

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016677.D
 Acq On : 02 Oct 2021 18:57
 Operator : CG/JU
 Sample : PB139503BS
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139503BS

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: BN016677.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.244	16	18	20	rBV	6801	9785	2.03%	0.123%
2	3.281	20	22	47	rVB	5505	27648	5.75%	0.347%
3	3.595	51	56	87	rVB	6741	33450	6.95%	0.420%
4	5.264	231	237	249	rBV	14812	57073	11.86%	0.716%
5	6.822	401	406	417	rBV	24311	62666	13.03%	0.786%
6	6.979	418	423	429	rVV	17871	39454	8.20%	0.495%
7	7.080	429	434	440	rVV	36191	75142	15.62%	0.943%
8	7.200	440	447	461	rVB	12448	33431	6.95%	0.420%
9	7.523	478	482	489	rVB	7145	15538	3.23%	0.195%
10	7.642	490	495	513	rVB2	51046	124842	25.95%	1.567%
11	7.956	524	529	538	rVB2	48805	111301	23.14%	1.397%
12	8.168	547	552	562	rVB	3415	8930	1.86%	0.112%
13	8.430	571	577	590	rBV3	21942	50722	10.54%	0.637%
14	8.696	594	598	601	rBV	5007	9495	1.97%	0.119%
15	8.784	601	605	606	rBV	32387	63798	13.26%	0.801%
16	8.822	606	608	616	rVB	27854	52110	10.83%	0.654%
17	9.342	645	649	652	rBV	47568	79873	16.60%	1.002%
18	9.520	660	663	666	rBV	3215	6254	1.30%	0.078%
19	9.596	666	669	680	rVB	8599	15861	3.30%	0.199%
20	9.836	684	688	702	rBV	15559	28392	5.90%	0.356%
21	10.052	702	705	716	rVB	4048	8870	1.84%	0.111%
22	10.407	729	733	735	rBV	107637	201060	41.80%	2.523%
23	10.457	735	737	741	rVV	107595	180098	37.44%	2.260%
24	10.571	743	746	756	rVV	29060	63712	13.24%	0.800%
25	10.749	756	760	763	rVB	32548	57694	11.99%	0.724%
26	11.307	801	804	814	rBV	1896	5146	1.07%	0.065%
27	11.709	852	865	898	rBV	13305	25629	5.33%	0.322%
28	12.003	920	931	939	rBV	59175	94647	19.68%	1.188%
