

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016616.D
 Acq On : 01 Oct 2021 02:23
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 2 Sample Multiplier: 1

Instrument :
 BNA_N
 LabSampleId :
 SSTDCCC0.4

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: BN016616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	21	rBV	8434	12514	2.38%	0.163%
2	3.585	51	55	77	rVB2	6241	30092	5.73%	0.392%
3	5.254	231	236	249	rBV2	14919	56041	10.67%	0.730%
4	6.822	401	406	418	rBV	23531	60916	11.59%	0.794%
5	6.978	418	423	429	rVV	17024	37680	7.17%	0.491%
6	7.080	429	434	440	rVV	36230	74414	14.16%	0.970%
7	7.200	440	447	460	rVB	12058	32675	6.22%	0.426%
8	7.522	478	482	489	rVB	6985	15410	2.93%	0.201%
9	7.642	490	495	514	rVB2	50914	124312	23.66%	1.620%
10	7.956	524	529	538	rVB2	49271	110596	21.05%	1.441%
11	8.168	547	552	557	rBV	3278	7900	1.50%	0.103%
12	8.429	571	577	590	rBV3	19716	49652	9.45%	0.647%
13	8.696	595	598	601	rBV	5173	9563	1.82%	0.125%
14	8.784	601	605	607	rBV	33347	72840	13.86%	0.949%
15	8.822	607	608	616	rVB	26954	40659	7.74%	0.530%
16	9.342	646	649	656	rBV	47362	77114	14.68%	1.005%
17	9.532	660	664	666	rVV	3397	6790	1.29%	0.088%
18	9.595	666	669	678	rVB	8683	15357	2.92%	0.200%
19	9.836	685	688	695	rBV	16118	27370	5.21%	0.357%
20	10.064	702	706	709	rBV	3842	8113	1.54%	0.106%
21	10.407	729	733	735	rBV	108785	195189	37.15%	2.543%
22	10.457	735	737	741	rVV	113795	185157	35.24%	2.413%
23	10.571	743	746	756	rVV	25372	60489	11.51%	0.788%
24	10.749	756	760	763	rVB	34615	57464	10.94%	0.749%
25	11.709	852	865	888	rBV	13007	24207	4.61%	0.315%
26	12.007	919	932	940	rBV	56914	94093	17.91%	1.226%
27	12.078	940	948	972	rVB	129190	208429	39.67%	2.716%
28	12.301	988	998	1020	rBV	125370	201528	38.36%	2.626%
29	12.695	1056	1059	1062	rBV	16388	27778	5.29%	0.362%
30	12.772	1062	1065	1071	rVB	12216	24168	4.60%	0.315%
31	12.886	1071	1074	1078	rBV	107956	198156	37.71%	2.582%
32	13.139	1091	1094	1097	rVB	81920	127421	24.25%	1.660%
33	13.736	1138	1141	1143	rBV	11539	16279	3.10%	0.212%
34	13.850	1147	1150	1153	rVB	18374	27010	5.14%	0.352%
35	13.990	1158	1161	1164	rVB	96453	152504	29.03%	1.987%
36	14.269	1180	1183	1185	rBV	138351	196610	37.42%	2.562%

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37	14.332	1185	1188	1191	rVB	169611	242626	46.18%	3.161%
38	14.637	1209	1212	1224	rBV3	15534	42966	8.18%	0.560%
39	14.814	1224	1226	1230	rVV	5058	9077	1.73%	0.118%
40	14.903	1230	1233	1243	rVB	7435	12055	2.29%	0.157%
41	15.106	1246	1249	1252	rBV	8204	10800	2.06%	0.141%
42	15.322	1263	1266	1270	rBV2	219923	347351	66.11%	4.526%
43	15.411	1270	1273	1280	rVB2	4185	9411	1.79%	0.123%
44	15.537	1280	1283	1287	rBV	33845	59215	11.27%	0.772%
45	15.614	1287	1289	1293	rVB2	39127	61146	11.64%	0.797%
46	15.766	1298	1301	1311	rVB2	12913	21607	4.11%	0.282%
47	16.226	1335	1338	1341	rBV2	59155	88991	16.94%	1.160%
48	16.324	1343	1346	1350	rVB	46814	71659	13.64%	0.934%
49	16.506	1358	1361	1372	rBV	19914	32319	6.15%	0.421%
50	16.677	1372	1375	1384	rBV	19951	34810	6.63%	0.454%
51	17.017	1400	1403	1405	rBV	93830	154484	29.40%	2.013%
52	17.066	1405	1407	1410	rVV	149015	213903	40.71%	2.787%
53	17.151	1411	1414	1434	rVV	105816	181014	34.45%	2.359%
54	17.431	1434	1437	1453	rVV	80994	130218	24.78%	1.697%
55	18.020	1482	1486	1504	rVB	5291	7708	1.47%	0.100%
56	19.063	1686	1696	1699	rBV	107186	153679	29.25%	2.002%
57	19.093	1699	1702	1741	rVB	177443	249648	47.51%	3.253%
58	19.460	1767	1776	1812	rBV	182857	244453	46.53%	3.185%
59	19.678	1813	1820	1846	rVV	104670	135928	25.87%	1.771%
60	20.378	1918	1921	1924	rBV	47247	54358	10.35%	0.708%
61	21.164	1992	1995	1997	rBV	51161	58134	11.06%	0.757%
62	21.217	1997	2000	2003	rVV2	201575	403667	76.83%	5.260%
63	21.270	2003	2005	2016	rVB	182998	254800	48.50%	3.320%
64	22.056	2075	2079	2082	rBV	51881	76026	14.47%	0.991%
65	22.803	2216	2228	2234	rBV	126015	204373	38.90%	2.663%
66	22.848	2234	2241	2274	rVB	136631	242430	46.14%	3.159%
67	23.382	2384	2397	2415	rBV	84901	187959	35.77%	2.449%
68	23.478	2415	2425	2472	rVB	93602	200464	38.15%	2.612%
69	24.083	2592	2602	2624	rBV	8776	16944	3.22%	0.221%
70	24.850	2815	2826	2855	rVB	8903	20671	3.93%	0.269%
71	25.767	3067	3094	3164	rBV3	138395	525412	100.00%	6.846%
72	26.452	3271	3294	3337	rBV	76355	241255	45.92%	3.143%
73	26.818	3386	3401	3429	rVB	2034	6819	1.30%	0.089%

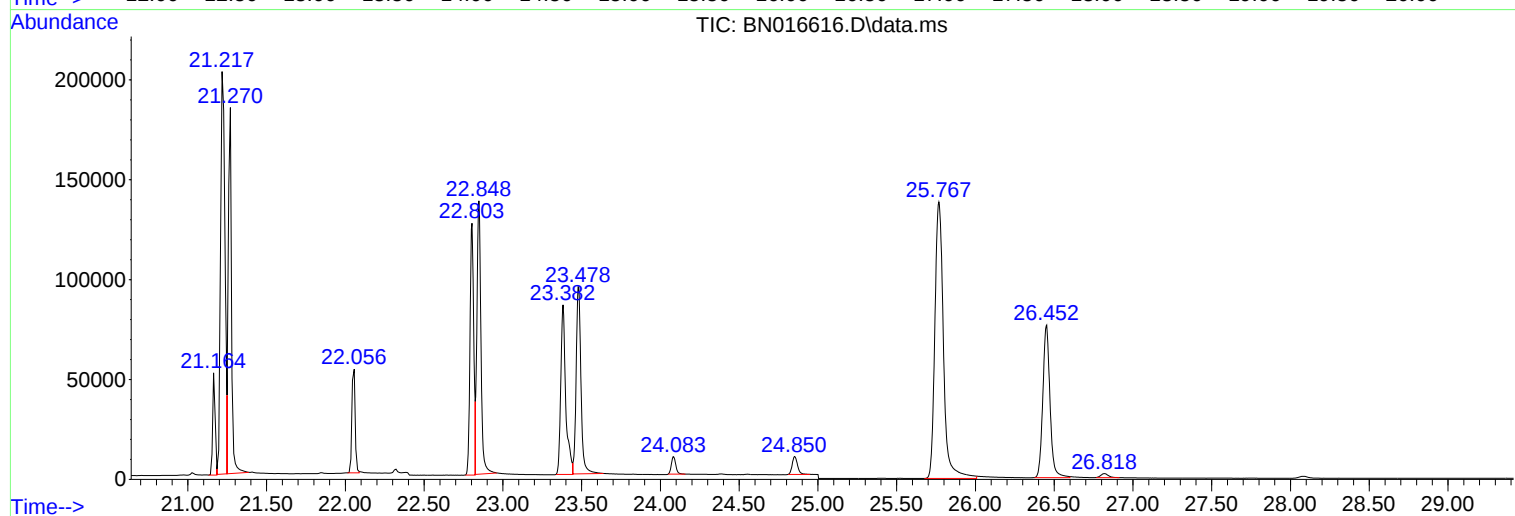
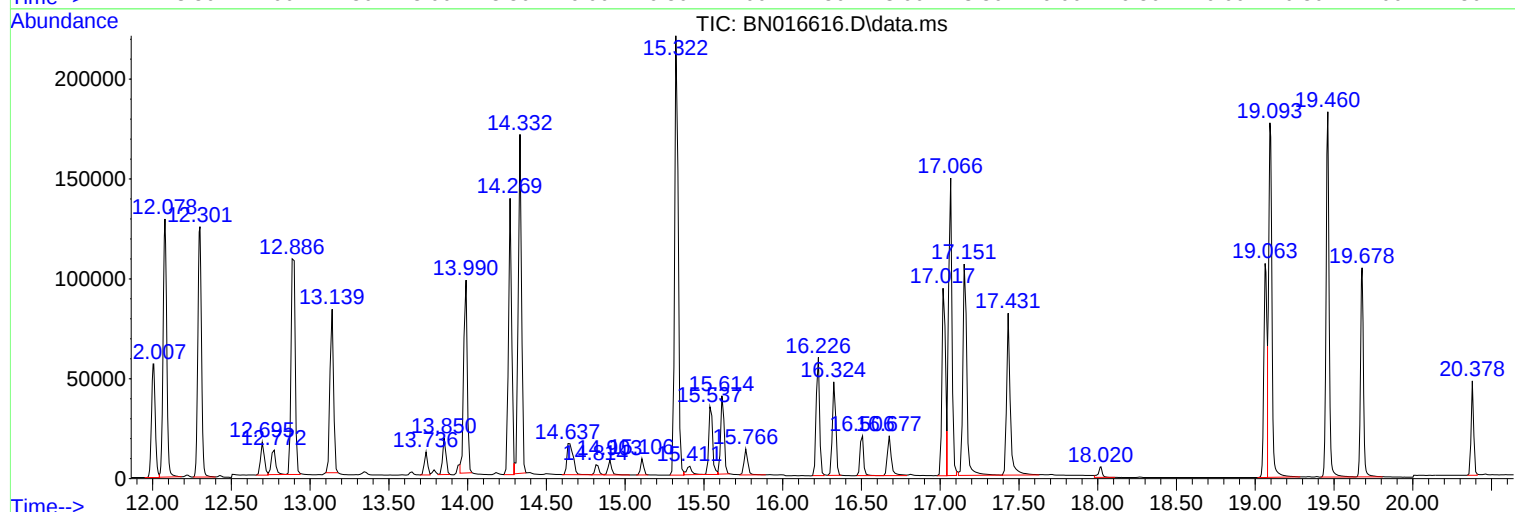
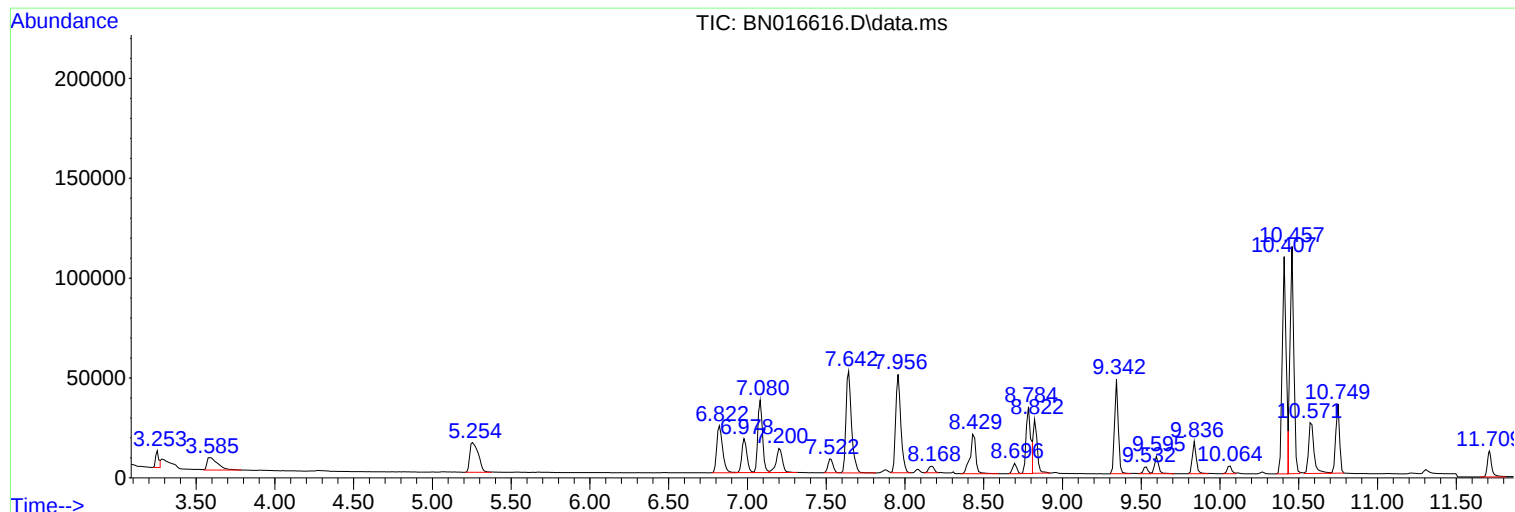
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

