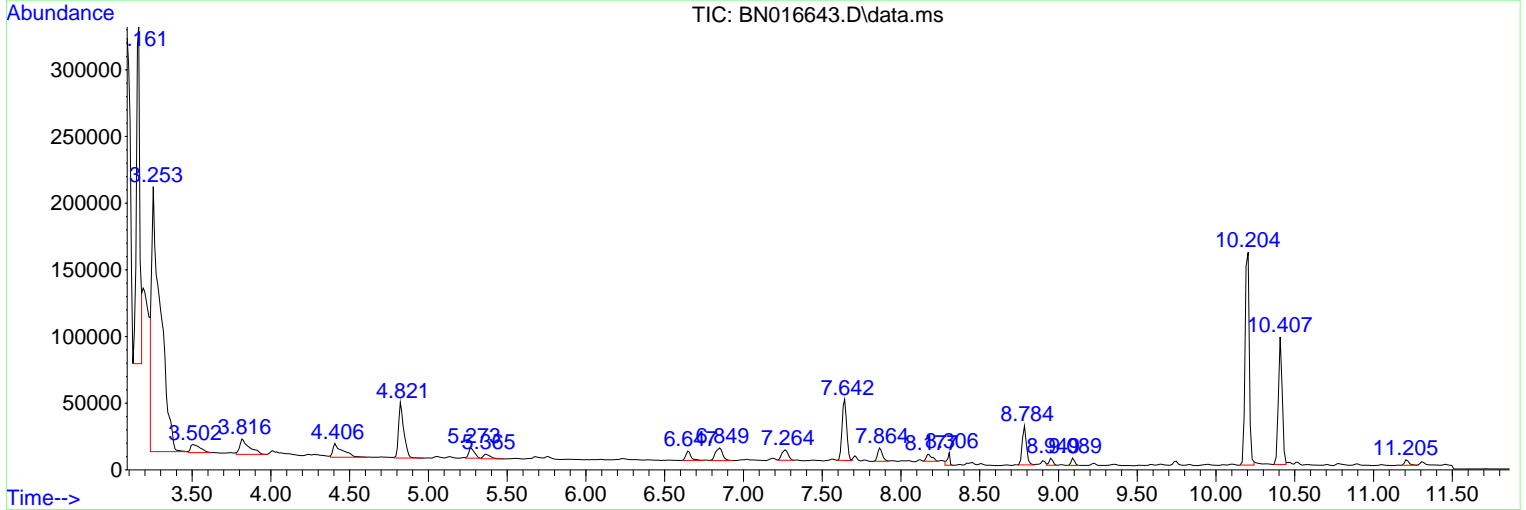
Sum of corrected areas: 3714011

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
ClientSampleId :
 MW201D-20210919

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 : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

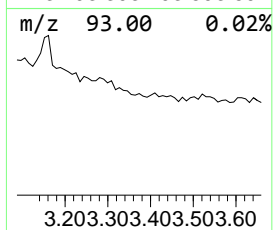
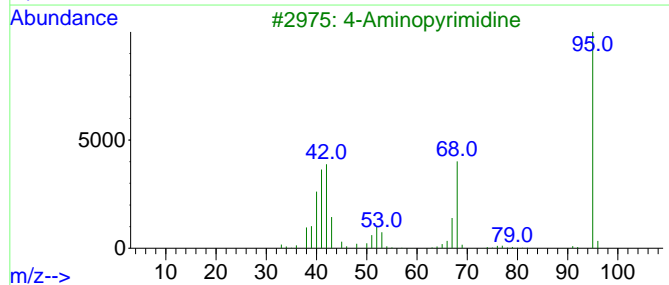
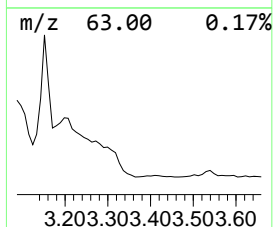
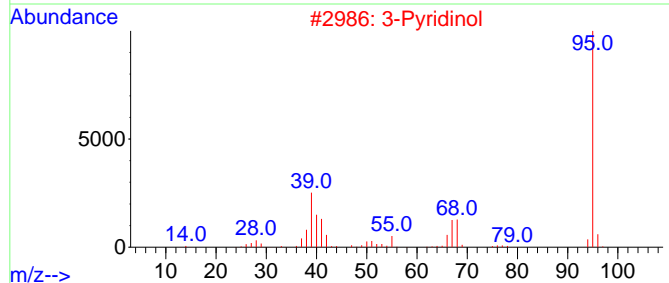
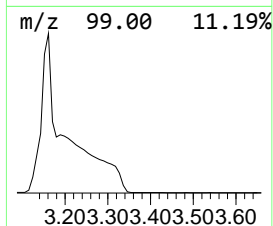
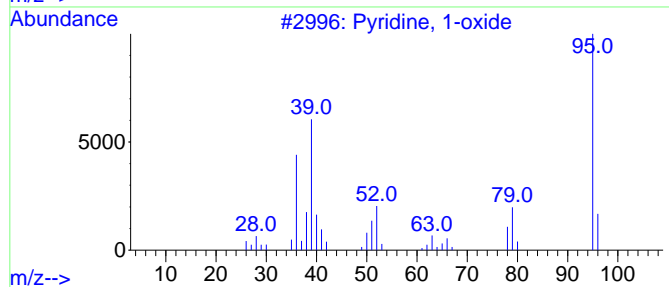
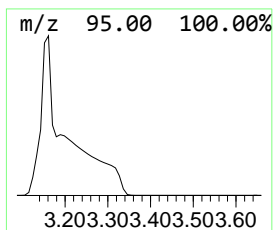
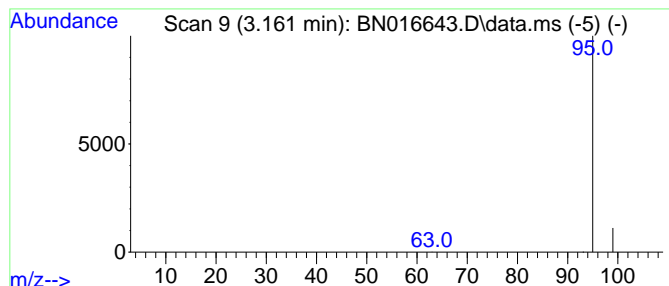
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	1.69 ng	397108	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 : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