29	12.078	939	948	972	rVV	127456	210982	43.86%	2.648%
30	12.296	987	997	1021	rVV	129732	204114	42.43%	2.561%
31	12.696	1056	1059	1062	rBV	17096	28539	5.93%	0.358%
32	12.772	1062	1065	1071	rVB	11746	24884	5.17%	0.312%
33	12.886	1071	1074	1078	rBV	120217	200202	41.62%	2.512%
34	13.140	1090	1094	1097	rBV	79140	131617	27.36%	1.652%
35	13.736	1138	1141	1143	rBV	11792	17068	3.55%	0.214%
36	13.850	1147	1150	1153	rVB	19465	27825	5.78%	0.349%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	13.939	1155	1157	1158	rBV	5223	8513	1.77%	0.107%
38	13.990	1158	1161	1164	rVB	92728	155103	32.24%	1.946%
39	14.269	1180	1183	1185	rBV	139307	198879	41.34%	2.496%
40	14.332	1185	1188	1191	rVB	167141	246906	51.33%	3.098%
41	14.637	1209	1212	1220	rBV3	16123	43109	8.96%	0.541%
42	14.814	1223	1226	1230	rBV	5387	9120	1.90%	0.114%
43	14.903	1230	1233	1236	rBV	7313	11108	2.31%	0.139%
44	15.106	1246	1249	1252	rBV	8938	11487	2.39%	0.144%
45	15.322	1263	1266	1269	rBV2	234885	355804	73.97%	4.465%
46	15.411	1271	1273	1280	rVV2	2739	6954	1.45%	0.087%
47	15.538	1280	1283	1287	rVV	38798	64058	13.32%	0.804%
48	15.614	1287	1289	1298	rVV2	42852	65436	13.60%	0.821%
49	15.766	1298	1301	1311	rVB2	13357	22513	4.68%	0.283%
50	16.227	1334	1338	1341	rBV2	59166	92583	19.25%	1.162%
51	16.324	1343	1346	1350	rVB	48987	73527	15.29%	0.923%
52	16.494	1358	1360	1372	rVB	20891	34336	7.14%	0.431%
53	16.677	1372	1375	1384	rBV	18738	34127	7.09%	0.428%
54	17.018	1400	1403	1405	rBV	101140	164510	34.20%	2.064%
55	17.066	1405	1407	1410	rVV	151115	220720	45.88%	2.770%
56	17.151	1411	1414	1434	rVB	115510	188859	39.26%	2.370%
57	17.431	1434	1437	1453	rBV	86167	140736	29.26%	1.766%