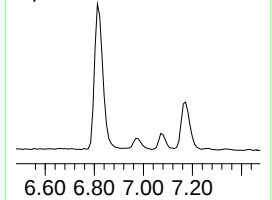
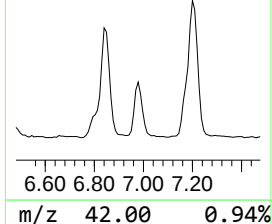
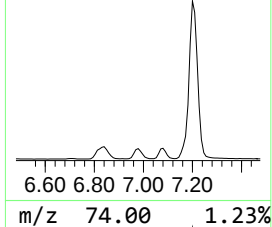
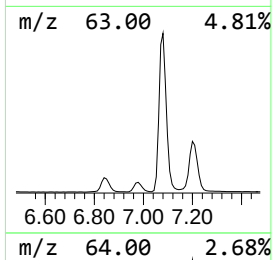
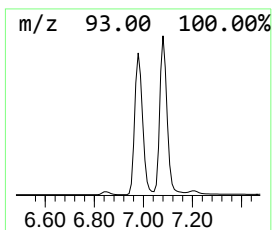
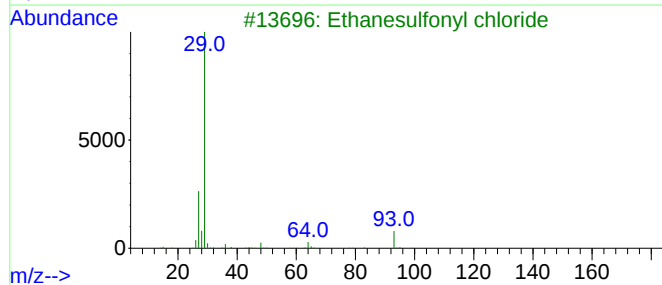
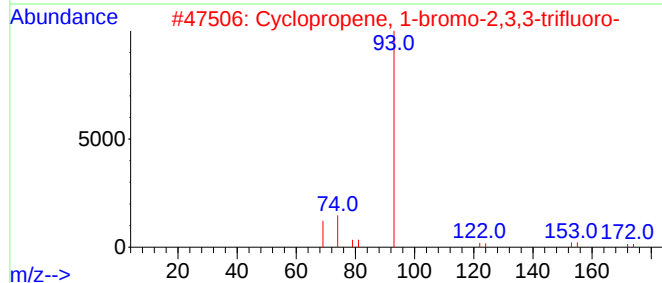
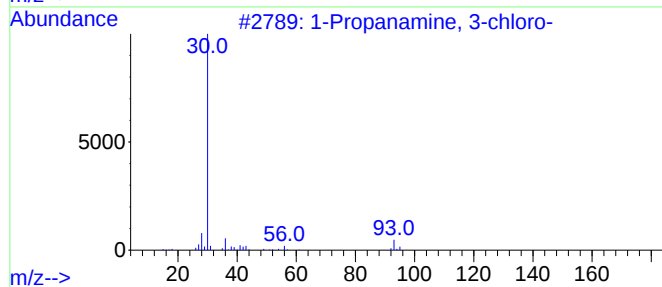
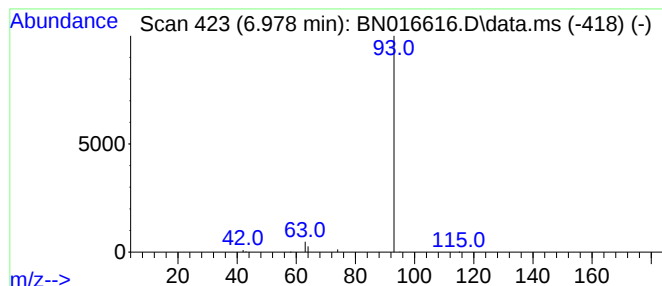
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.12 ng	37680	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
2		Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3		Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	1
4		Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	1
5		Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1



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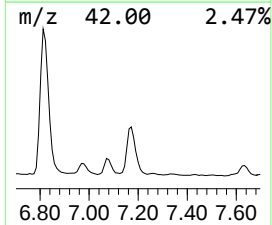
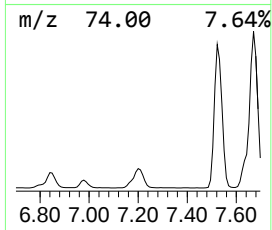
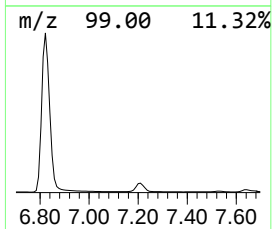
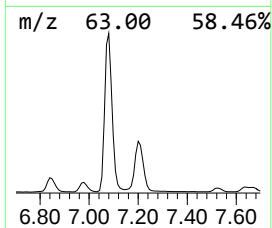
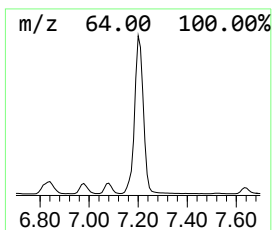
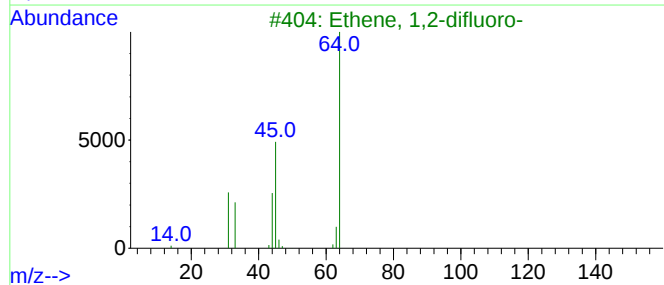
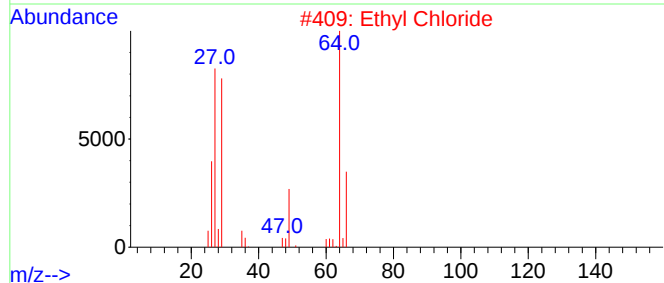
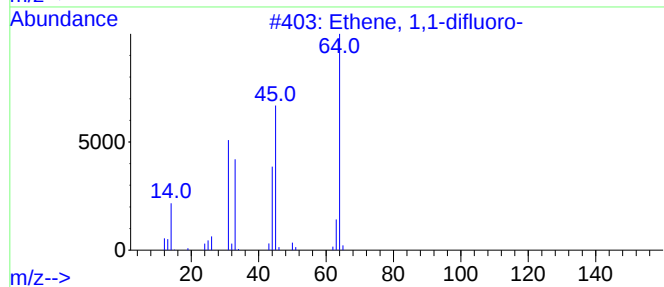
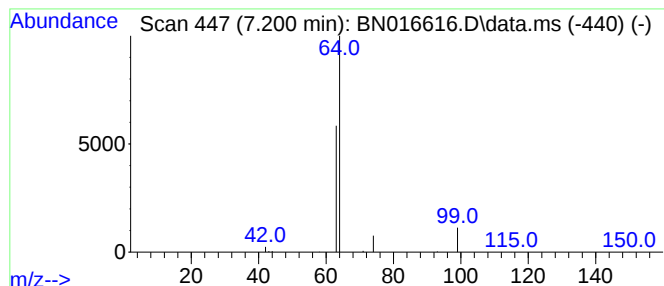
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	32675	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
4			Sulfur dioxide	64	O2S	007446-09-5	3
5			(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2



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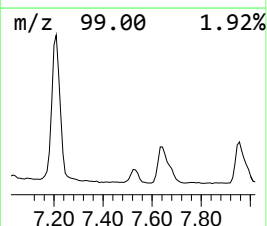
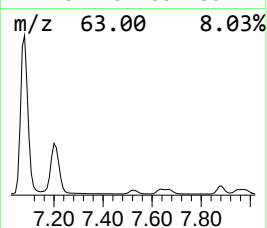
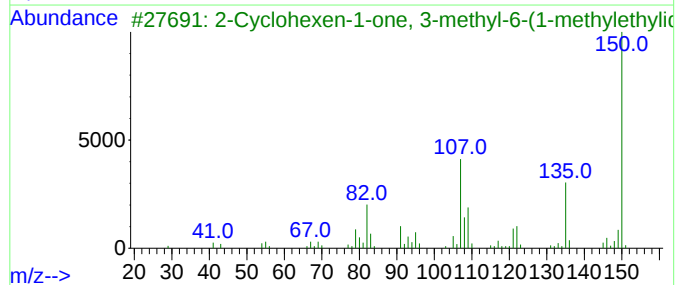
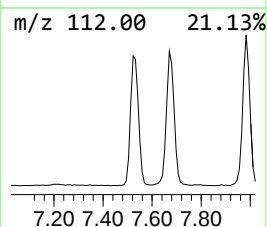
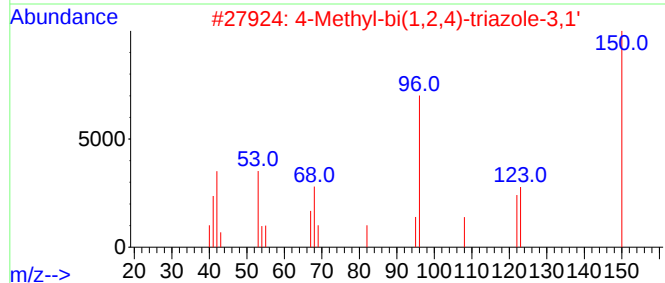
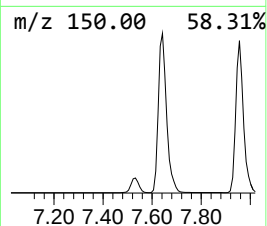
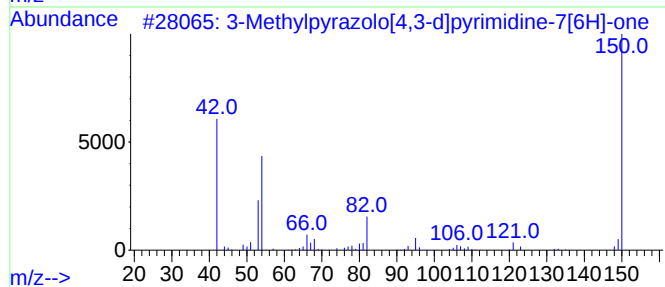
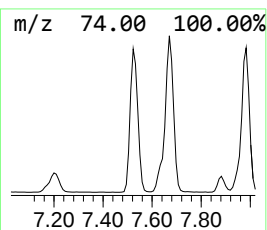
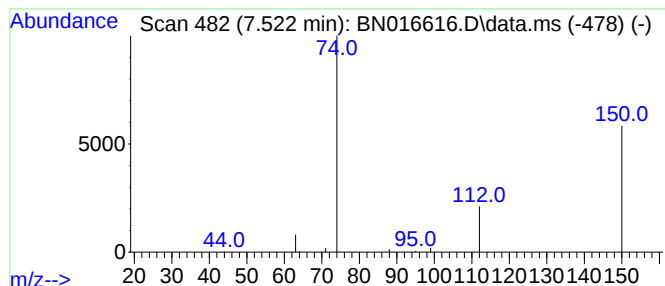
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Methylpyrazolo[4,3-d]pyri... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	15410	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
2		4-Methyl-bi(1,2,4)-triazole-3,1'	150	C5H6N6	063523-89-7	2
3		2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
4		Thiirane, methyl-	74	C3H6S	001072-43-1	2
5		N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2