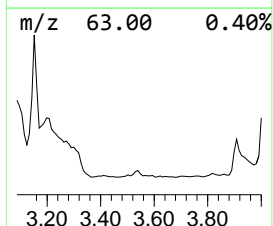
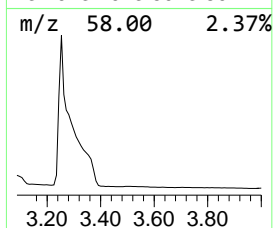
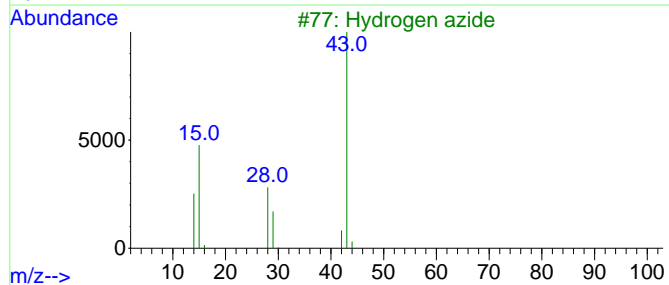
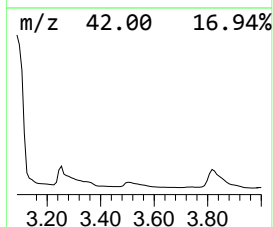
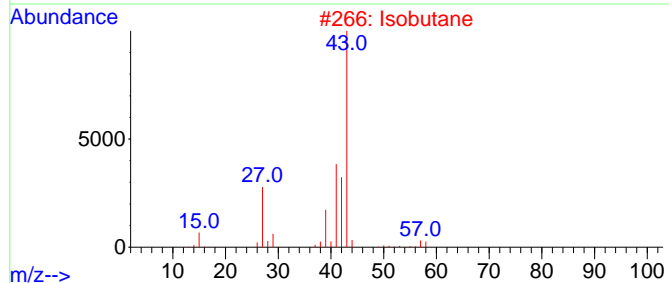
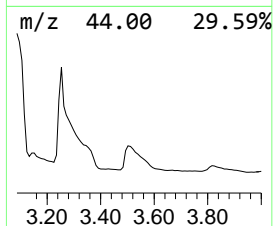
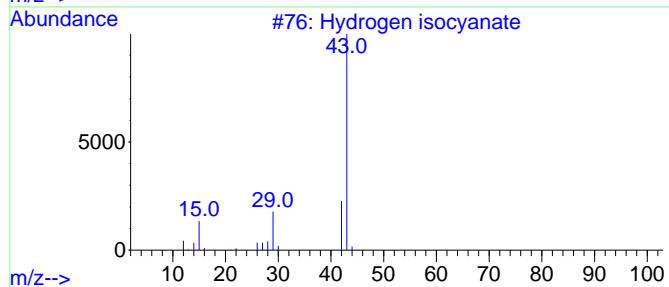
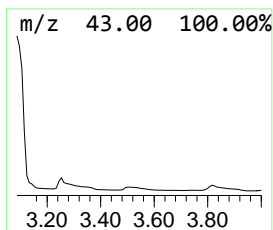
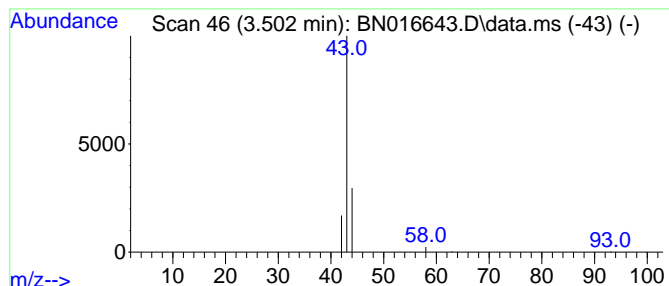
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Hydrogen isocyanate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.502	0.11 ng	25363	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hydrogen isocyanate	43	CHNO	000075-13-8	3
2		Isobutane	58	C4H10	000075-28-5	3
3		Hydrogen azide	43	HN3	007782-79-8	3
4		Acetaldehyde	44	C2H4O	000075-07-0	2
5		Ethylene oxide	44	C2H4O	000075-21-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

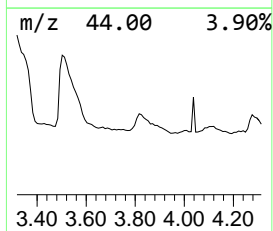
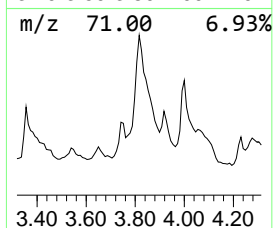
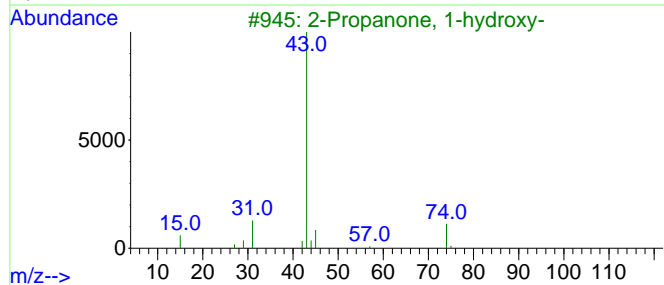
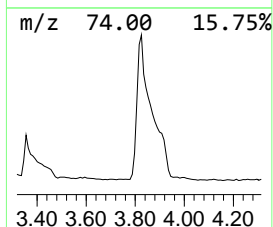
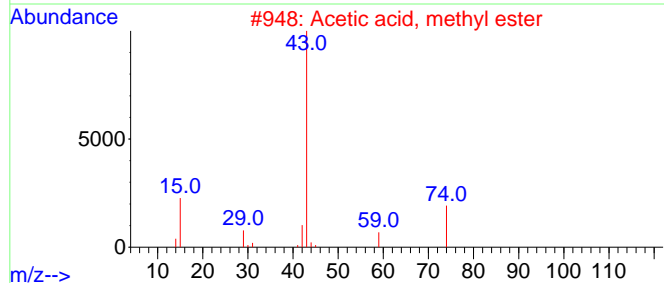
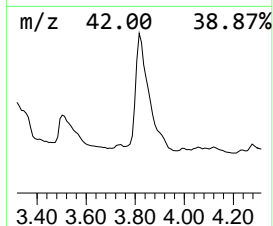
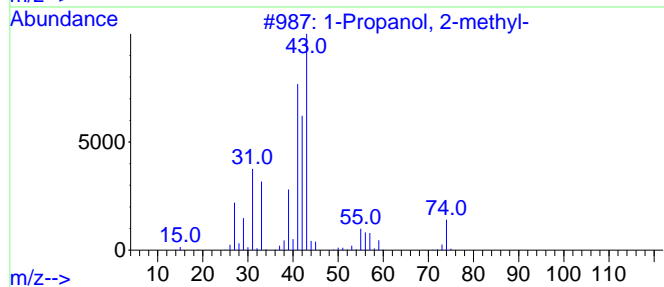
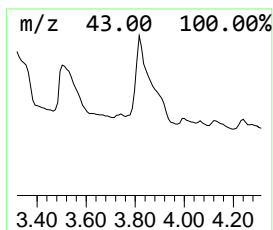
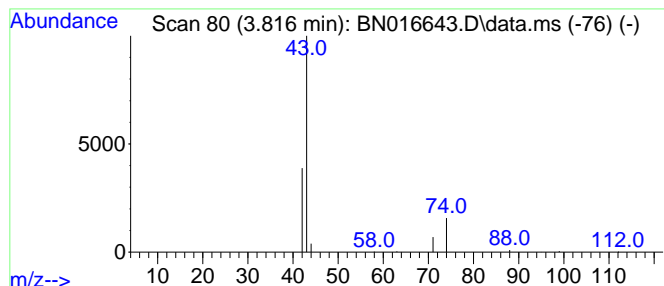
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 3 1-Propanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.21 ng	48563	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	5
2		Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
3		2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
4		Hydrogen isocyanate	43	CHNO	000075-13-8	3
5		Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