58	18.016	1482	1485	1506	rVB8	5887	7951	1.65%	0.100%
59	19.063	1686	1696	1699	rBV	122665	170901	35.53%	2.145%
60	19.093	1699	1702	1747	rVB	194812	270096	56.15%	3.389%
61	19.460	1767	1776	1805	rBV	198518	270329	56.20%	3.392%
62	19.679	1813	1820	1862	rVB	116234	147413	30.64%	1.850%
63	20.378	1918	1921	1924	rBV	51355	61736	12.83%	0.775%
64	21.164	1992	1995	1997	rBV	50346	66352	13.79%	0.833%
65	21.217	1997	2000	2003	rVV2	213350	435506	90.53%	5.465%
66	21.270	2003	2005	2017	rVB	209177	285603	59.37%	3.584%
67	22.056	2076	2079	2082	rBV	75826	94217	19.59%	1.182%
68	22.807	2217	2229	2235	rBV	131022	213756	44.44%	2.682%
69	22.851	2235	2242	2297	rVB	136621	262905	54.65%	3.299%
70	23.385	2384	2398	2416	rBV	85678	195355	40.61%	2.452%
71	23.485	2416	2427	2488	rVB	100370	218420	45.41%	2.741%
72	24.084	2593	2602	2622	rBV	5609	11264	2.34%	0.141%
73	24.854	2817	2827	2852	rVB2	5683	12656	2.63%	0.159%
74	25.771	3066	3095	3171	rBV3	116554	481040	100.00%	6.037%
75	26.456	3273	3295	3356	rBV	67239	226910	47.17%	2.848%

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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

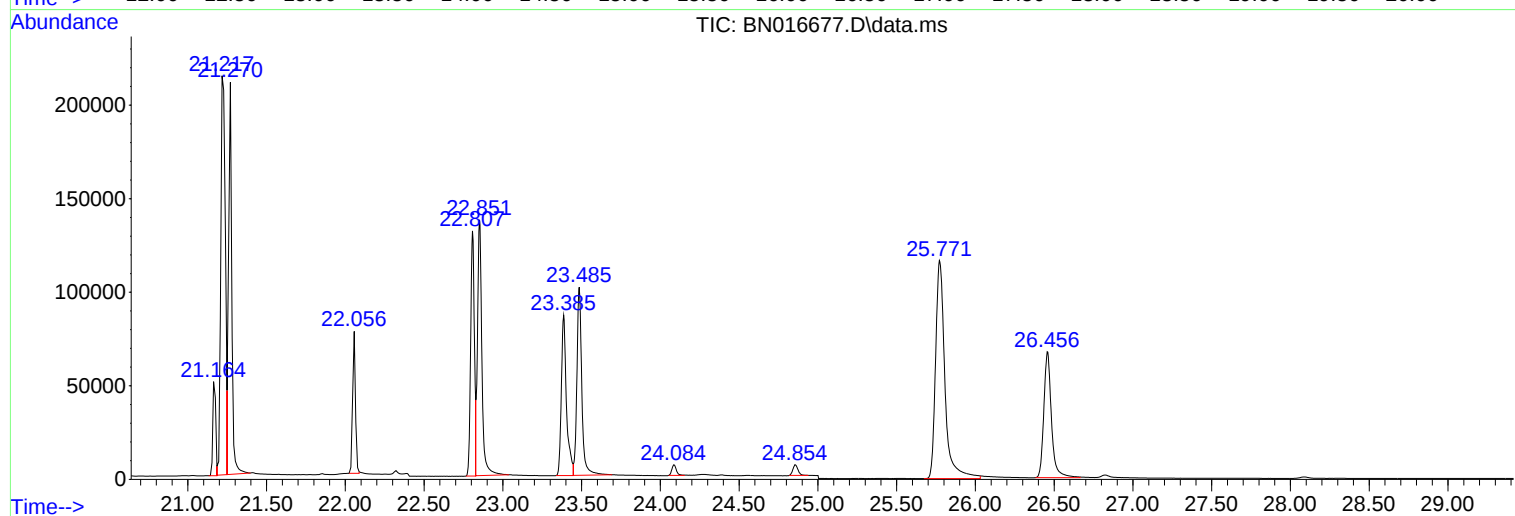
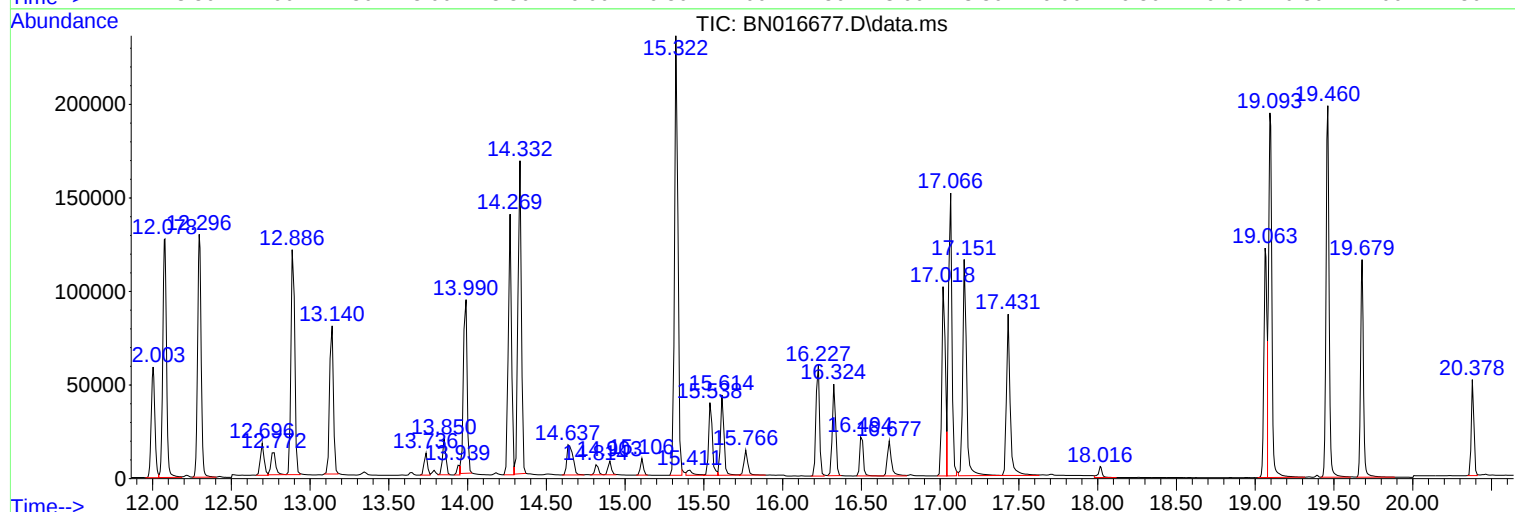
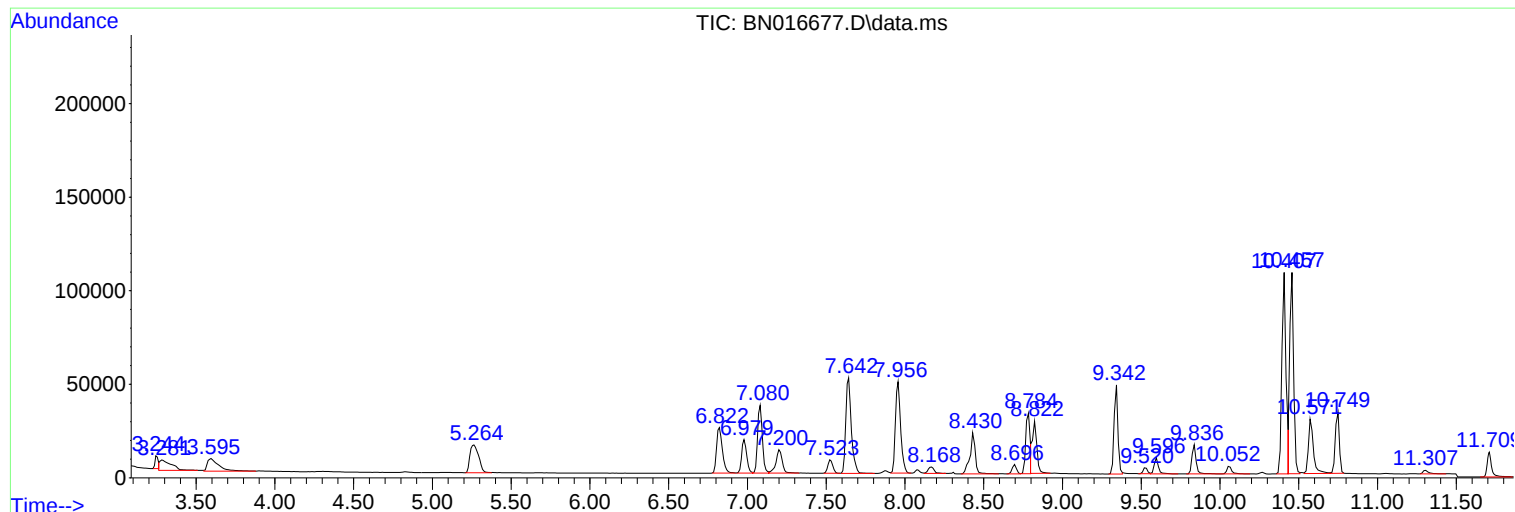
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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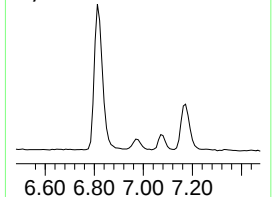
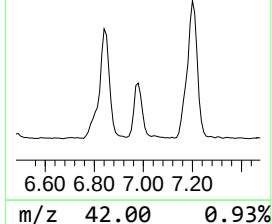
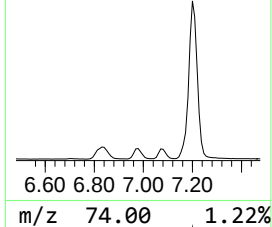
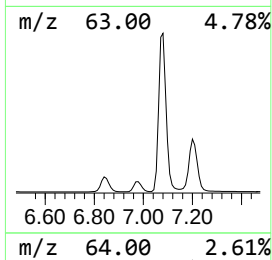
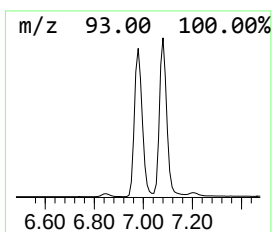
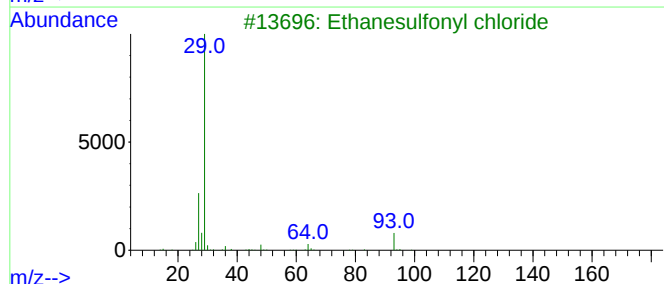
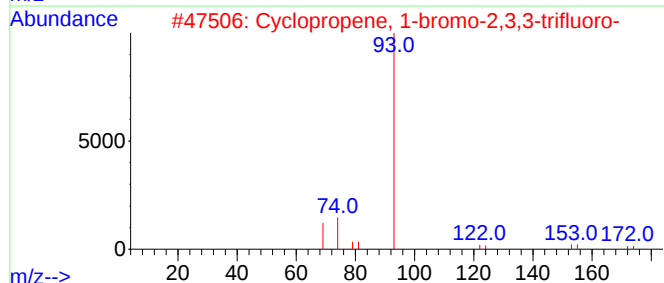
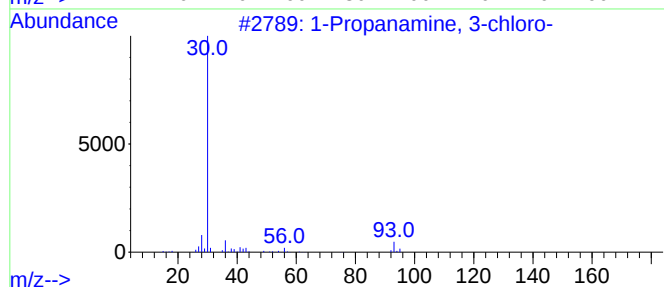
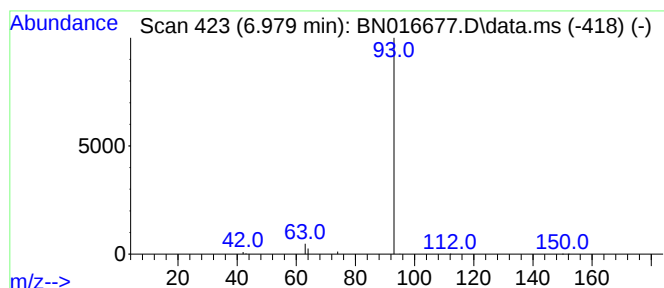