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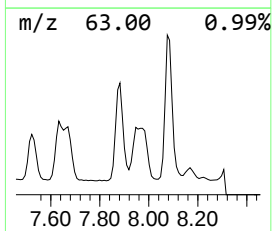
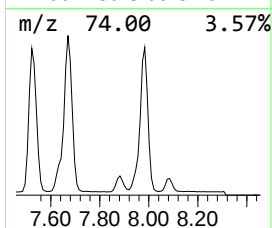
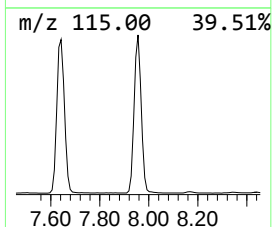
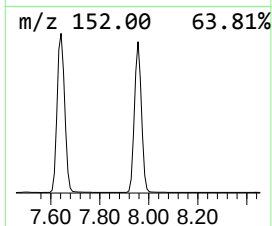
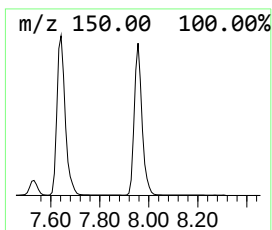
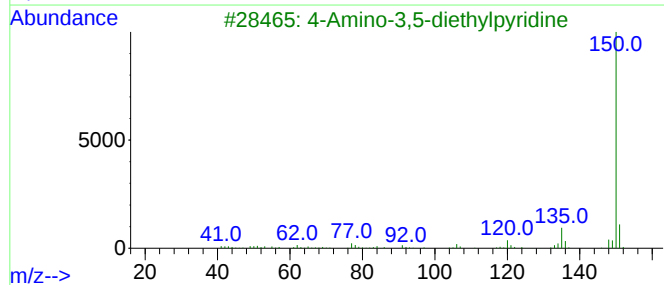
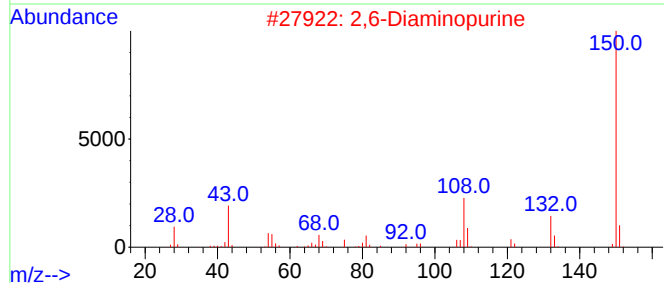
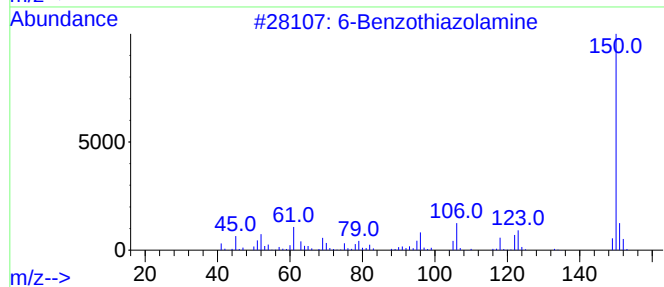
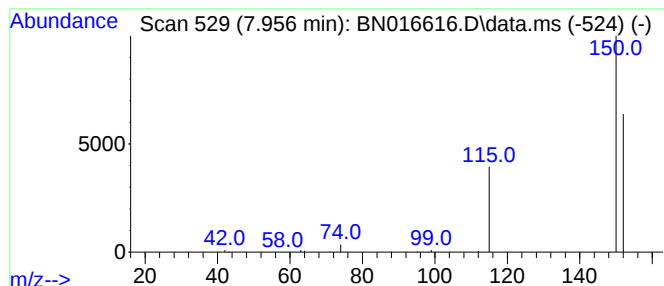
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	110596	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		6-Benzothiazolamine	150	C7H6N2S	000533-30-2	4
2		2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
3		4-Amino-3,5-diethylpyridine	150	C9H14N2	1000128-75-1	2
4		Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	2
5		2-Benzimidazolethiol	150	C7H6N2S	000583-39-1	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
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LabSampleId :
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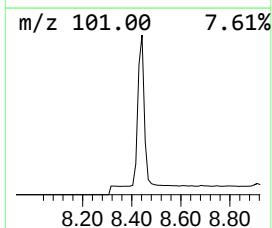
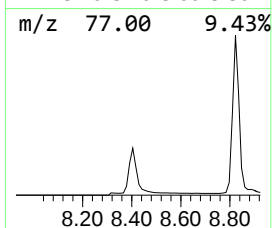
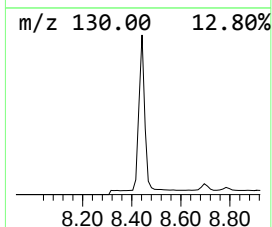
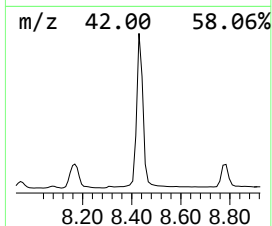
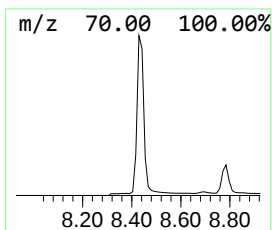
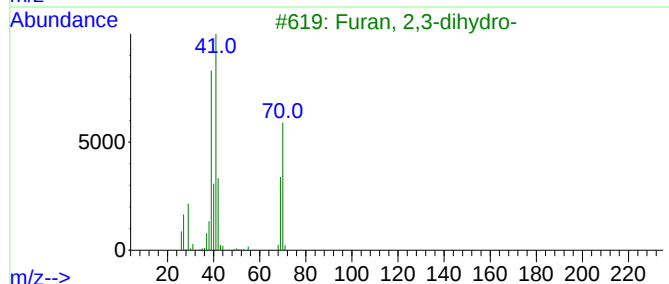
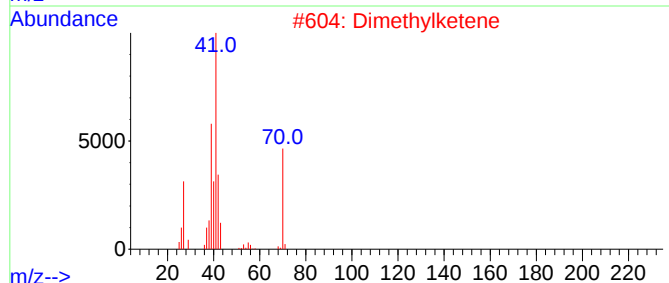
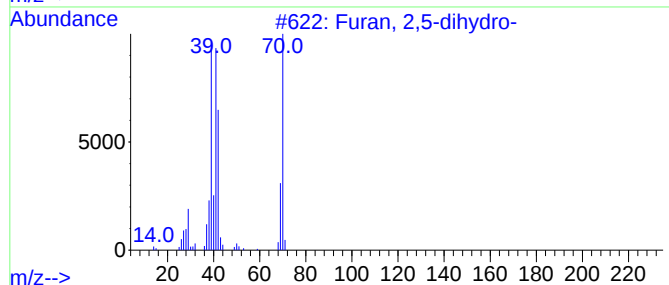
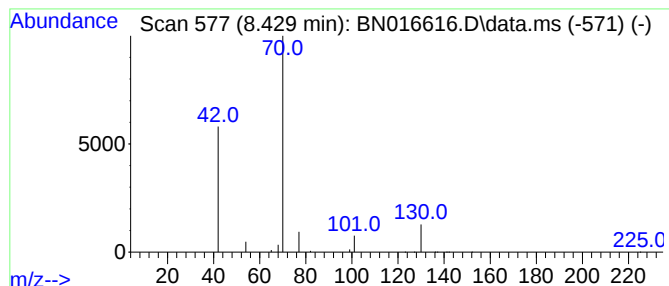
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Furan, 2,5-dihydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.16 ng	49652	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2			Dimethylketene	70	C4H6O	000598-26-5	5
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4
5			1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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LabSampleId :
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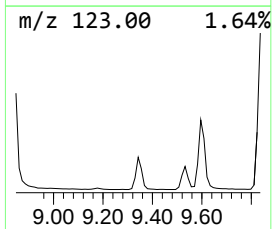
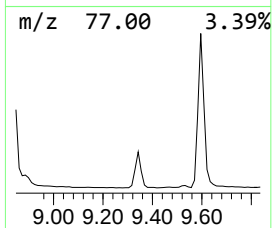
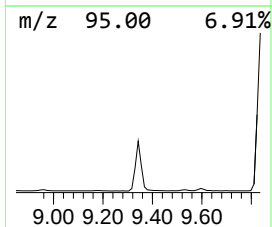
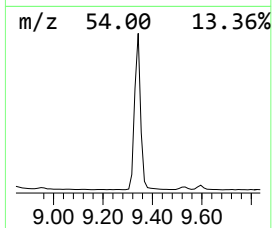
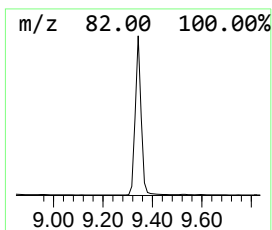
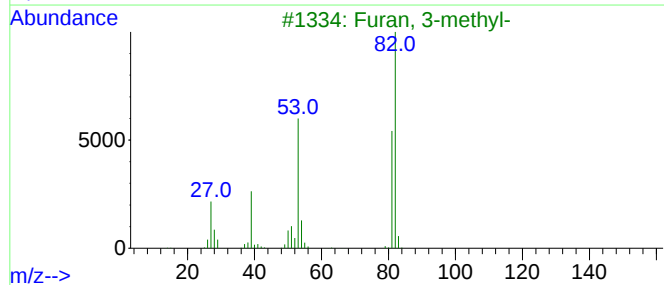
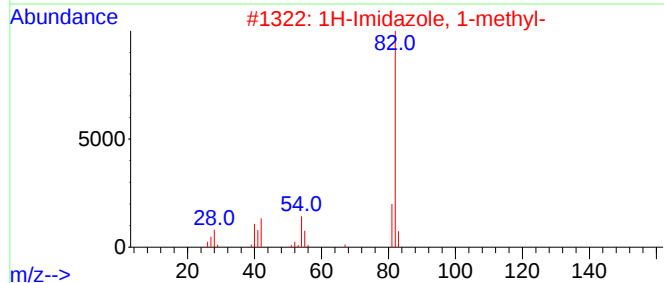
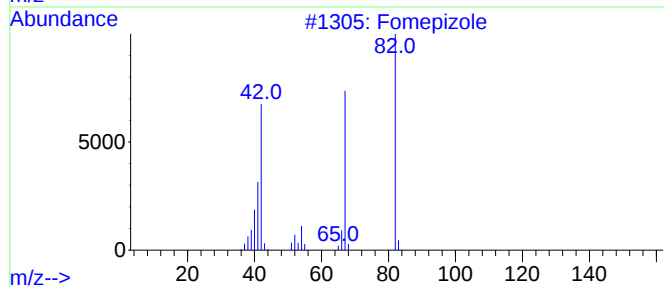
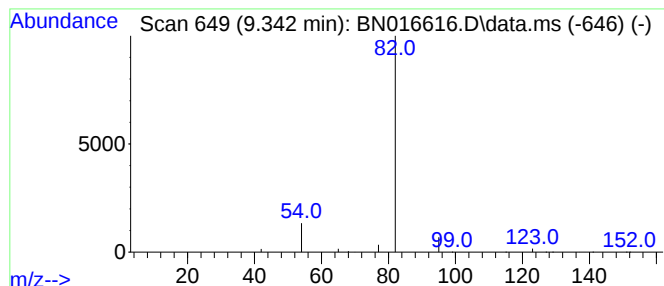
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	77114	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fomepizole	82	C4H6N2	007554-65-6	5
2			1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
3			Furan, 3-methyl-	82	C5H6O	000930-27-8	4
4			Furan, 2-methyl-	82	C5H6O	000534-22-5	4
5			3-Aminocrotononitrile	82	C4H6N2	001118-61-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
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Misc :
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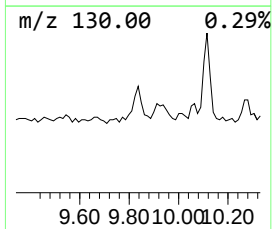
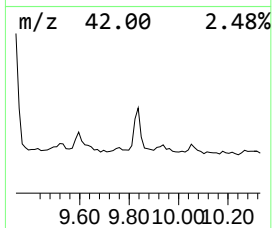
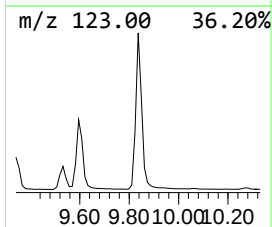
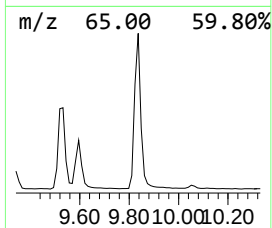
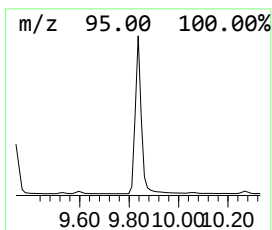
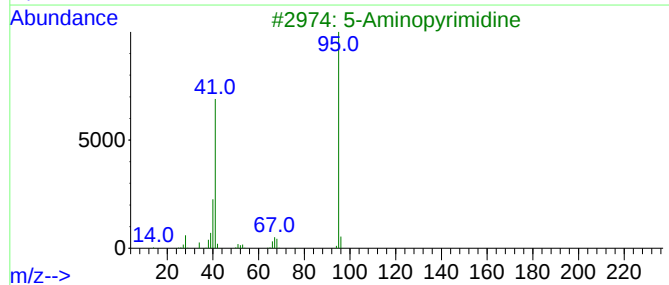
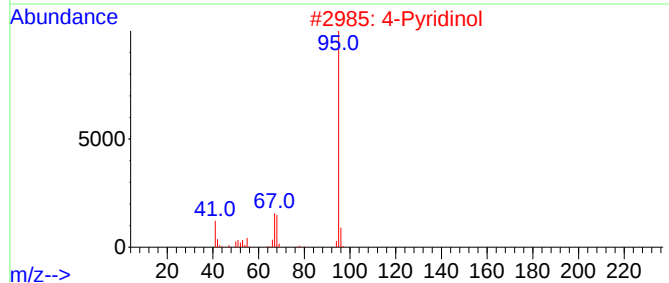
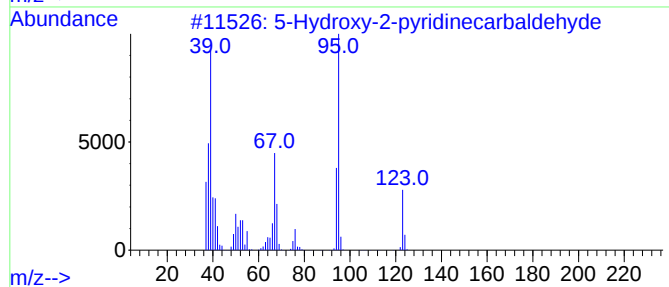
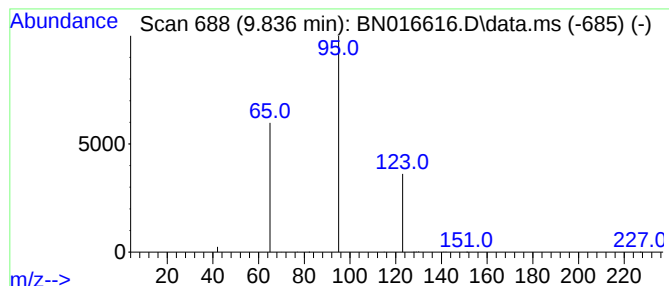
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Hydroxy-2-pyridinecarbal... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	27370	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2		4-Pyridinol	95	C5H5NO	000626-64-2	4
3		5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
4		3-Pyridinol	95	C5H5NO	000109-00-2	2
5		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
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Misc :
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Instrument :
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LabSampleId :
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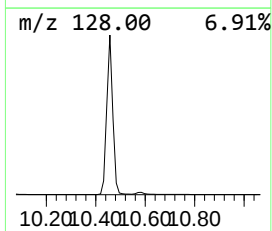
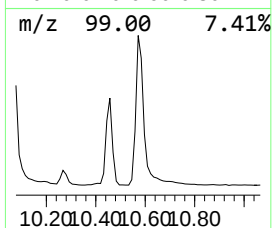
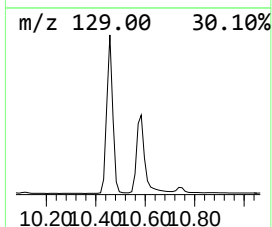
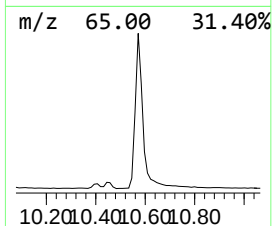
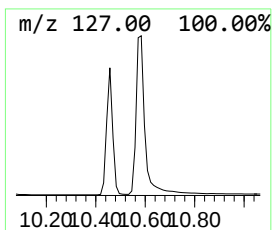
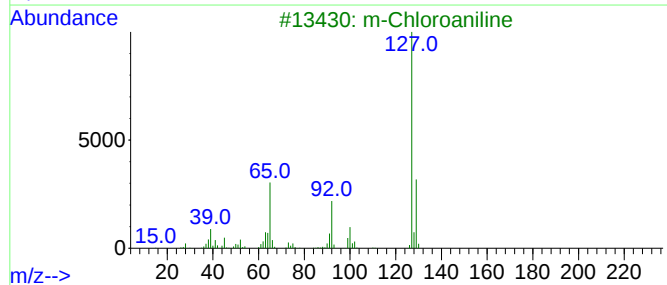
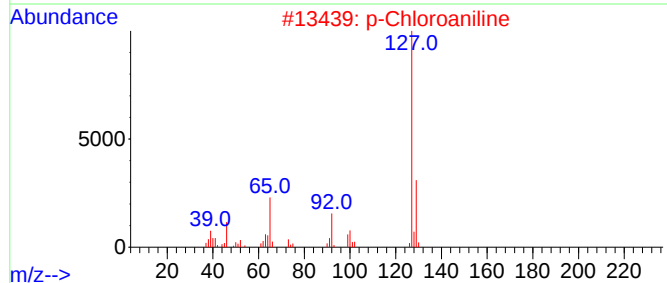
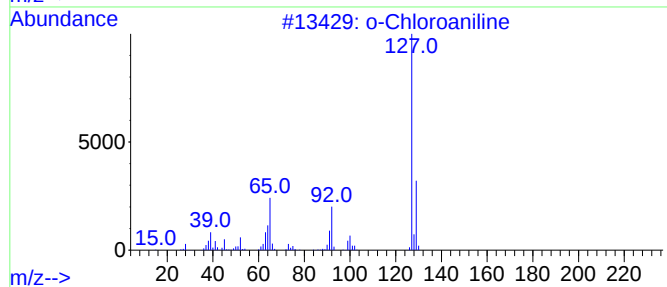
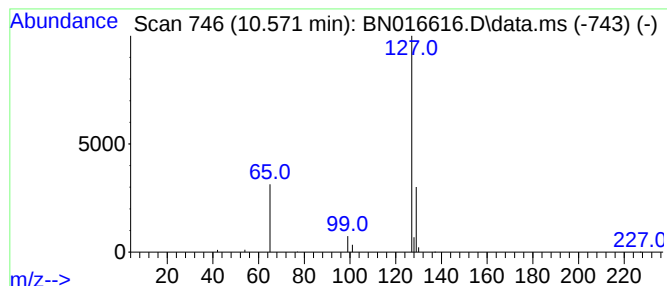
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	60489	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Chloroaniline	127	C6H6ClN	000095-51-2	90
2			p-Chloroaniline	127	C6H6ClN	000106-47-8	90
3			m-Chloroaniline	127	C6H6ClN	000108-42-9	90
4			4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5			Picloxydine	474	C20H24Cl2N10	005636-92-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
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Misc :
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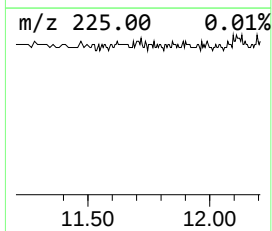
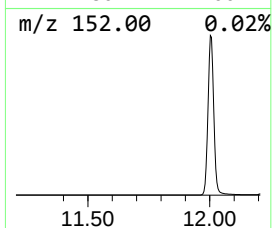
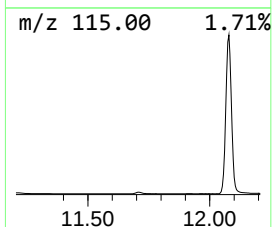
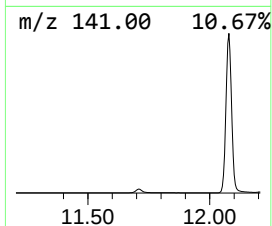
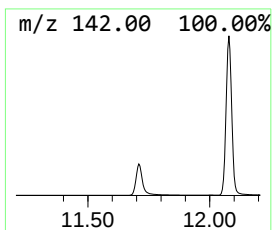
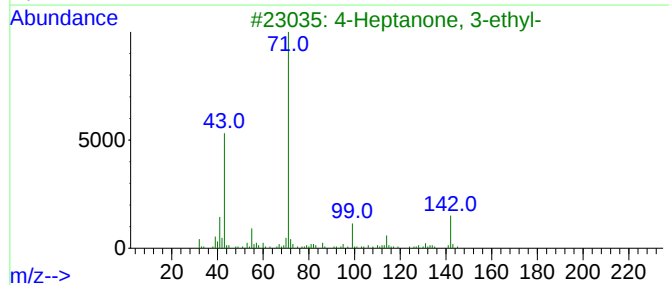
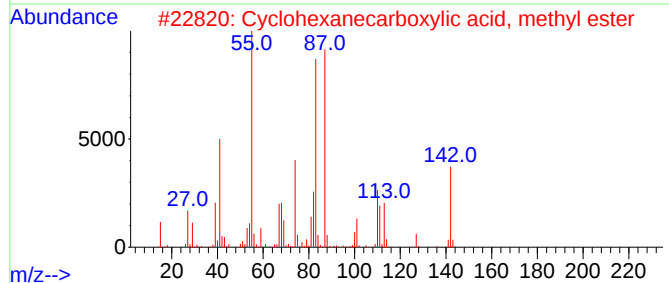
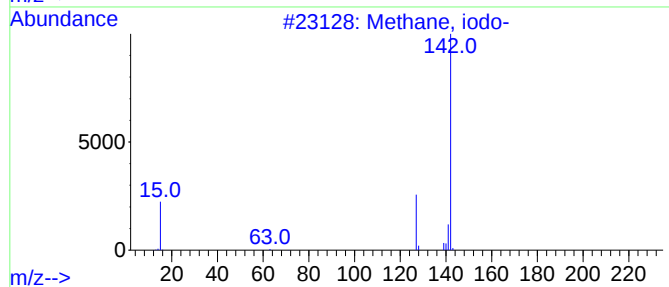
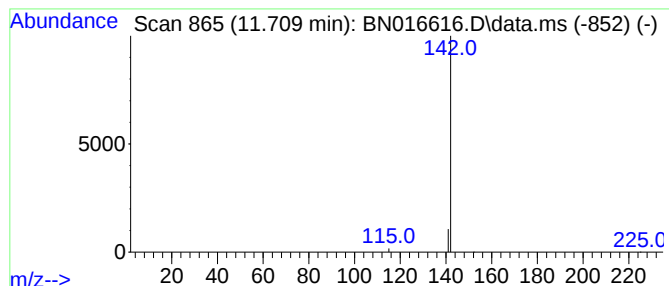
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	24207	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, iodo-	142	CH3I	000074-88-4	4
2			Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	4
3			4-Heptanone, 3-ethyl-	142	C9H18O	001528-25-2	3
4			Cyclohexane carboxylic acid hydr...	142	C7H14N2O	038941-47-8	3
5			2-Butanone, diethylhydrazone	142	C8H18N2	028236-94-4	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
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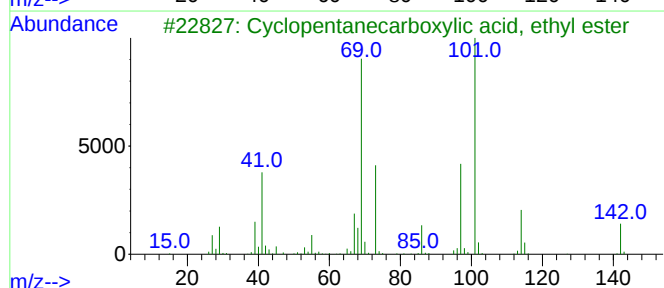
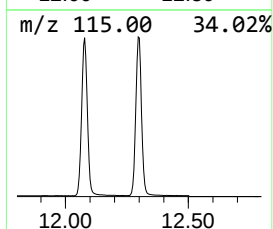
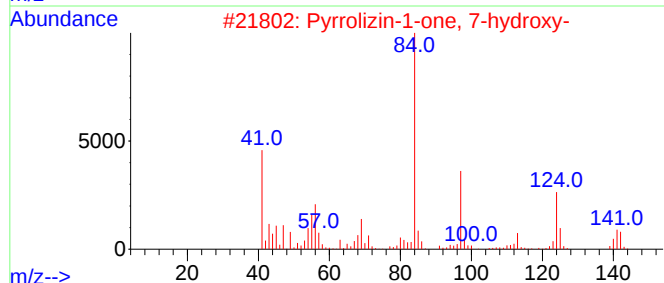
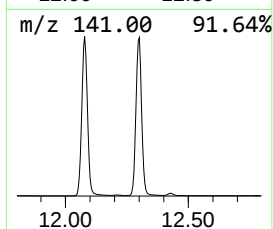
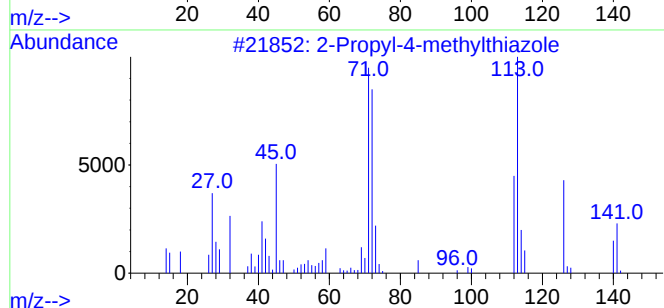
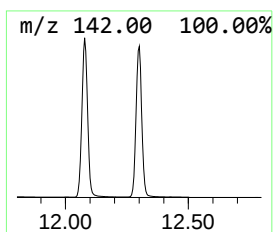
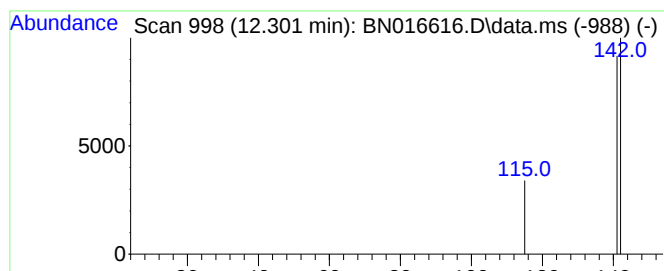
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.41 ng	201528	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2		Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3		Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4		2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5		2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