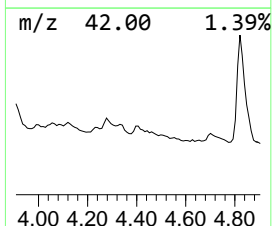
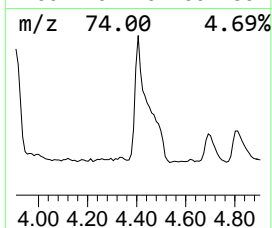
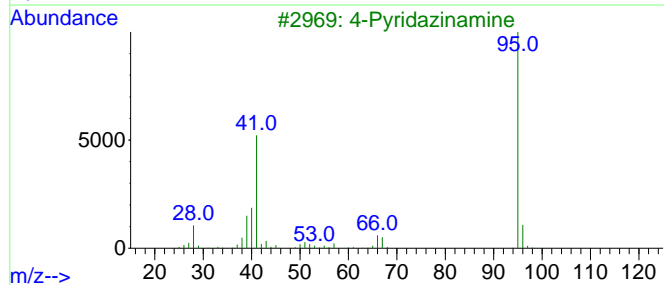
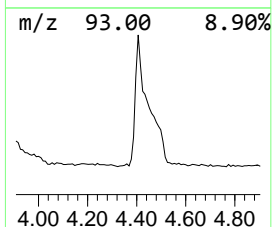
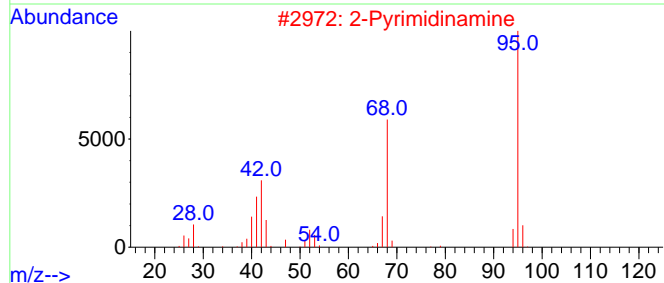
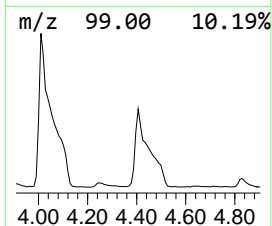
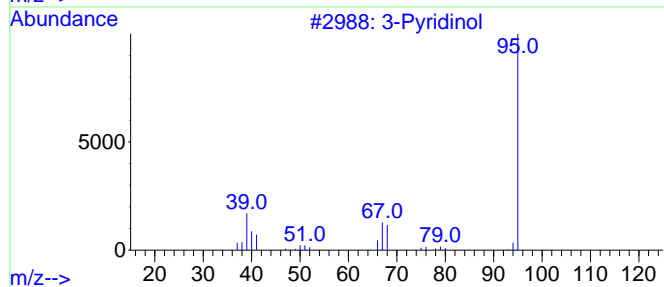
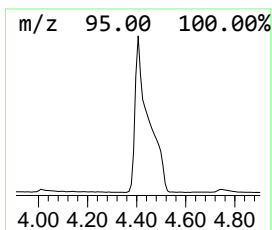
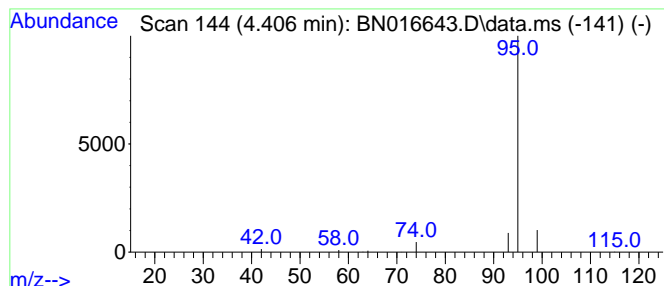
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 4 3-Pyridinol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.406	0.18 ng	42771	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pyridinol	95	C5H5NO	000109-00-2	2
2		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
3		4-Pyridazinamine	95	C4H5N3	020744-39-2	2
4		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
5		4-Pyridinone	95	C5H5NO	1000433-50-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

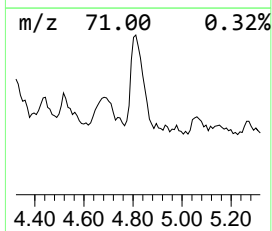
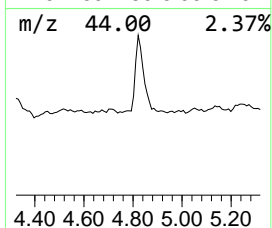
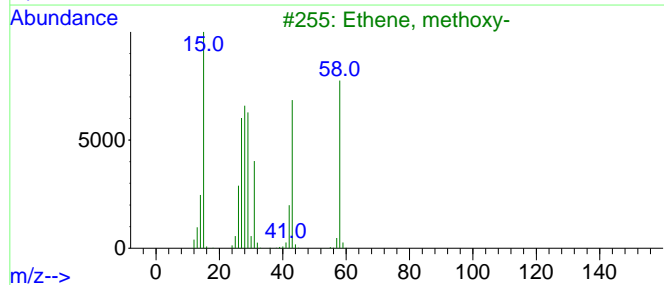
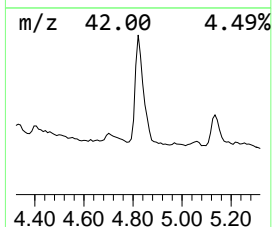
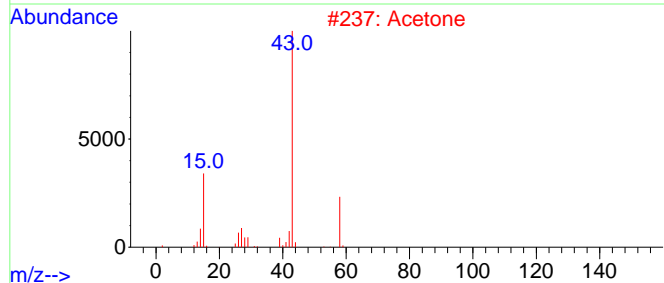
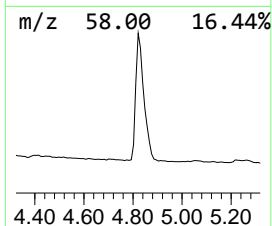
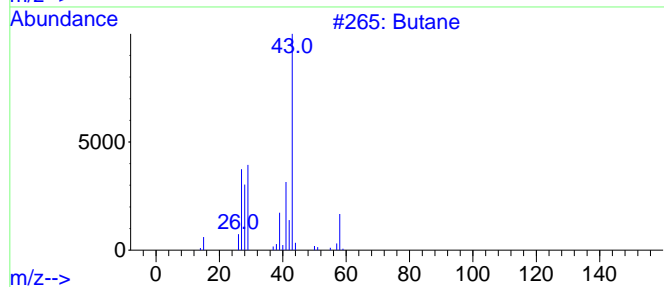
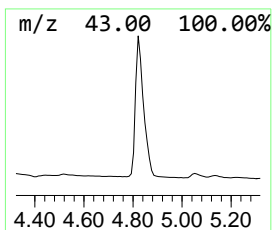
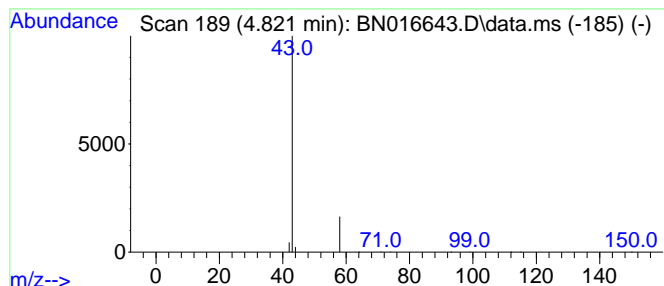
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.41 ng	96825	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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleID :
 MW201D-20210919