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.13 ng	39454	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			Ethanesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1



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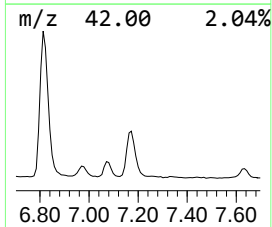
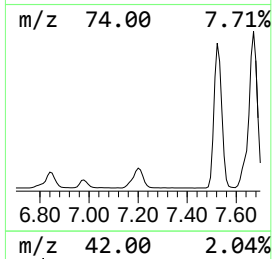
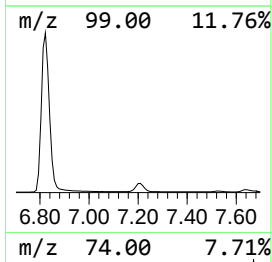
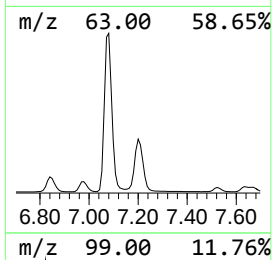
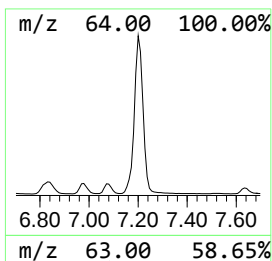
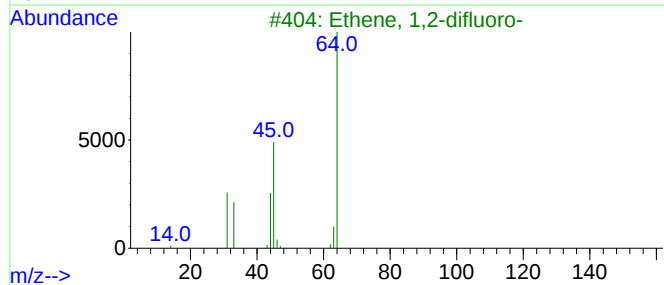
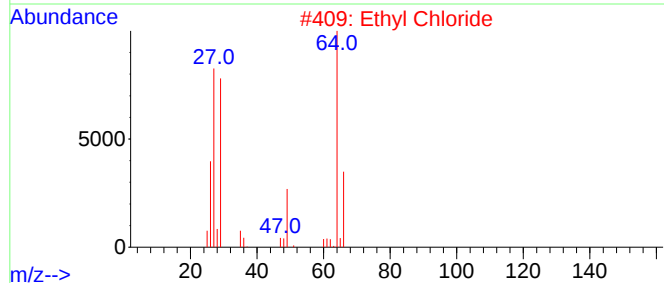
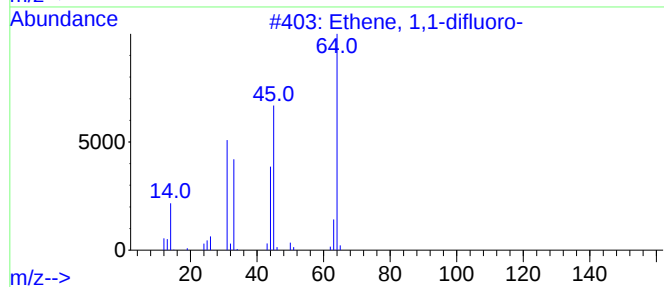
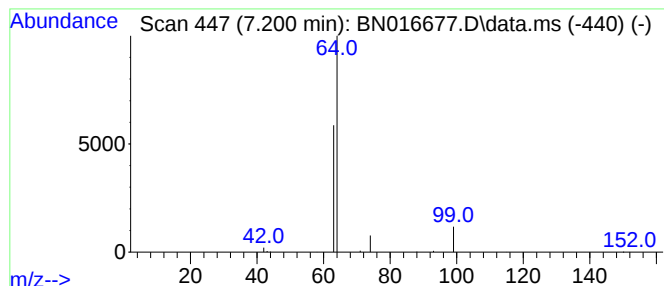
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	33431	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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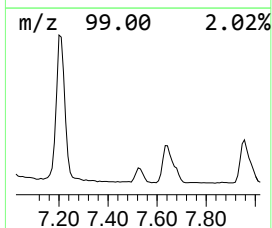
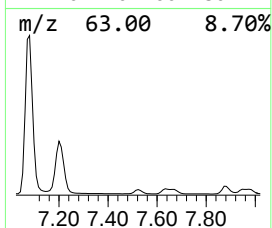
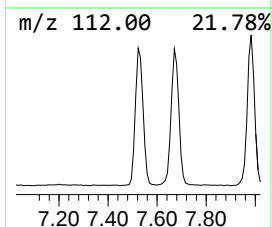
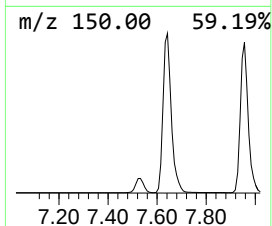
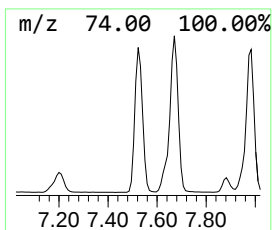
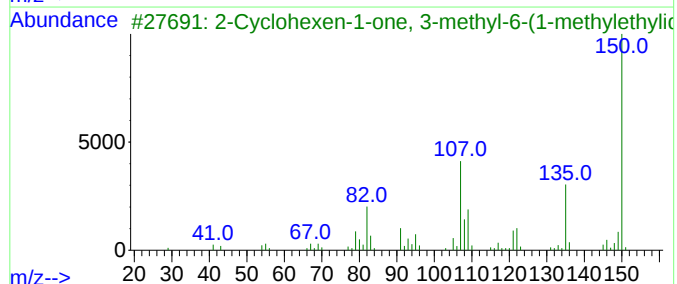
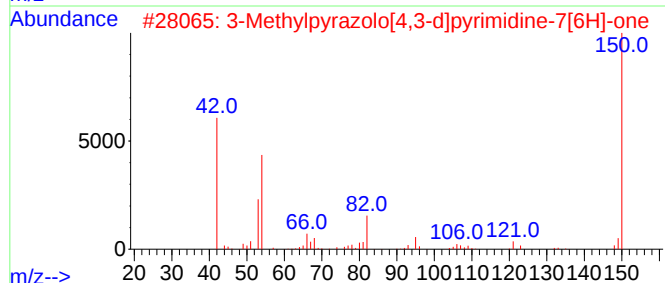
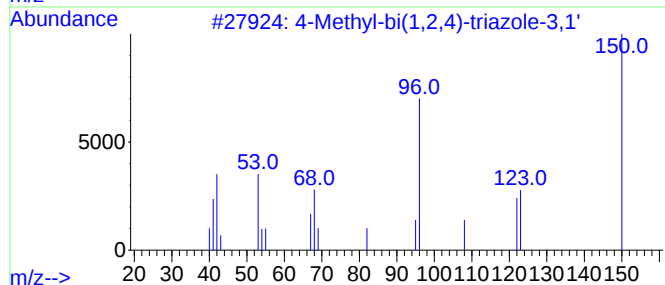
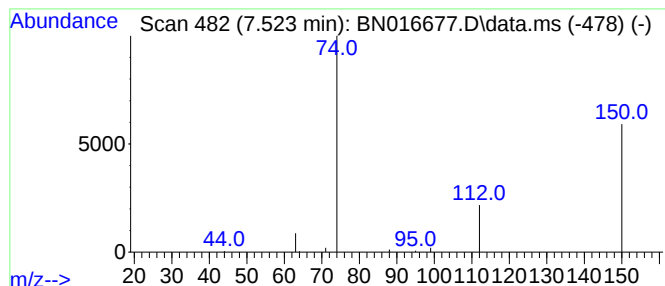
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Methyl-bi(1,2,4)-triazole... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	15538	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-bi(1,2,4)-triazole-3,1'	150	C5H6N6	063523-89-7	2
2			3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
3			2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
4			N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2
5			Propanoic acid	74	C3H6O2	000079-09-4	2



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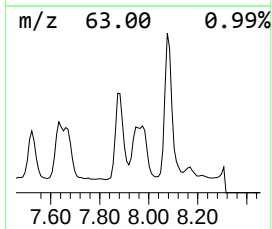