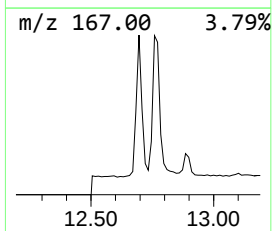
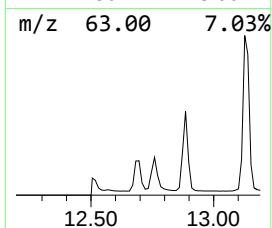
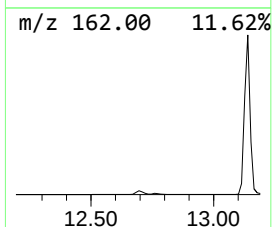
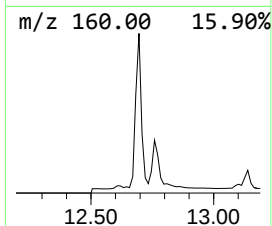
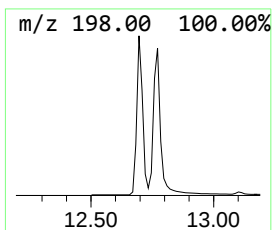
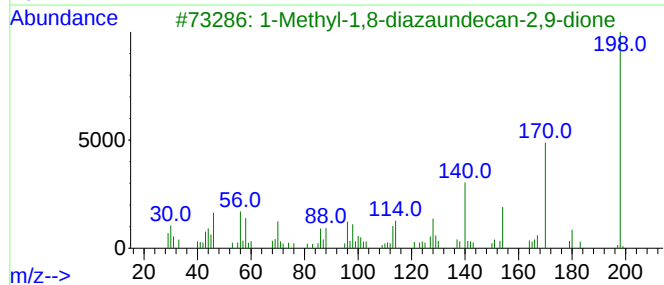
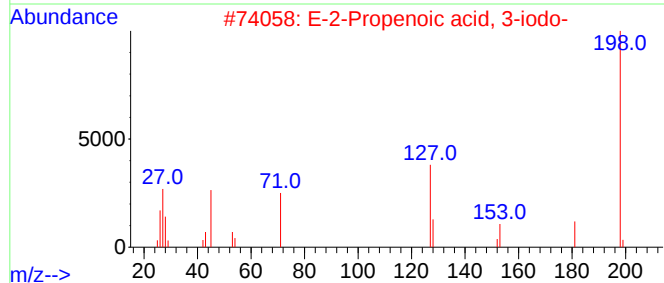
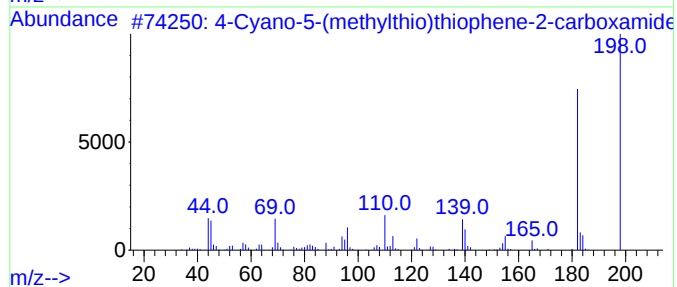
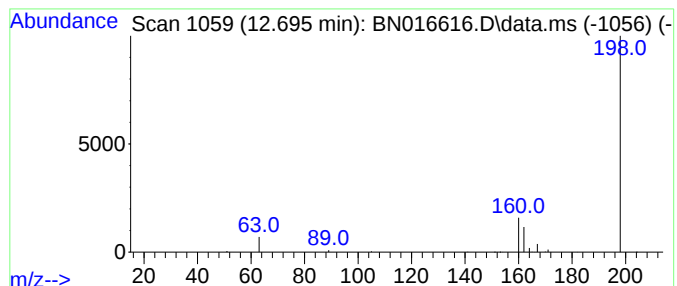
Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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 4-Cyano-5-(methylthio)thiop... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.695	0.06 ng	27778	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Cyano-5-(methylthio)thiophene-...		198	C7H6N2OS2	1000267-39-2	3
2	E-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-7	3
3	1-Methyl-1,8-diazaundecan-2,9-dione		198	C10H18N2O2	1000298-94-5	3
4	Z-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-8	3
5	Thiazolo[5,4-d]pyrimidine, 5-ami...		198	C6H6N4S2	019835-31-5	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