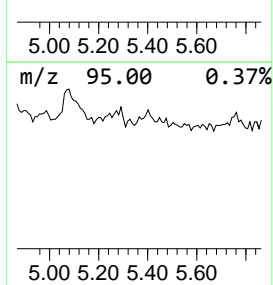
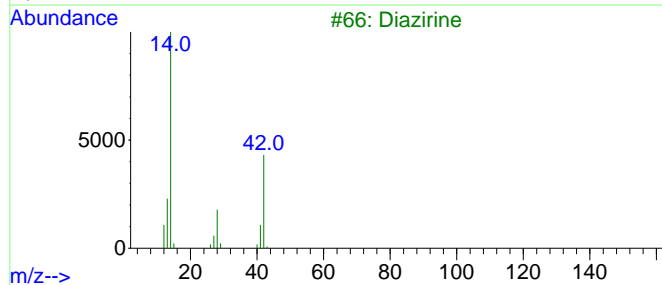
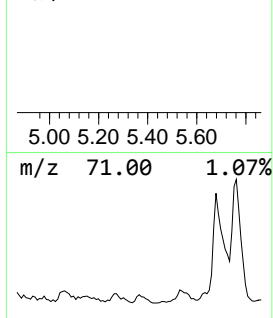
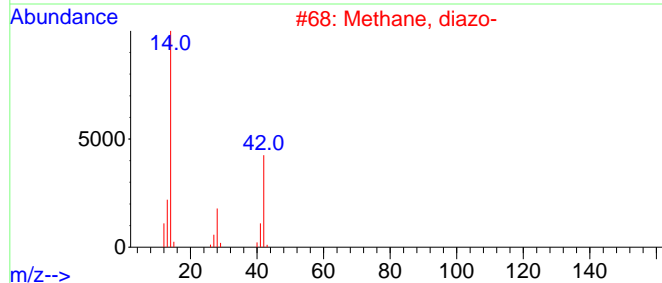
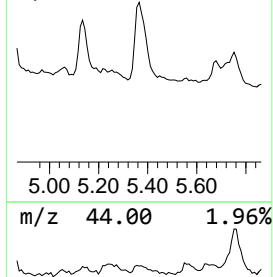
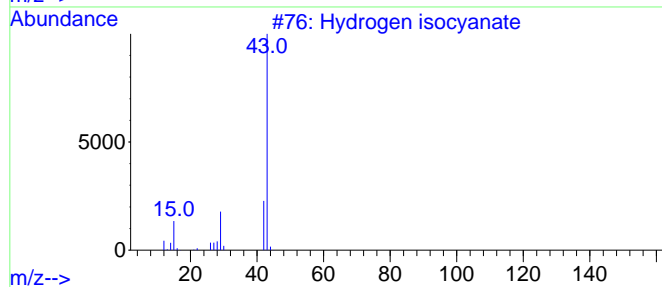
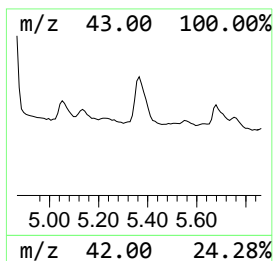
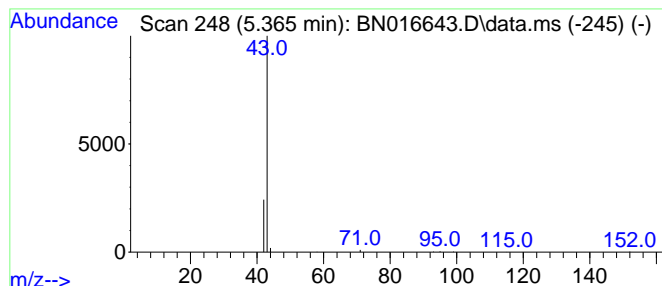
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Hydrogen isocyanate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.365	0.04 ng	10380	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			Methane, diazo-	42	CH2N2	000334-88-3	2
3			Diazirine	42	CH2N2	1000305-84-1	2
4			Ketene	42	C2H2O	000463-51-4	2
5			Cyclobutylamine	71	C4H9N	002516-34-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

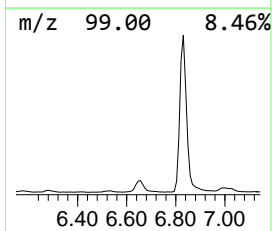
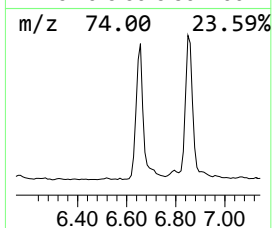
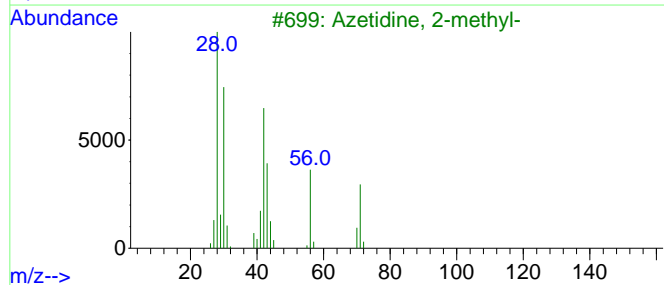
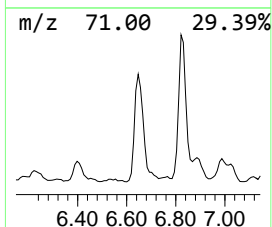
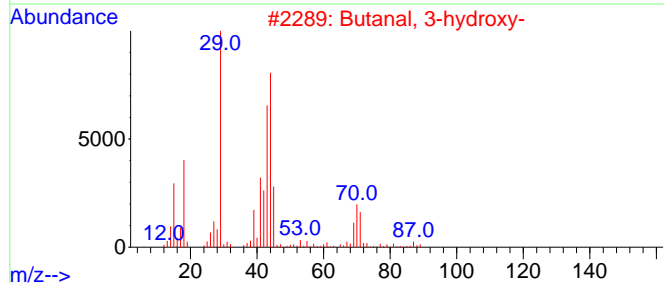
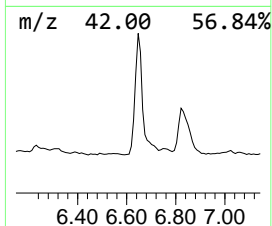
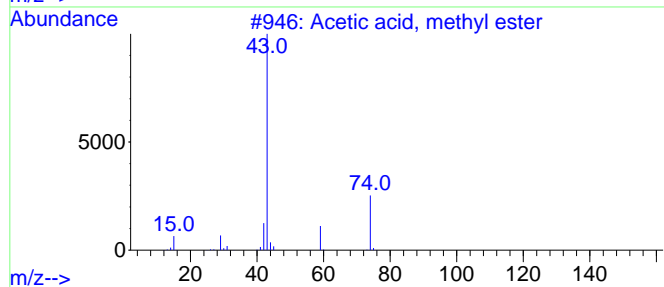
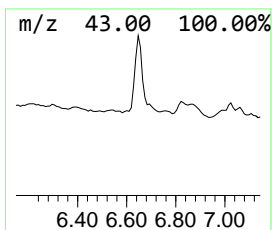
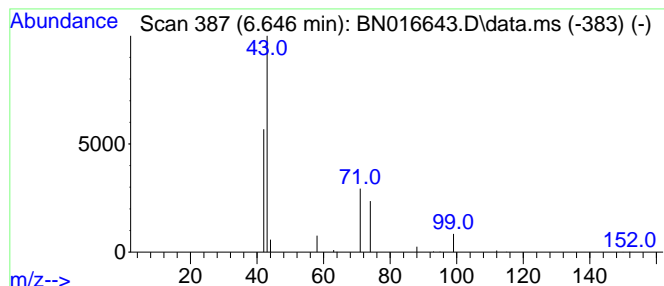
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Acetic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.07 ng	15593	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		Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	4
3		Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
4		Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
5		Isobutane	58	C4H10	000075-28-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