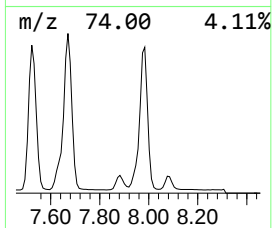
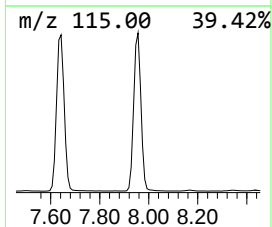
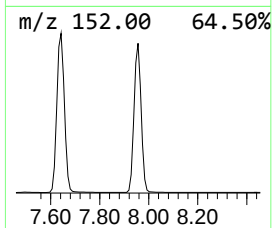
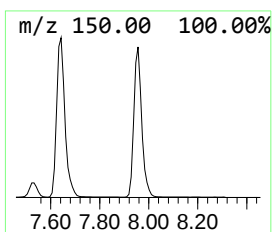
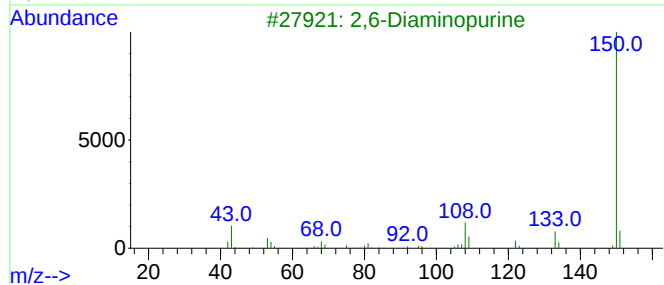
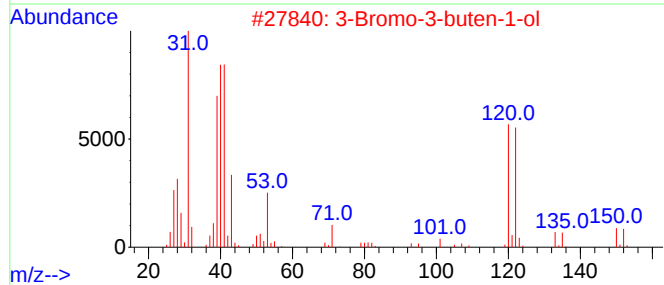
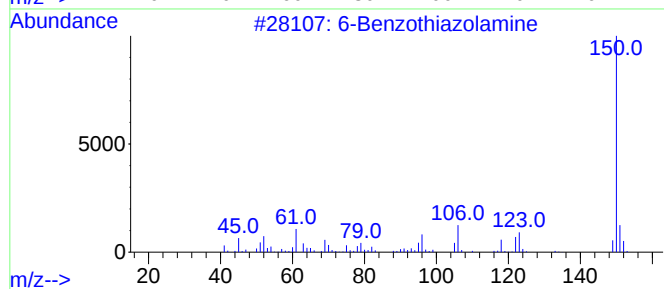
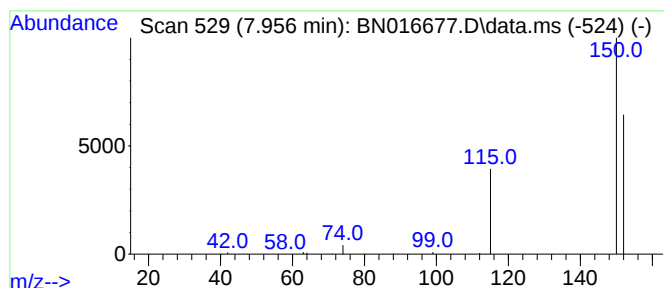
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	111301	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		3-Bromo-3-buten-1-ol	150	C4H7BrO	076334-36-6	3
3		2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
4		9-Methylpoxanthine	150	C6H6N4O	000875-31-0	2
5		5,6,7,8-Tetrahydro-6-oxopteridine	150	C6H6N4O	051036-16-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

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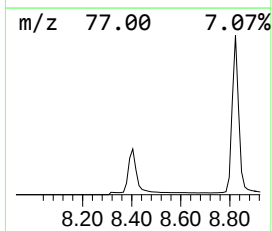
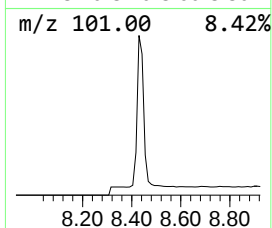
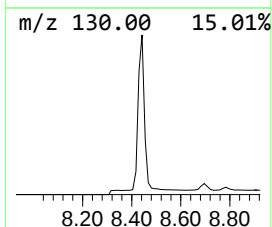
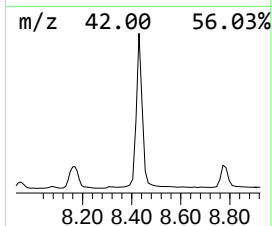
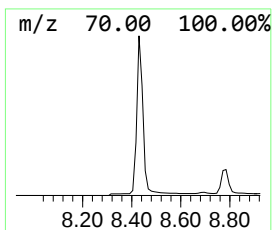
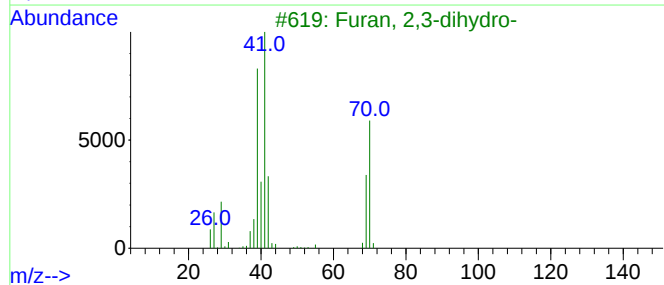
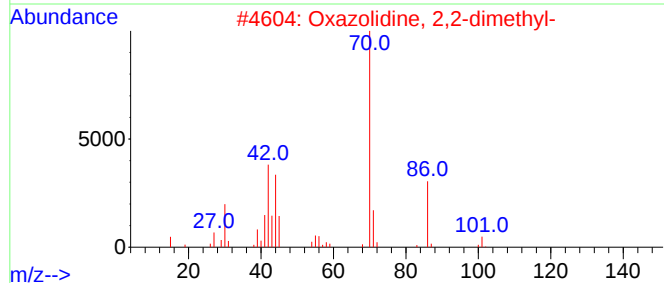
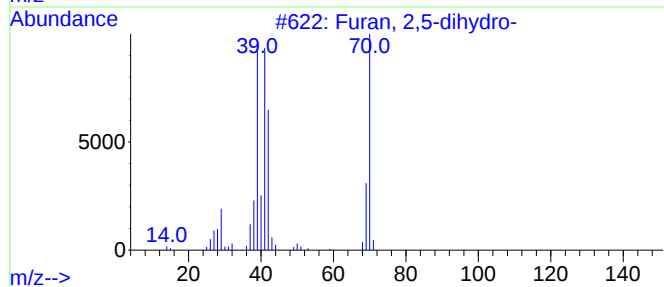
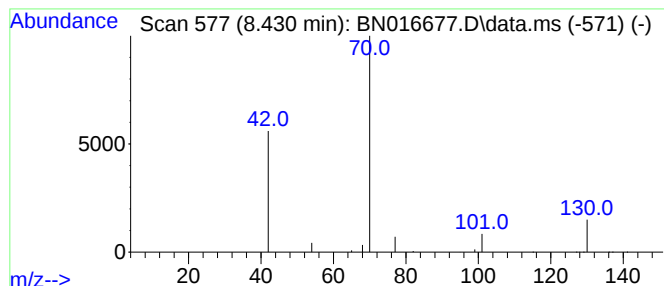
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
8.430	0.16 ng	50722	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			Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4			Dimethylketene	70	C4H6O	000598-26-5	5
5			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
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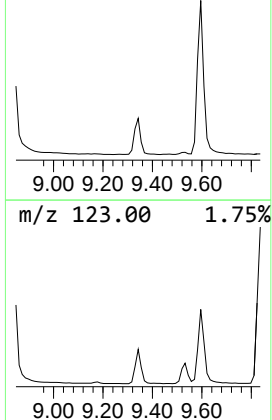
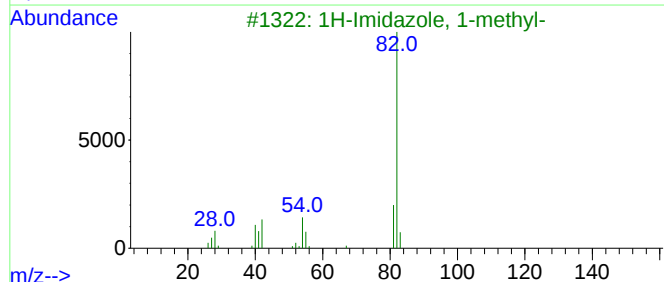
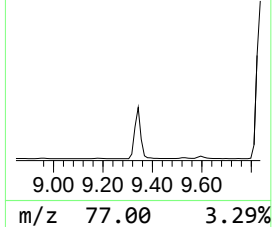
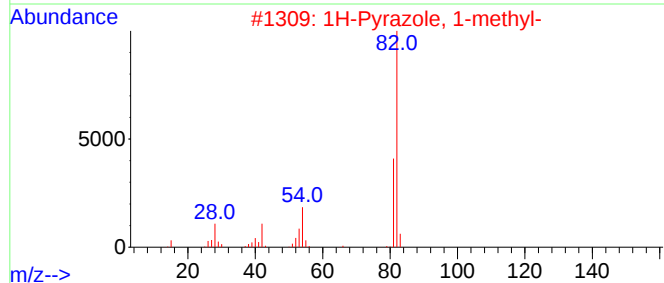
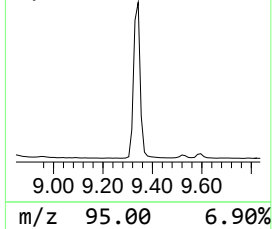