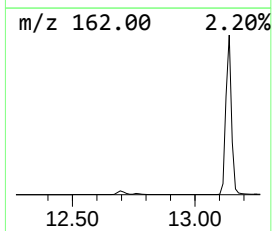
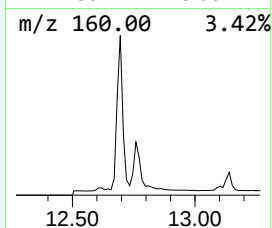
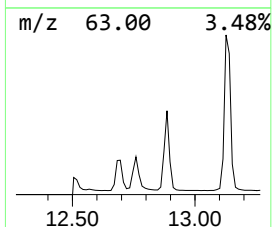
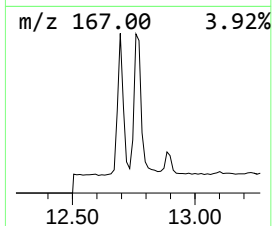
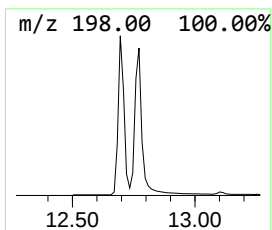
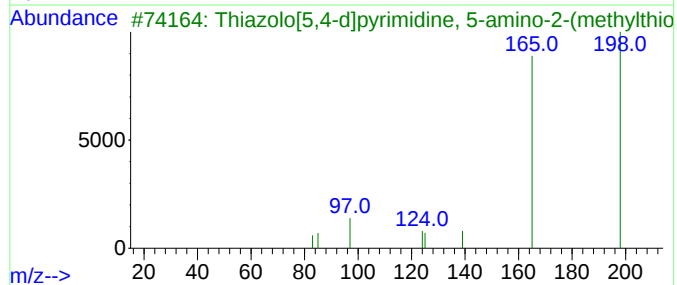
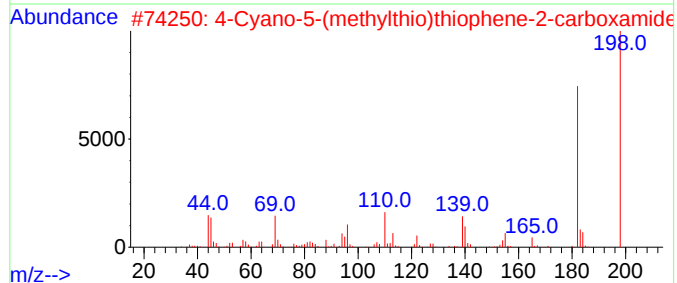
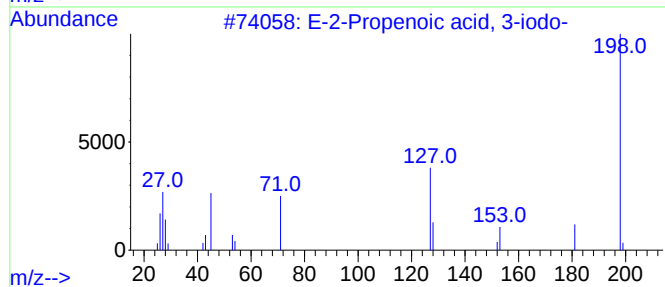
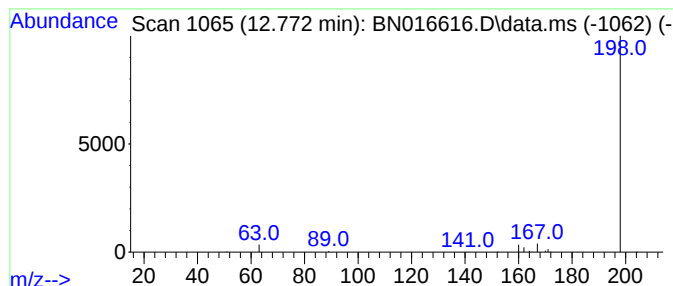
Instrument :
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LabSampleId :
SSTDCCC0.4