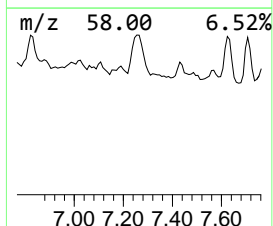
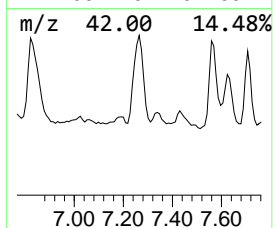
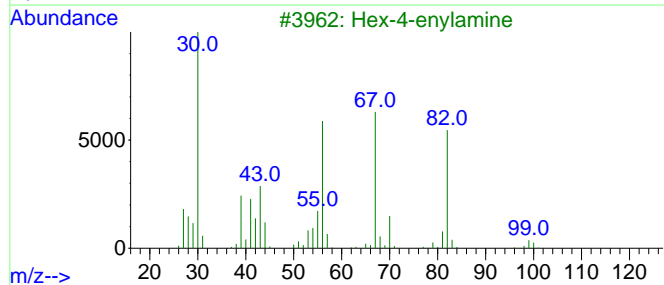
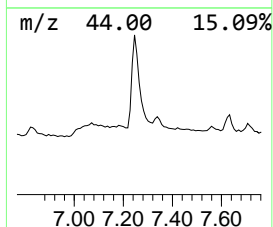
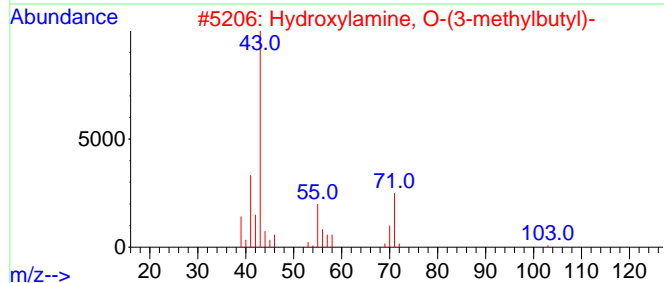
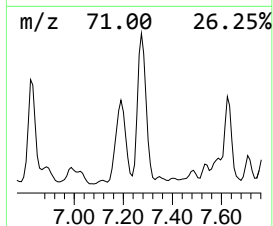
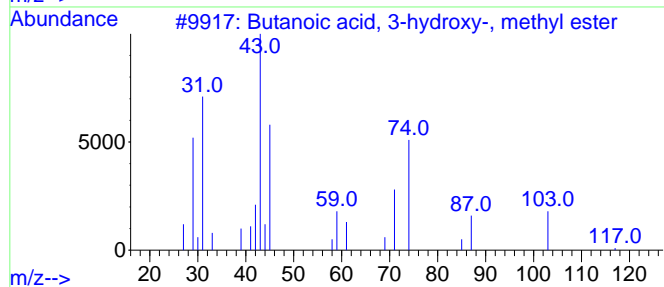
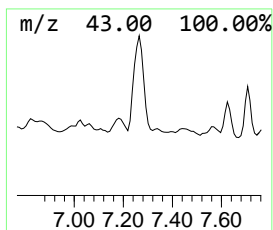
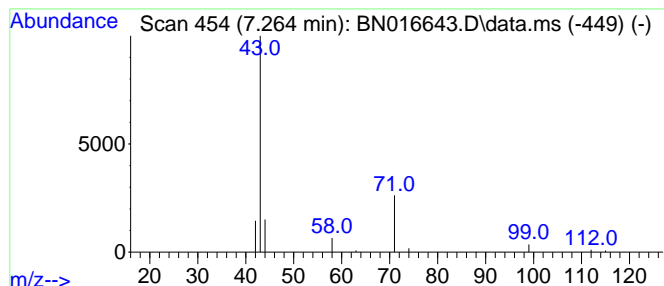
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Butanoic acid, 3-hydroxy-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.09 ng	21979	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hydroxy-, methyl...	118	C5H10O3	001487-49-6	9
2			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
3			Hex-4-enylamine	99	C6H13N	055108-01-5	5
4			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	4
5			1-Hepten-4-ol	114	C7H14O	003521-91-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

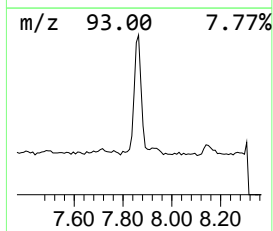
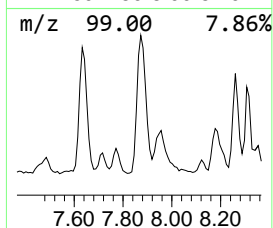
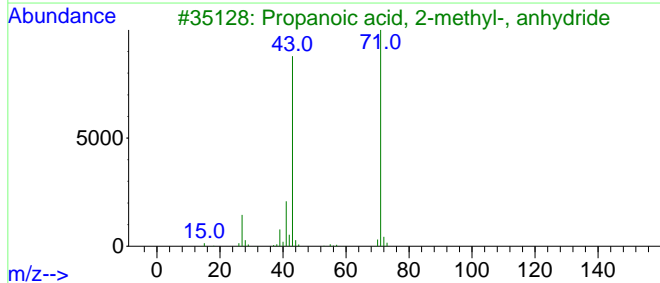
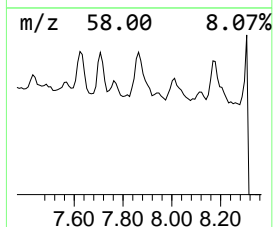
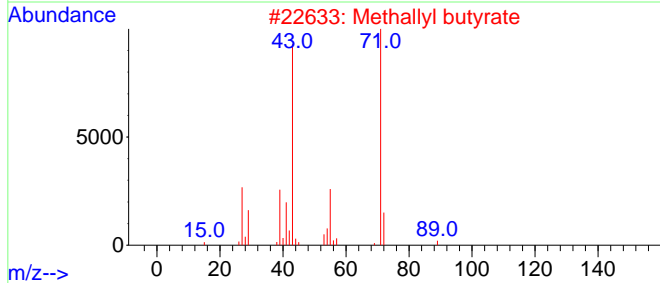
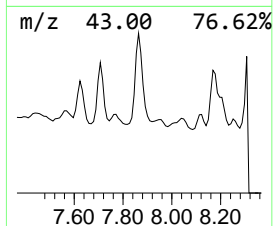
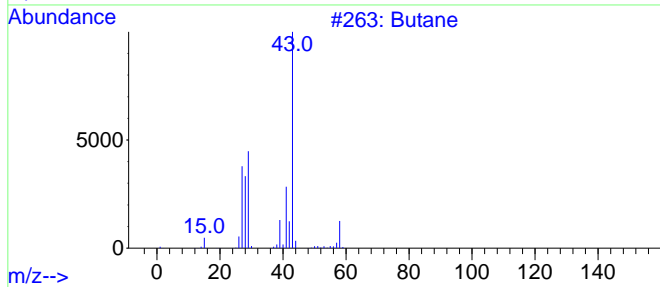
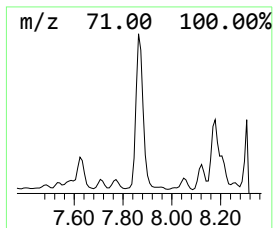
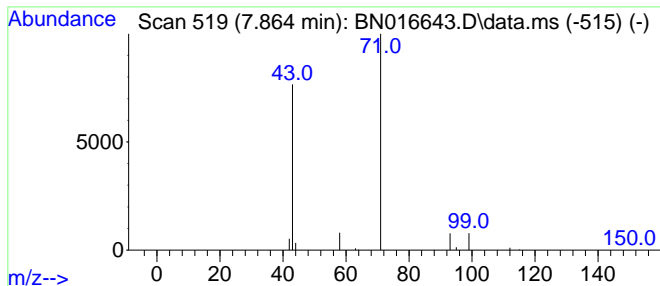
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.09 ng	21013	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		3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
5		Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