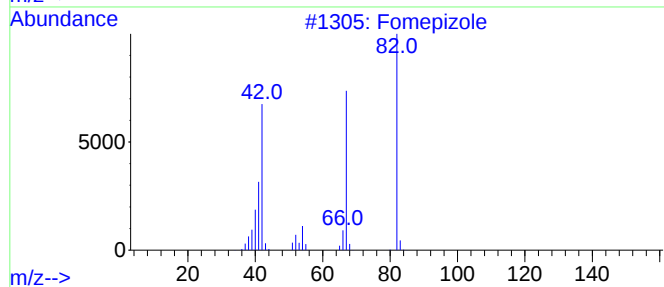
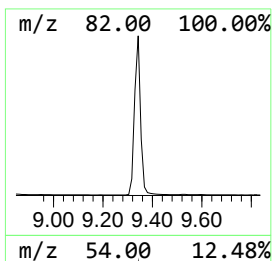
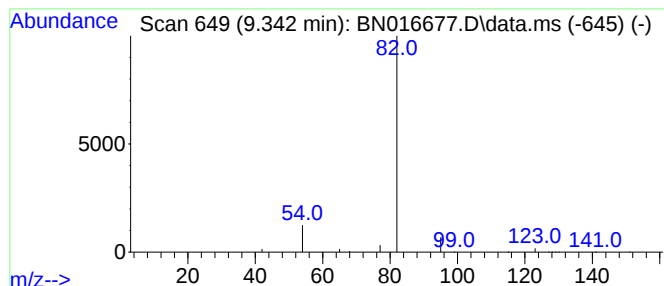
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	79873	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fomepizole	82	C4H6N2	007554-65-6	5
2			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	4
3			1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
4			Furan, 3-methyl-	82	C5H6O	000930-27-8	4
5			Furan, 2-methyl-	82	C5H6O	000534-22-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
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Instrument :
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ClientSampleId :
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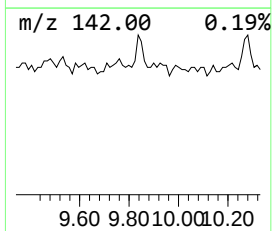
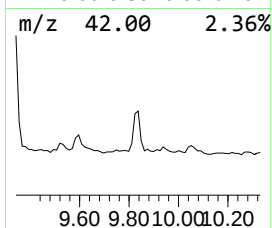
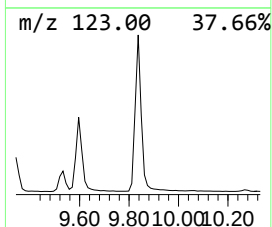
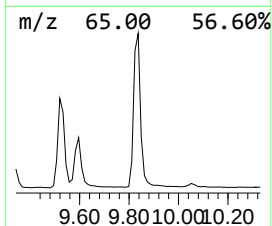
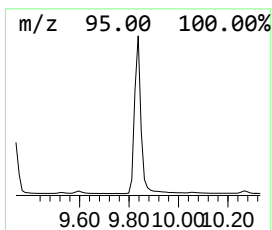
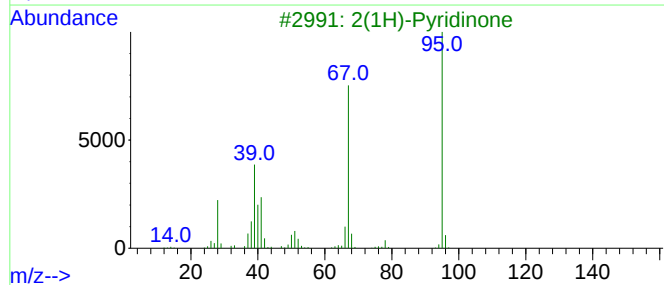
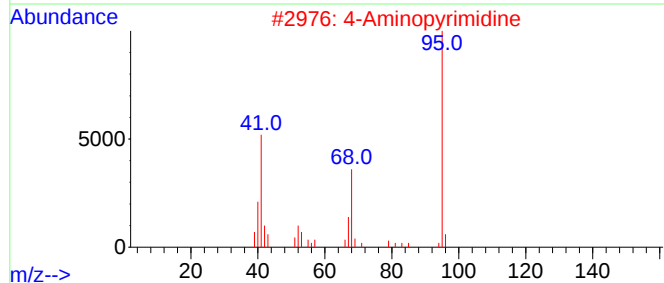
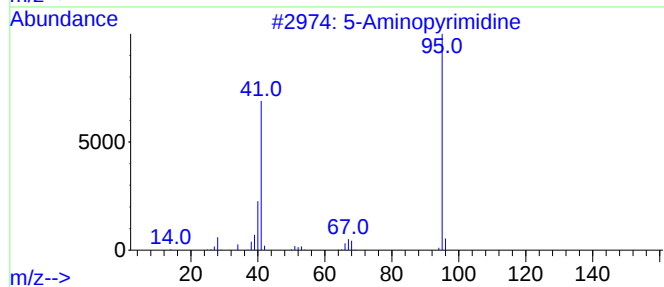
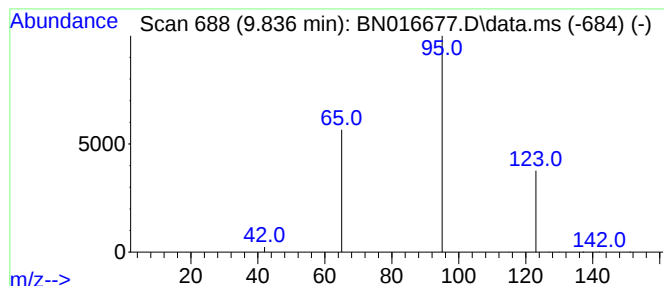
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Aminopyrimidine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	28392	Naphthalene-d8	10.407

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
2		4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
3		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
4		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5		Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
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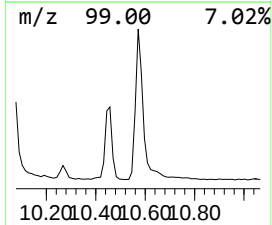
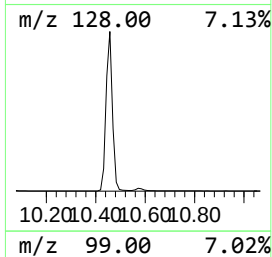
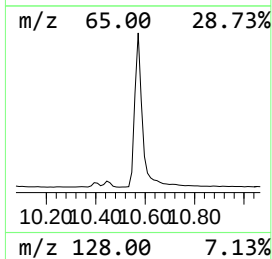