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 E-2-Propenoic acid, 3-iodo- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.772	0.05 ng	24168	Acenaphthene-d10			14.269
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	E-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-7	3
2	4-Cyano-5-(methylthio)thiophene-...		198	C7H6N2OS2	1000267-39-2	3
3	Thiazolo[5,4-d]pyrimidine, 5-ami...		198	C6H6N4S2	019835-31-5	3
4	Z-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-8	3
5	Methyl 2-(dimethylhydrazono)-3,3...		198	C6H9F3N2O2	1000489-35-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

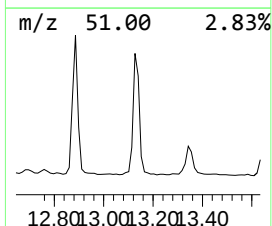
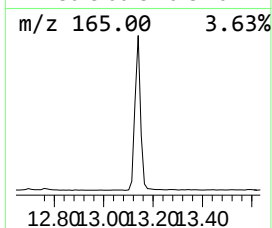
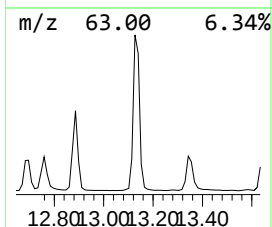
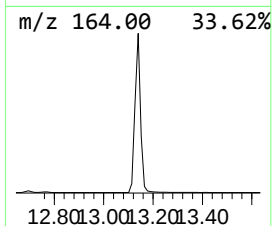
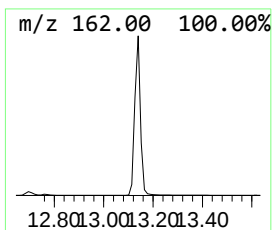
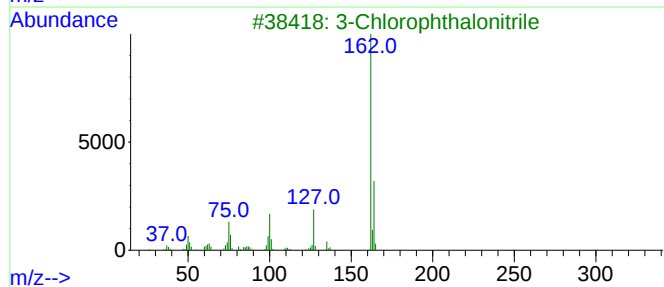
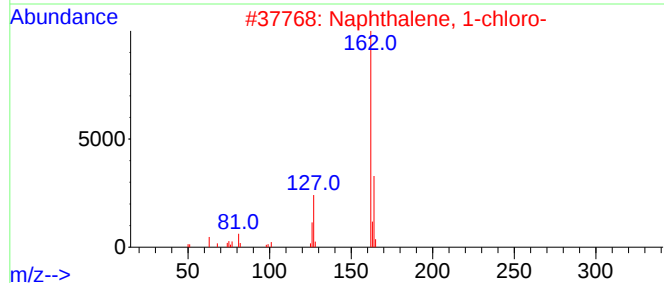
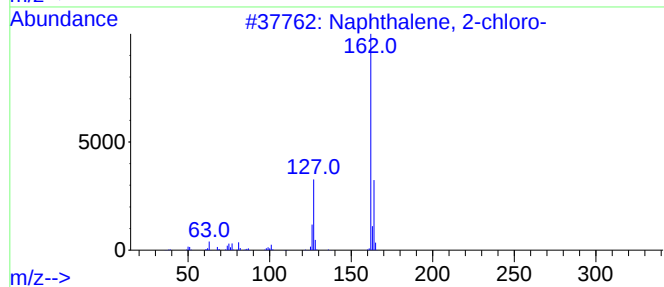
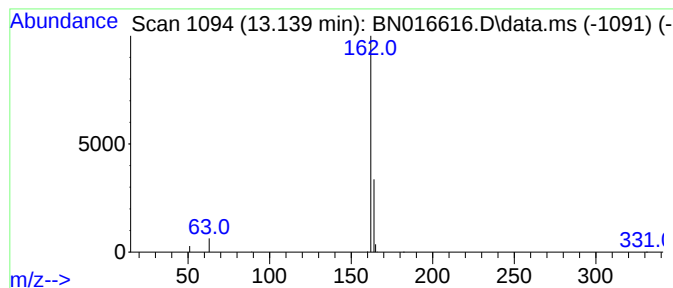
Instrument :
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LabSampleId :
SSTDCCC0.4

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 Naphthalene, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.140	0.26 ng	127421	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 2-chloro-		162	C10H7Cl	000091-58-7	74
2	Naphthalene, 1-chloro-		162	C10H7Cl	000090-13-1	74
3	3-Chlorophthalonitrile		162	C8H3ClN2	076241-79-7	7
4	2-Chloroisophthalonitrile		162	C8H3ClN2	028442-78-6	7
5	2-Amino-4-chloro-1,3-thiazole-5-...		162	C4H3ClN2OS	076874-79-8	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

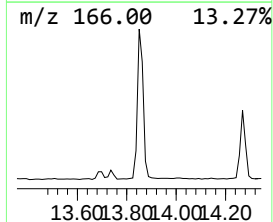
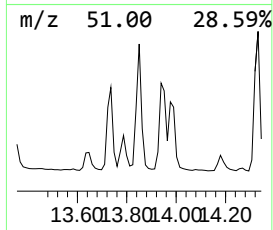
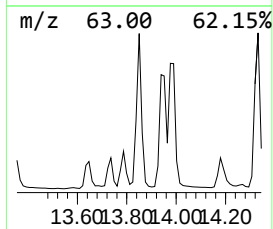
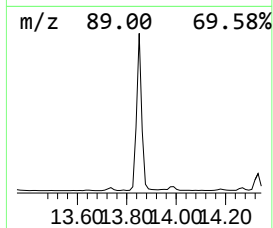
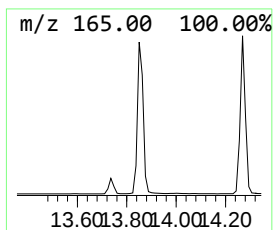
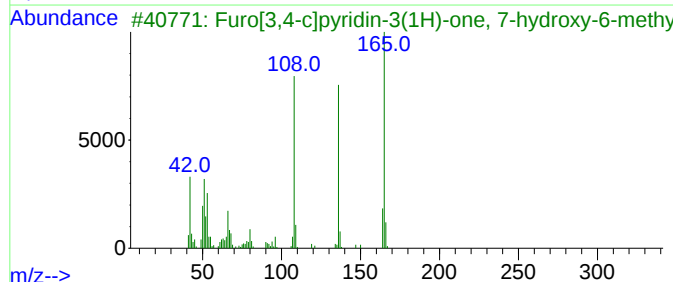
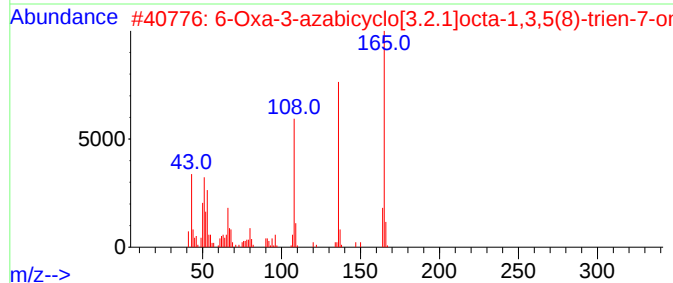
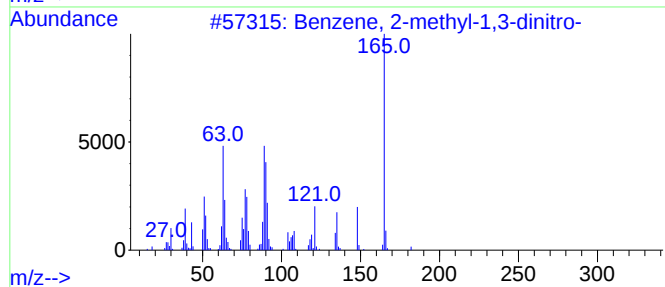
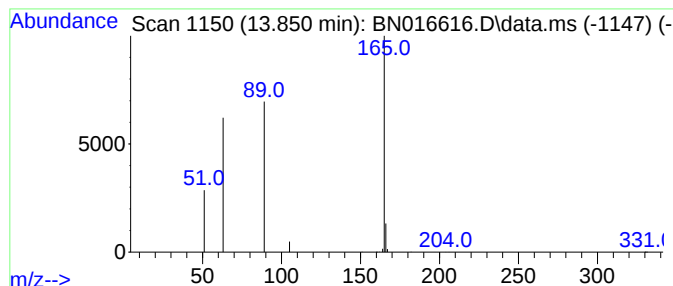
Instrument :
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.850	0.05 ng	27010	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	83
2	6-Oxa-3-azabicyclo[3.2.1]octa-1,...		165	C8H7NO3	055255-96-4	9
3	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
4	7-Hydroxy-2,4-dihydro-1,4-benzox...		165	C8H7NO3	067193-97-9	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