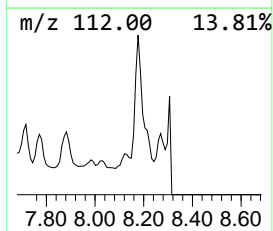
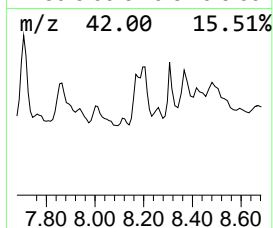
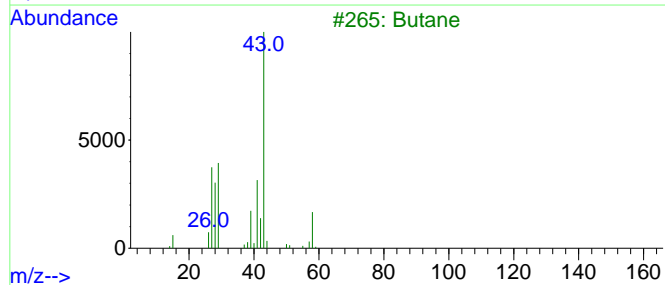
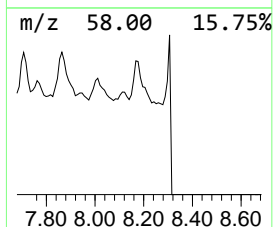
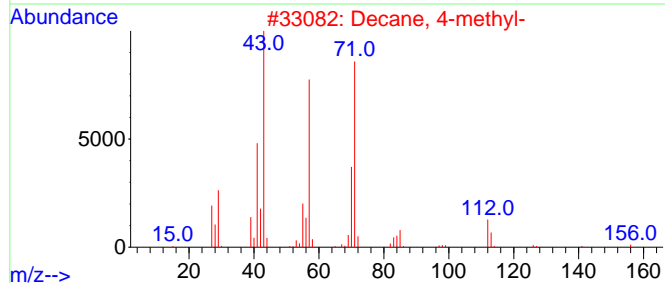
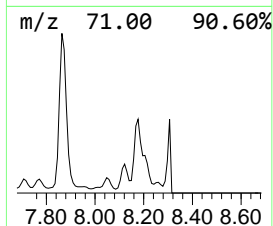
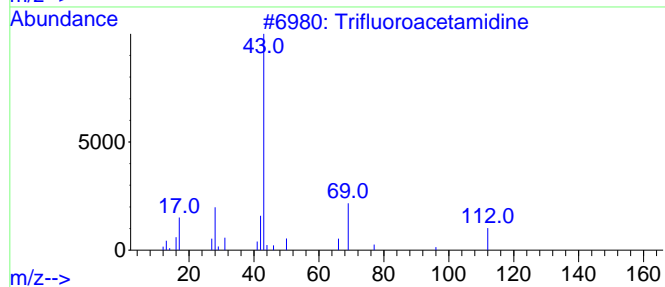
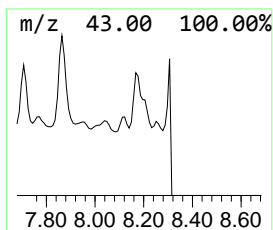
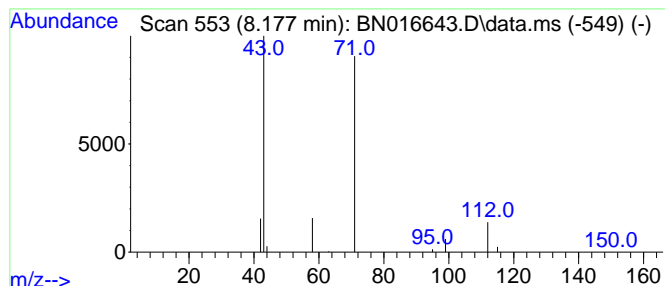
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Trifluoroacetamide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.177	0.06 ng	13559	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetamide	112	C2H3F3N2	000354-37-0	9
2		Decane, 4-methyl-	156	C11H24	002847-72-5	9
3		Butane	58	C4H10	000106-97-8	7
4		1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	5
5		3-Penten-2-one, 3,4-dimethyl-	112	C7H12O	000684-94-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

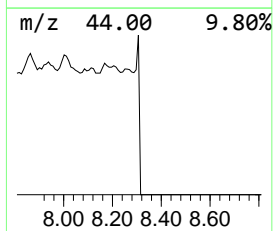
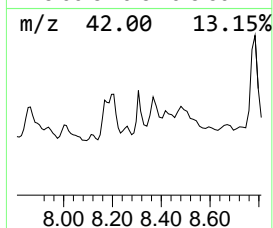
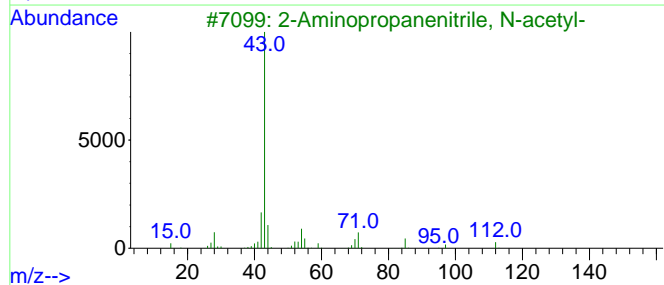
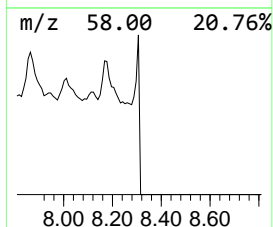
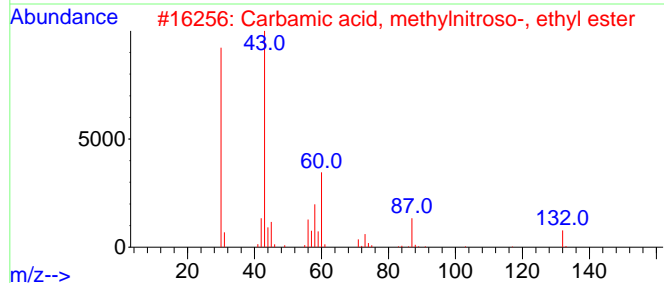
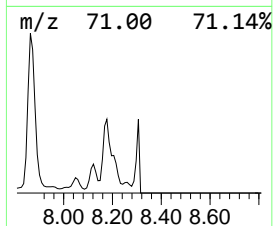
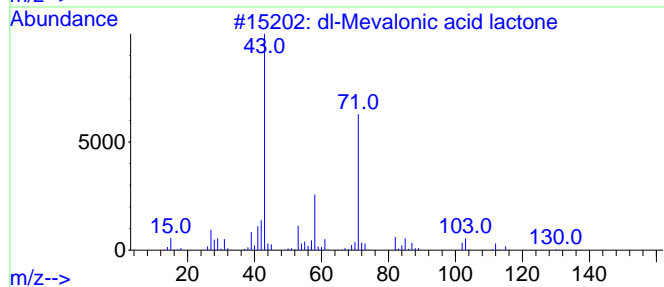
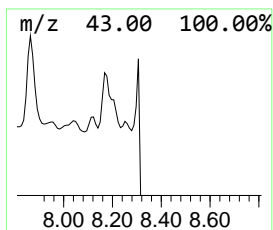
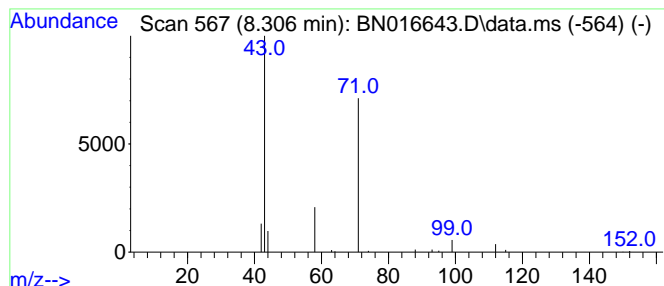
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 dl-Mevalonic acid lactone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.05 ng	10900	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	39
2		Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9
3		2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	7
4		Butane	58	C4H10	000106-97-8	5
5		Acetone	58	C3H6O	000067-64-1	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