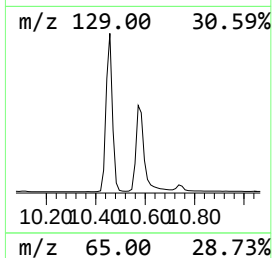
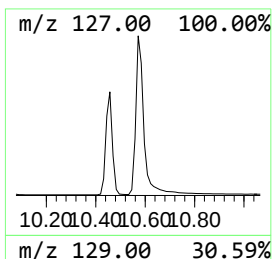
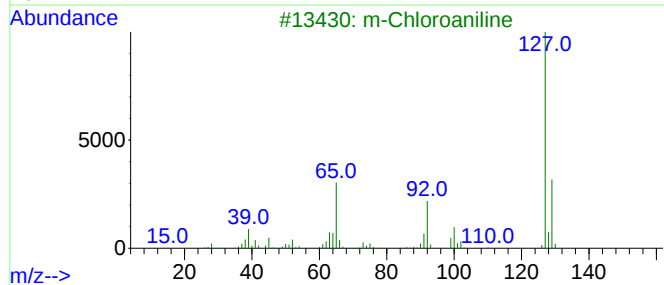
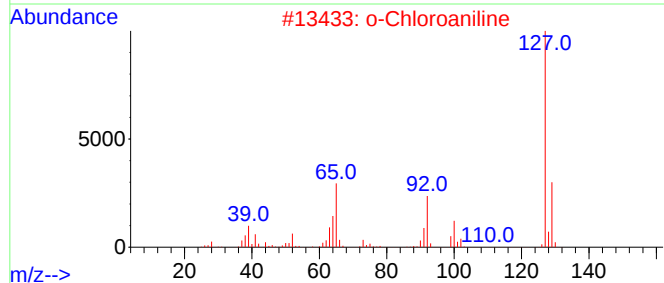
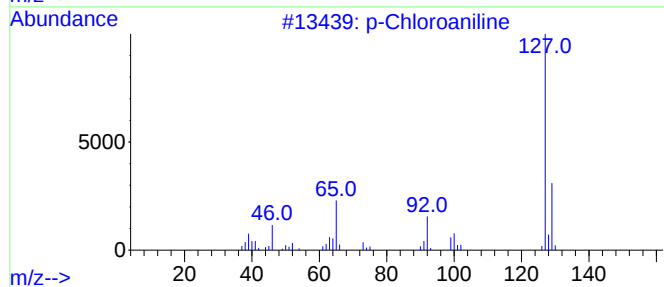
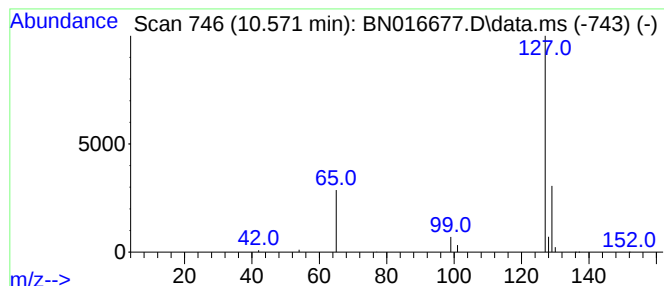
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.13 ng	63712	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Chloroaniline	127	C6H6ClN	000106-47-8	90
2			o-Chloroaniline	127	C6H6ClN	000095-51-2	90
3			m-Chloroaniline	127	C6H6ClN	000108-42-9	90
4			4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5			Pyridine, 2-chloro-6-methyl-	127	C6H6ClN	018368-63-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
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Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

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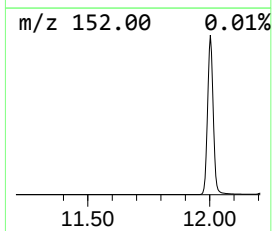
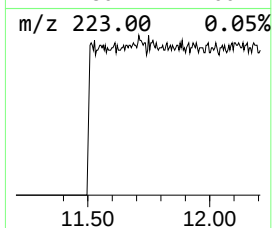
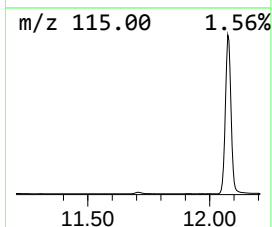
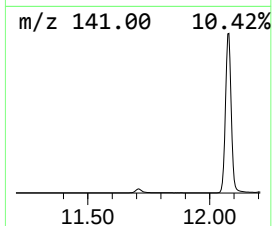
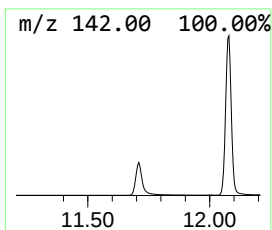
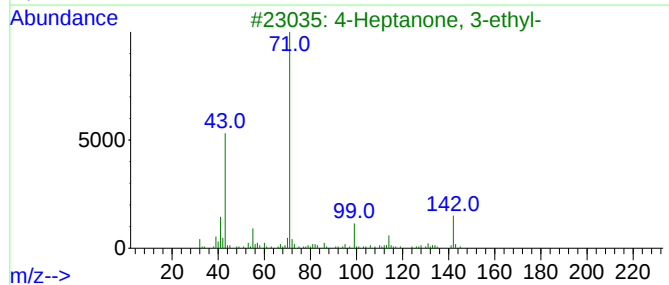
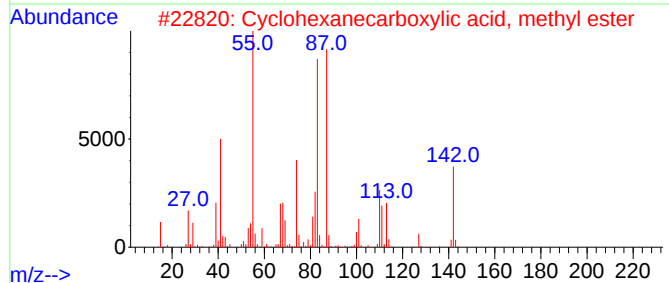
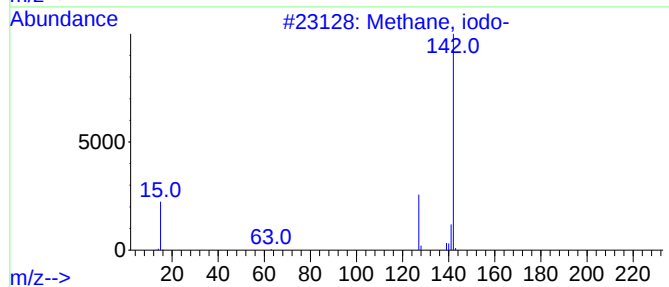
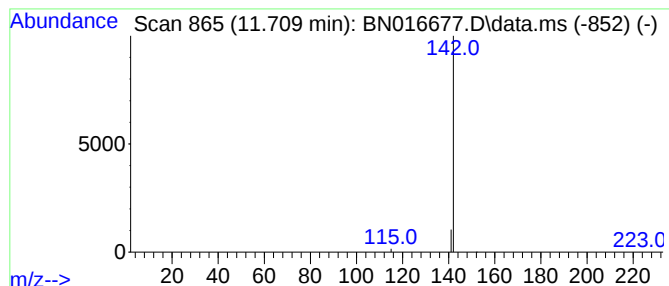
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	25629	Naphthalene-d8	10.407

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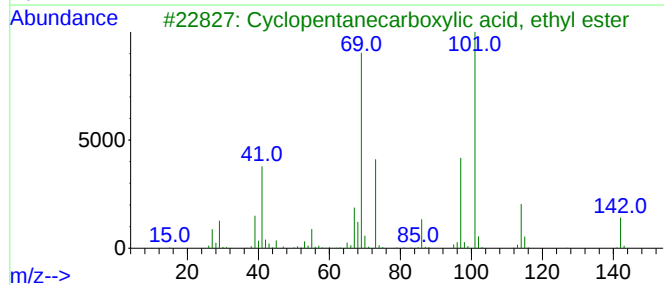
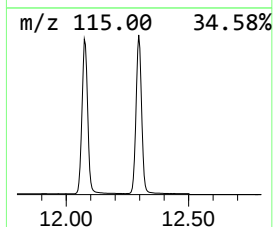
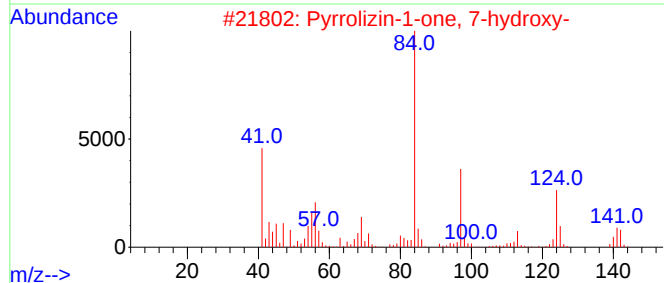
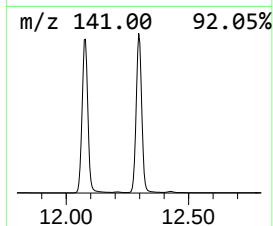
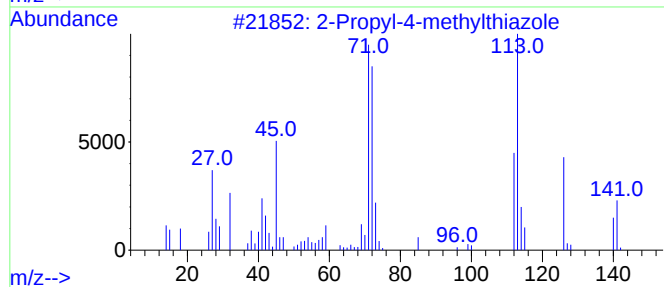
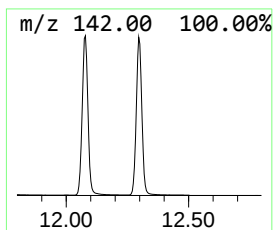
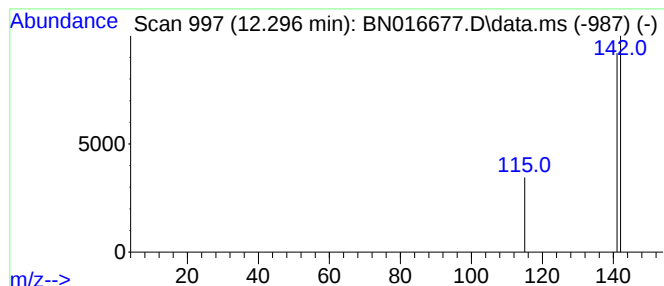
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.41 ng	204114	Naphthalene-d8	10.407