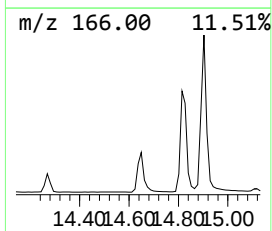
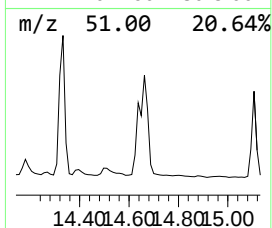
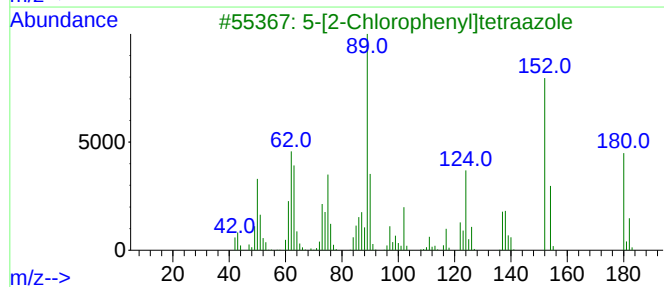
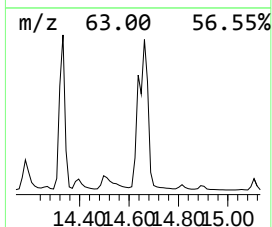
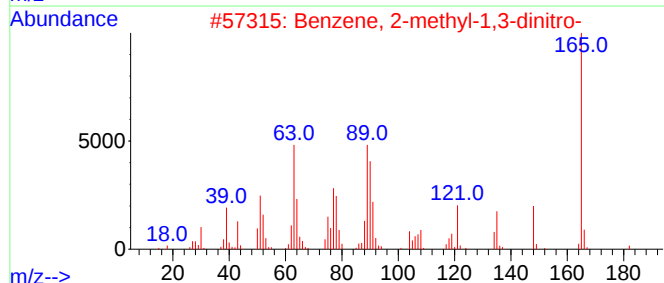
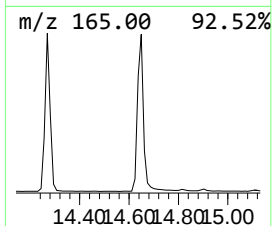
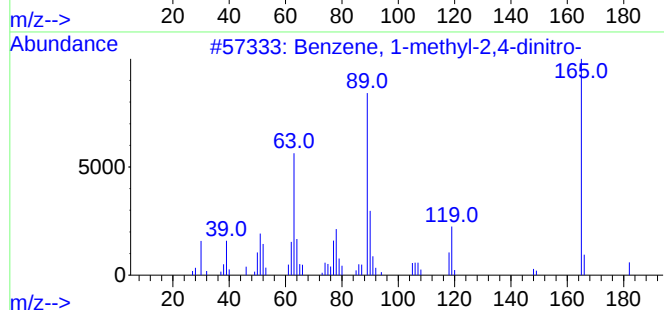
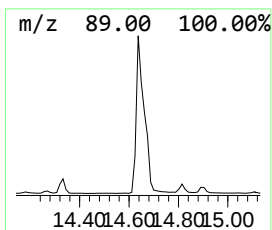
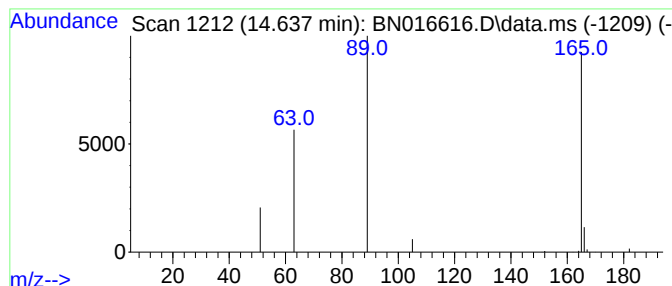
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	42966	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	74
2			Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3			5-[2-Chlorophenyl]tetrazole	180	C7H5ClN4	050907-46-5	9
4			6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9
5			2-Chloromethyl-1,3-dichloro-2-me...	174	C5H9Cl3	001067-09-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

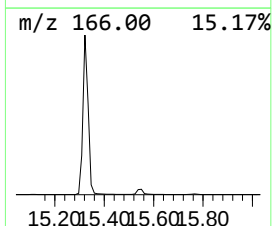
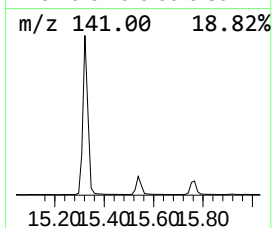
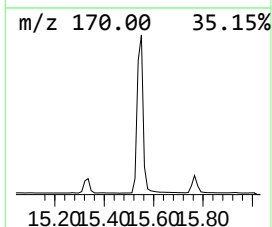
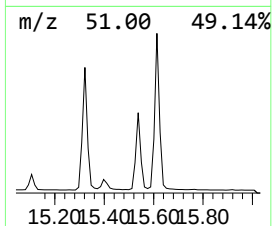
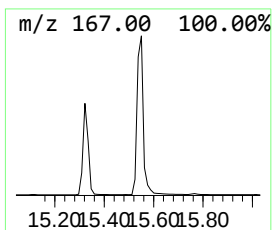
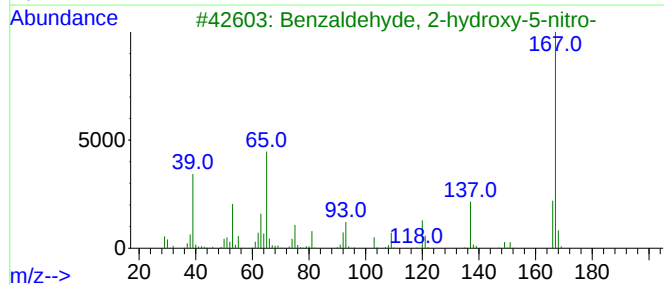
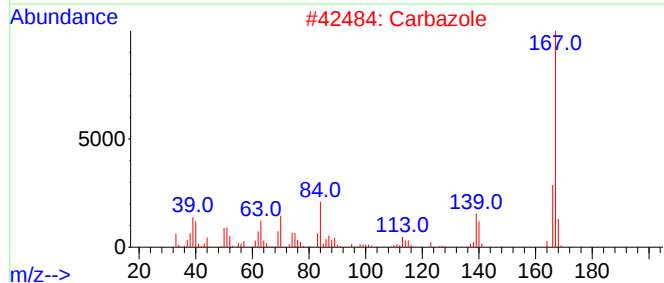
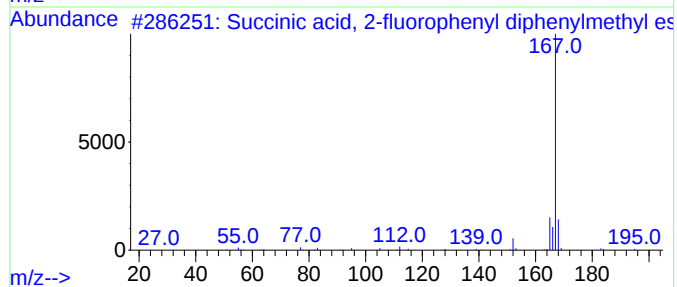
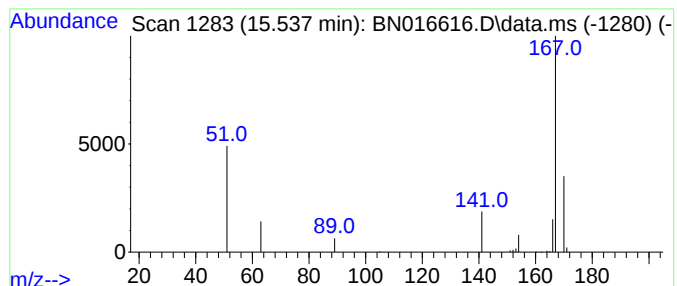
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	59215	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19F04	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5N04	000097-51-8	5
4			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5			2-Chloro-6-methylphenyl isocyanate	167	C8H6ClNO	019241-34-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
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LabSampleId :
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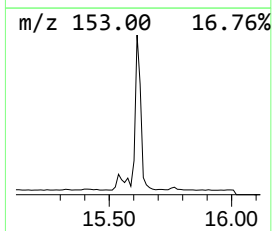
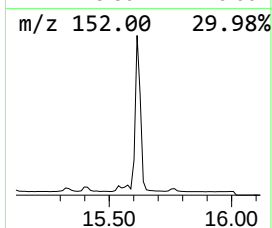
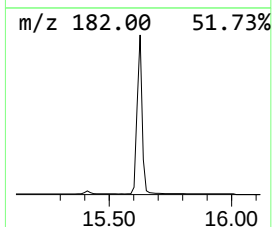
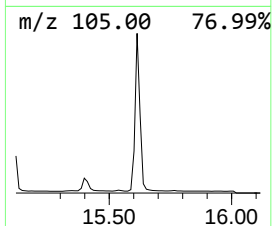
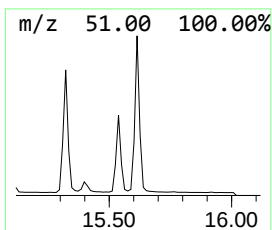
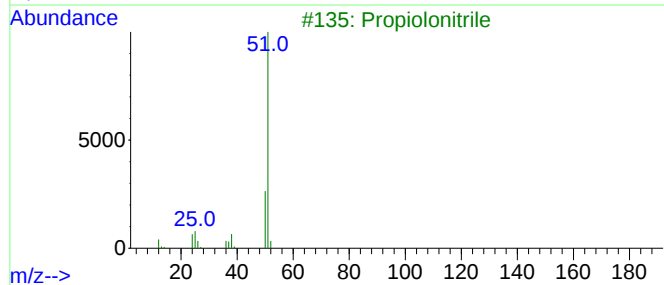
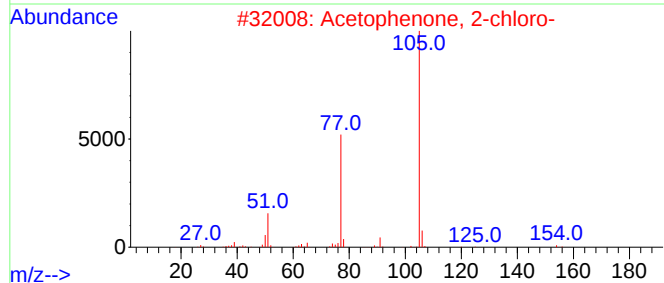
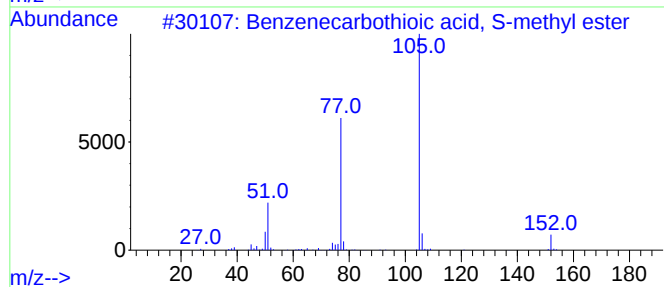
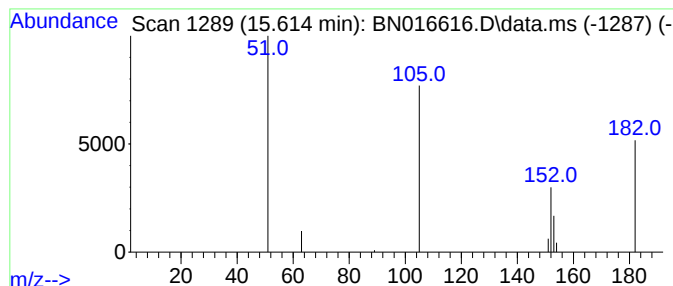
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzenecarbothioic acid, S-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.12 ng	61146	Acenaphthene-d10	14.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
3		Propiolonitrile	51	C3HN	001070-71-9	3
4		Benzenethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3
5		Propanal, 2-(benzoyloxy)-, (R)-	178	C10H10O3	078871-04-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
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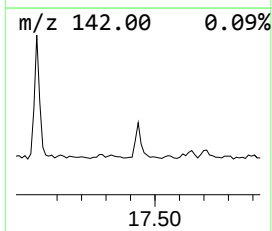
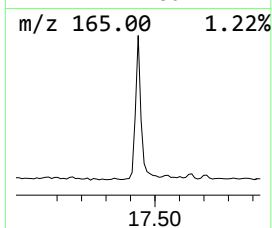
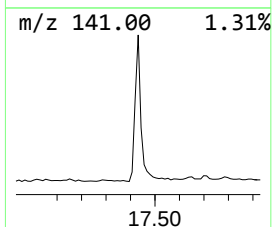
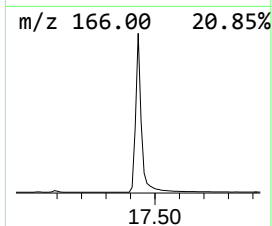
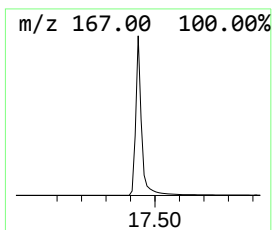
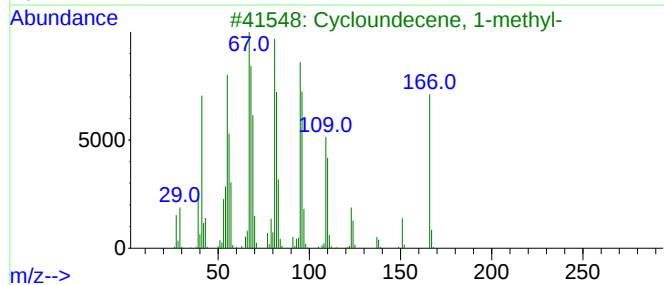
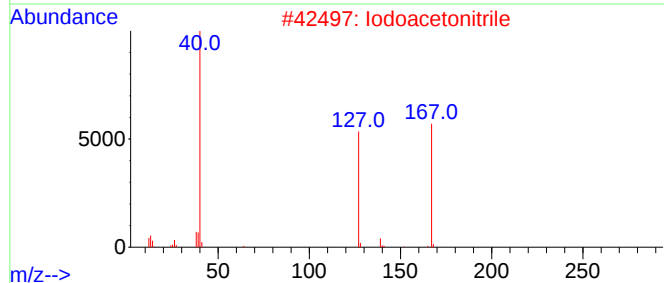
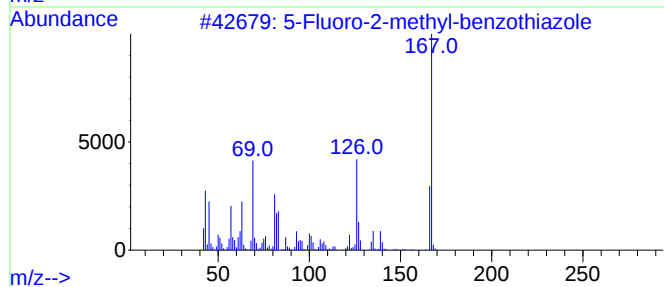
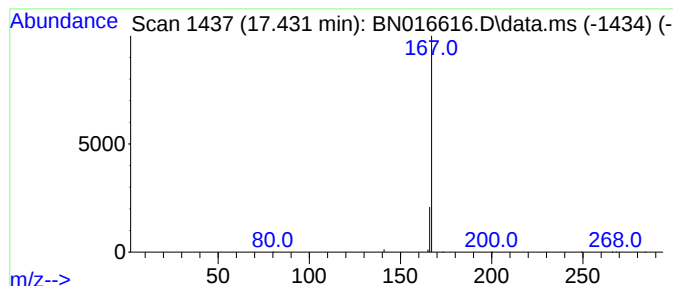
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.34 ng	130218	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Fluoro-2-methyl-benzothiazole	167	C8H6FN5	000399-75-7	5
2		Iodoacetoneitrile	167	C2H2IN	000624-75-9	4
3		Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
4		1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
5		1-Cyclopropanecarbonylpiperidin...	167	C9H13NO2	063463-43-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