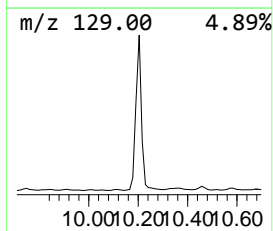
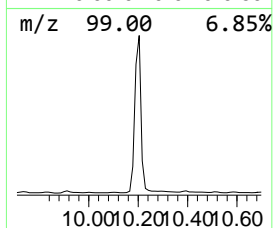
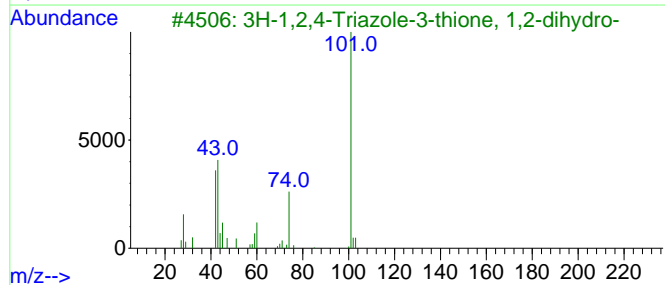
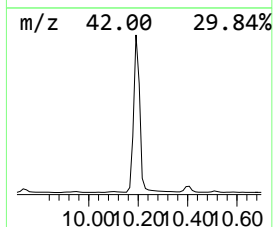
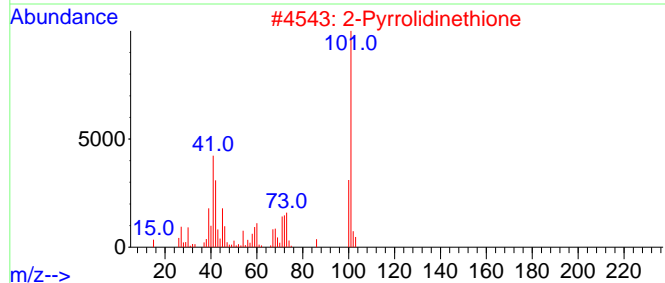
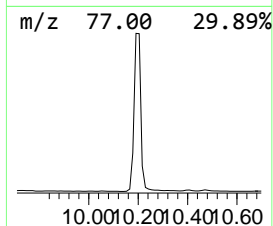
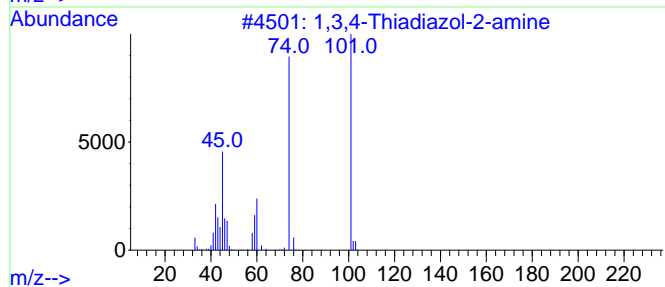
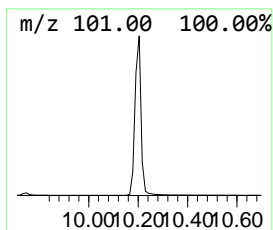
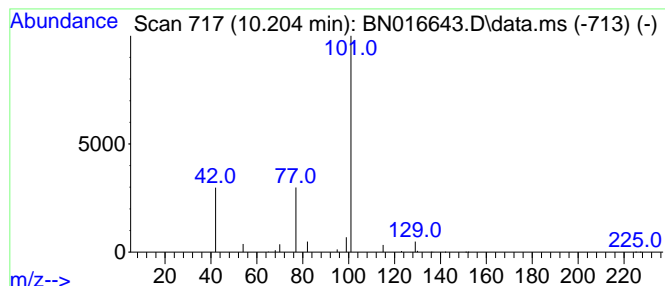
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 1,3,4-Thiadiazol-2-amine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	0.72 ng	293172	Naphthalene-d8	10.407

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	4
2		2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4
3		3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	4
4		Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	4
5		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

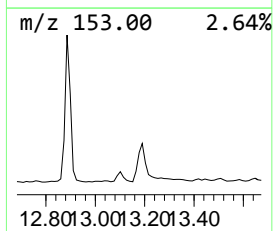
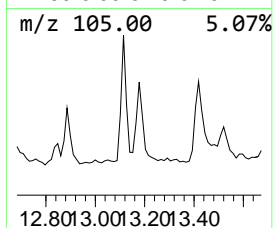
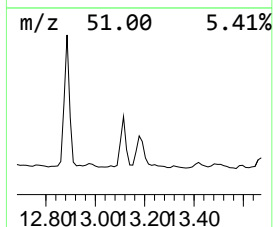
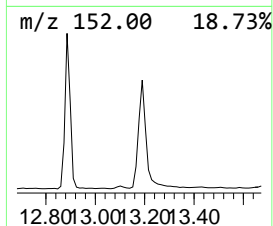
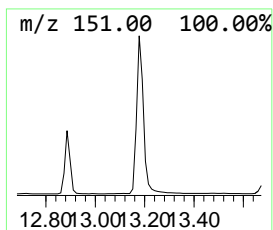
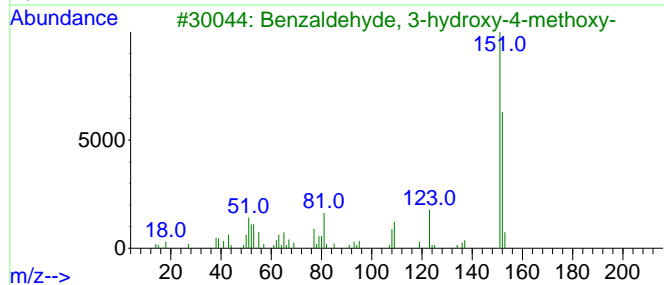
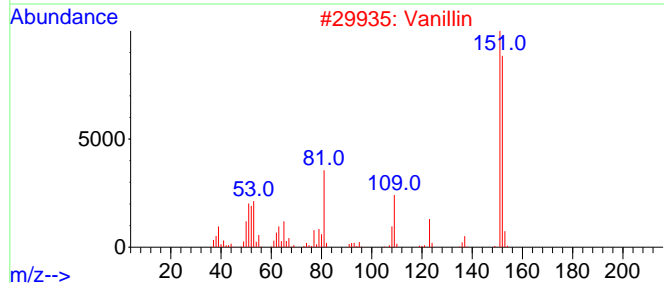
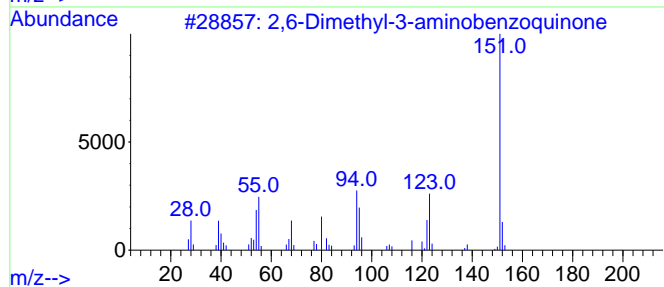
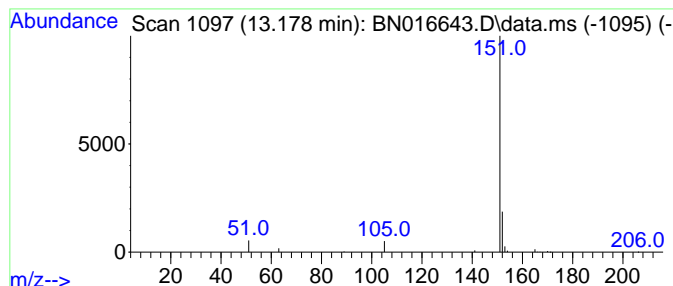
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 13 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.05 ng	21482	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		Vanillin	152	C8H8O3	000121-33-5	5
3		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	4
4		1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	4
5		Benzenaminium, 2-hydroxy-N,N,N-t...	151	C9H13NO	031061-58-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

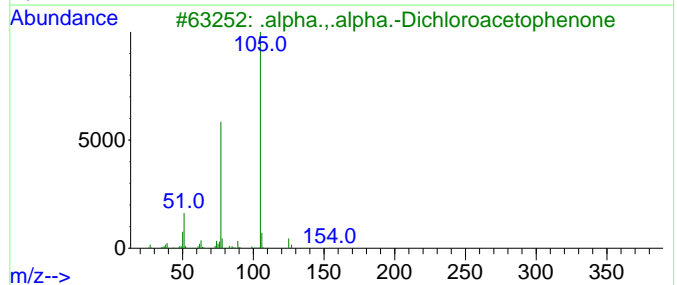
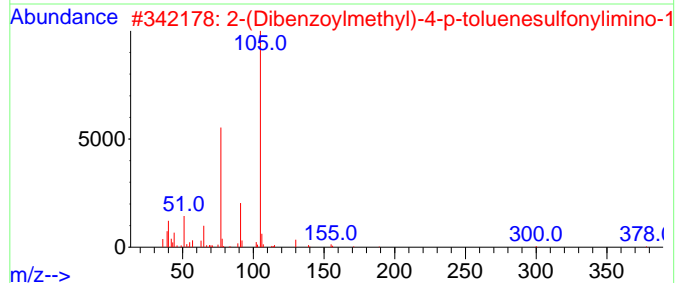
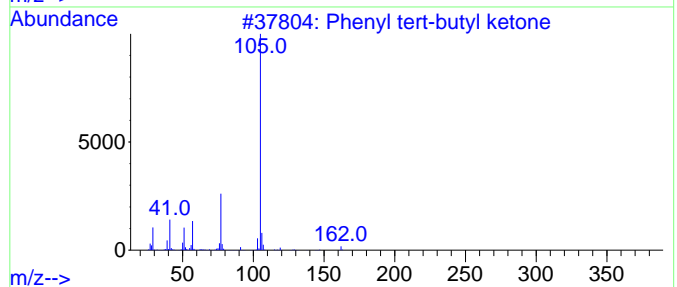
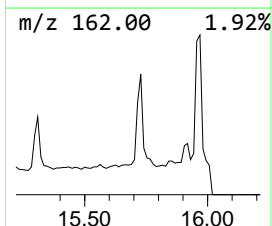
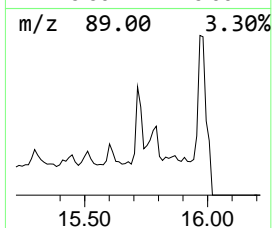
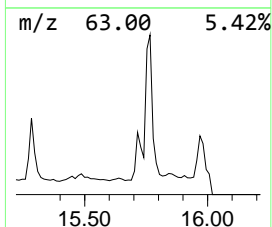
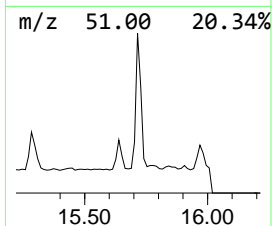
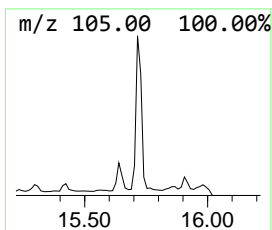
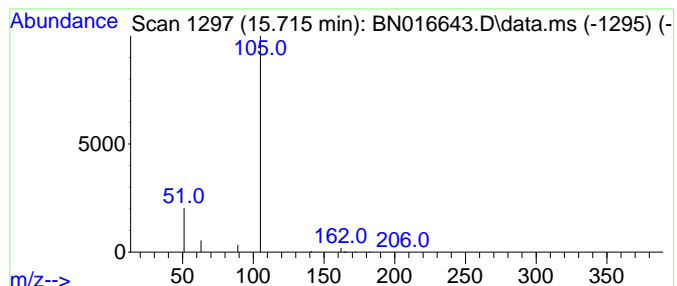
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 Phenyl tert-butyl ketone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	0.05 ng	18893	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenyl tert-butyl ketone	162	C11H14O	000938-16-9	3
2		2-(Dibenzoylmethyl)-4-p-toluenes...	533	C32H23NO5S	300360-29-6	2
3		.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	2
4		Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	2
5		Propanoic acid, 2-(benzoylamino)...	283	C17H17NO3	074923-17-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016643.D
 Acq On : 01 Oct 2021 19:34
 Operator : CG/JU
 Sample : M3833-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW201D-20210919

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	1.7	ng	397108	1	7.642	94016	0.4
Hydrogen isocya...	3.502	0.1	ng	25363	1	7.642	94016	0.4
1-Propanol, 2-m...	3.816	0.2	ng	48563	1	7.642	94016	0.4
3-Pyridinol	4.406	0.2	ng	42771	1	7.642	94016	0.4
Butane	4.821	0.4	ng	96825	1	7.642	94016	0.4
Hydrogen isocya...	5.365	0.0	ng	10380	1	7.642	94016	0.4
Acetic acid, me...	6.646	0.1	ng	15593	1	7.642	94016	0.4
Butanoic acid, ...	7.264	0.1	ng	21979	1	7.642	94016	0.4
Butane	7.864	0.1	ng	21013	1	7.642	94016	0.4
Trifluoroacetam...	8.177	0.1	ng	13559	1	7.642	94016	0.4
dl-Mevalonic ac...	8.306	0.0	ng	10900	1	7.642	94016	0.4
1,3,4-Thiadiaz...	10.204	0.7	ng	293172	2	10.407	162898	0.4
2,6-Dimethyl-3-...	13.178	0.0	ng	21482	3	14.269	189620	0.4
Phenyl tert-but...	15.715	0.0	ng	18893	4	17.017	157878	0.4