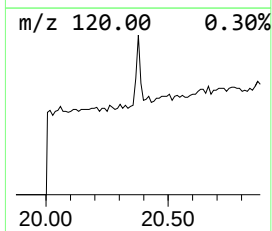
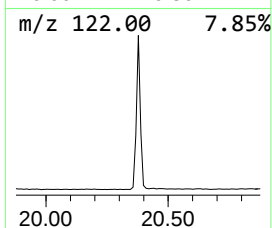
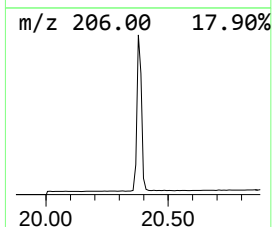
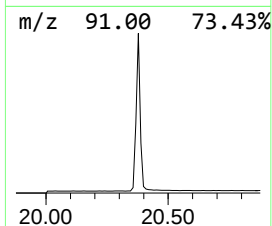
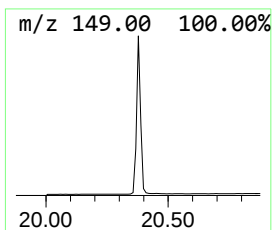
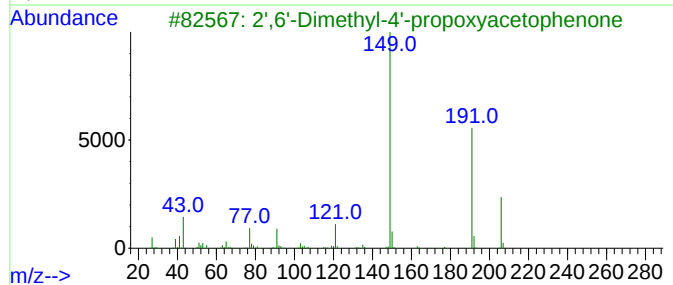
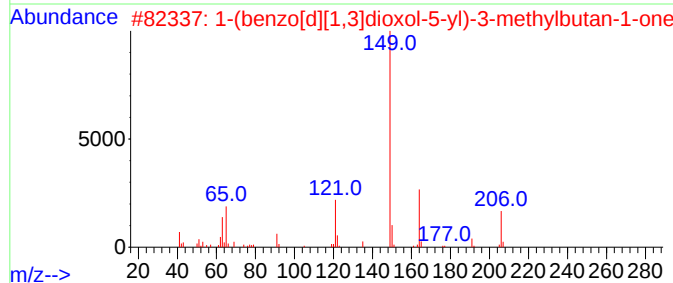
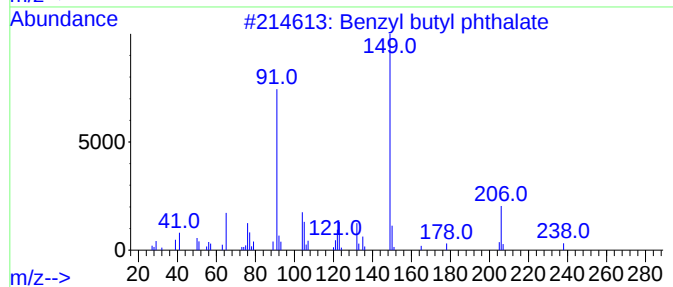
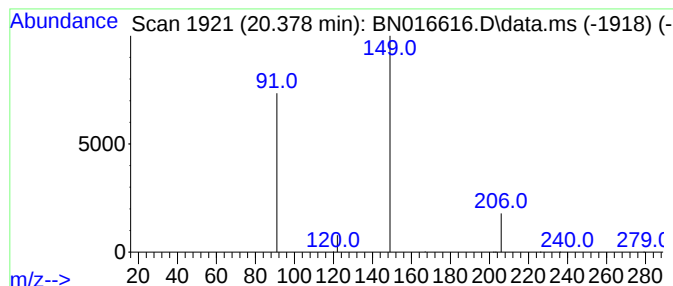
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.05 ng	54358	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl butyl phthalate	312	C19H20O4	000085-68-7	43
2			1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3			2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4			2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
5			1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016616.D
Acq On : 01 Oct 2021 02:23
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

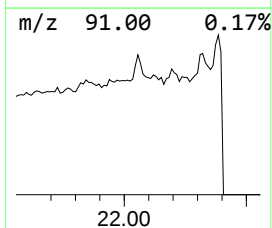
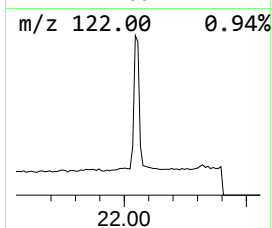
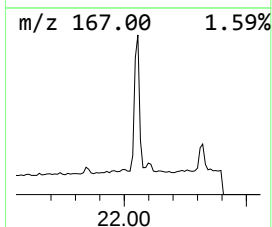
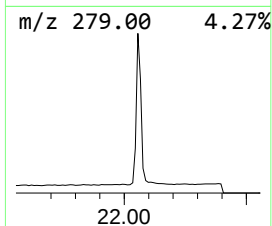
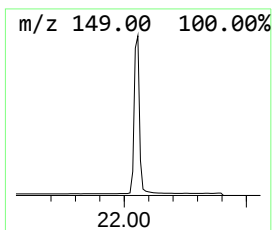
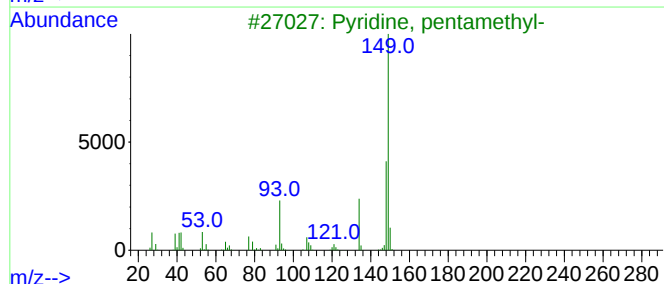
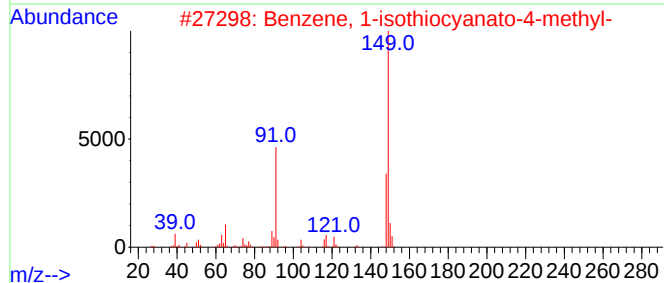
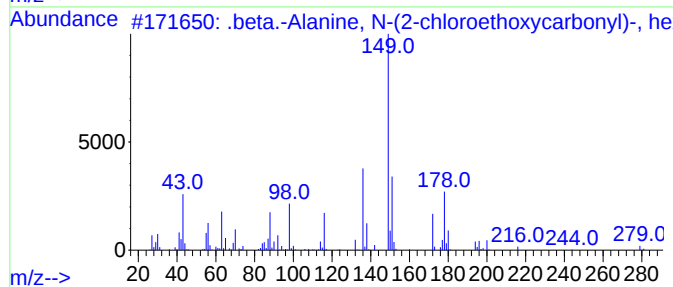
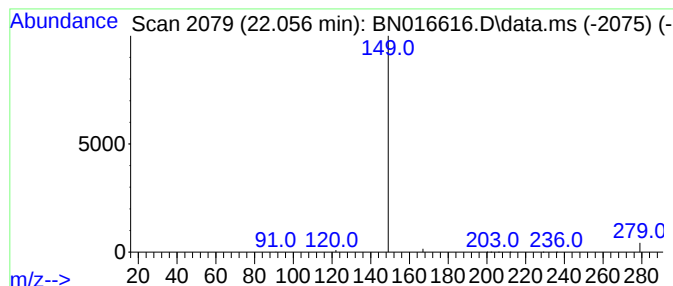
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	76026	Chrysene-d12	21.227

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2		Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
3		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4		m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
5		3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016616.D
 Acq On : 01 Oct 2021 02:23
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 2 Sample Multiplier: 1

Instrument :
 BNA_N
 LabSampleId :
 SSTDCCC0.4

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
1-Propanamine, ...	6.978	0.1	ng	37680	1	7.642	124312	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32675	1	7.642	124312	0.4
3-Methylpyrazol...	7.522	0.0	ng	15410	1	7.642	124312	0.4
6-Benzothiazola...	7.956	0.4	ng	110596	1	7.642	124312	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	49652	1	7.642	124312	0.4
Fomepizole	9.342	0.2	ng	77114	2	10.406	195189	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	27370	2	10.406	195189	0.4
o-Chloroaniline	10.571	0.1	ng	60489	2	10.406	195189	0.4
Methane, iodo-	11.709	0.0	ng	24207	2	10.406	195189	0.4
2-Propyl-4-meth...	12.301	0.4	ng	201528	2	10.406	195189	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	27778	3	14.269	196610	0.4
E-2-Propenoic a...	12.772	0.0	ng	24168	3	14.269	196610	0.4
Naphthalene, 2-...	13.140	0.3	ng	127421	3	14.269	196610	0.4
Benzene, 2-meth...	13.850	0.1	ng	27010	3	14.269	196610	0.4
Benzene, 1-meth...	14.637	0.1	ng	42966	3	14.269	196610	0.4
Succinic acid, ...	15.537	0.1	ng	59215	3	14.269	196610	0.4
Benzenecarbothi...	15.614	0.1	ng	61146	3	14.269	196610	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	130218	4	17.017	154484	0.4
Benzyl butyl ph...	20.378	0.1	ng	54358	5	21.227	403667	0.4
.beta.-Alanine,...	22.056	0.1	ng	76026	5	21.227	403667	0.4