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



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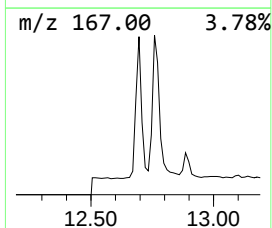
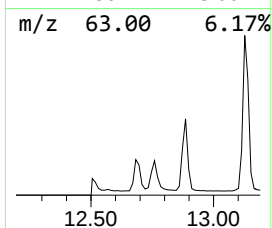
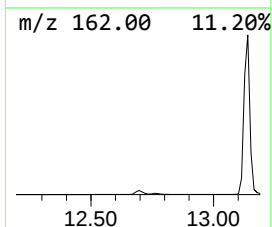
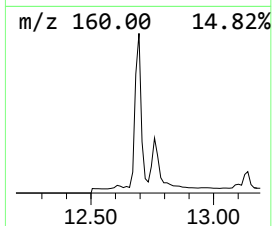
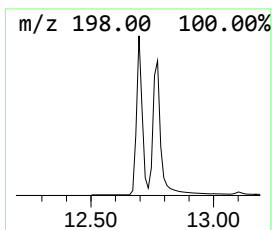
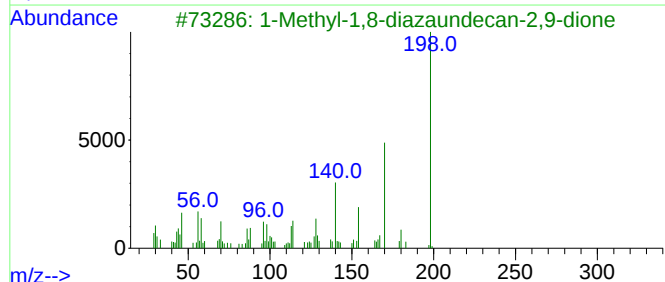
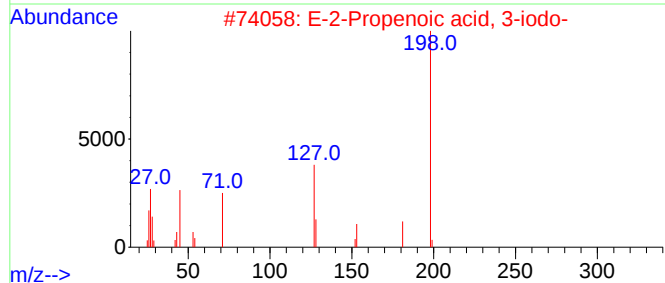
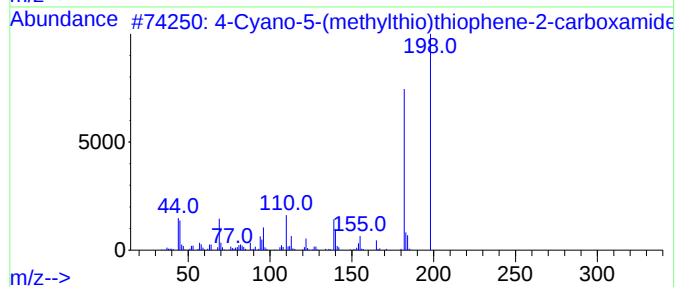
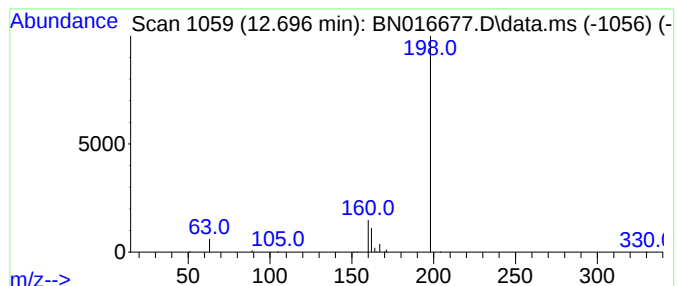
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	28539	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 : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139503BS

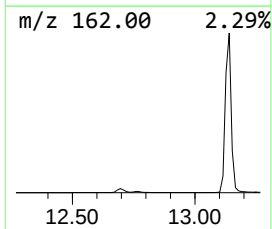
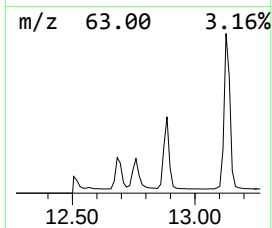
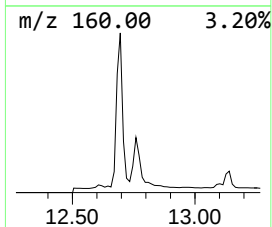
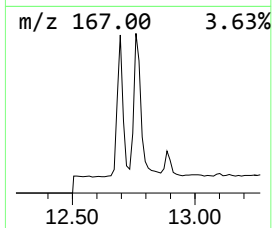
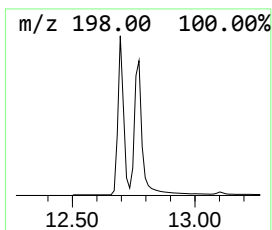
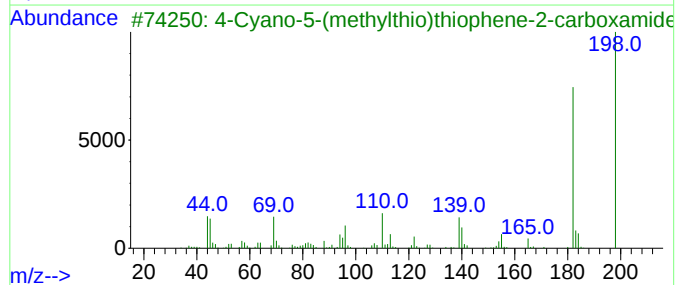
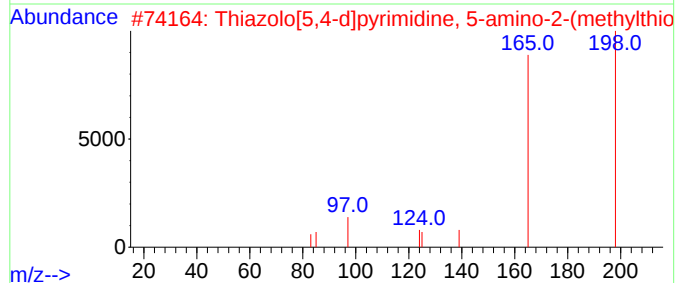
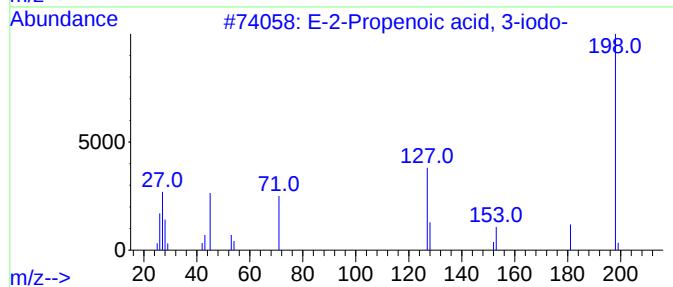
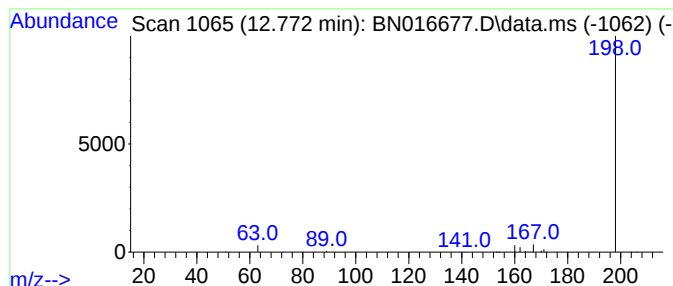
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.05 ng	24884	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			Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
3			4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
4			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5			Imidazolidine-2,4,5-trione, 1,3-...	198	C7H6N2O5	115083-04-0	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

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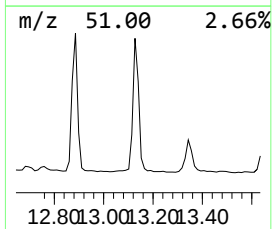
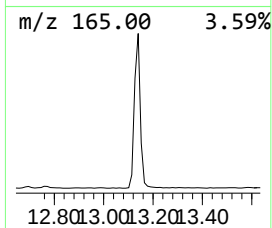
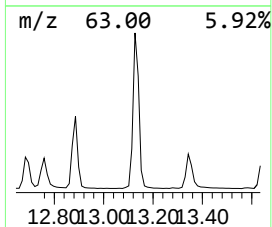
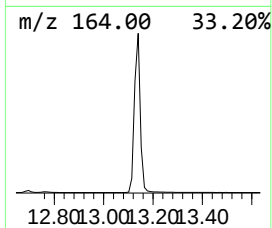
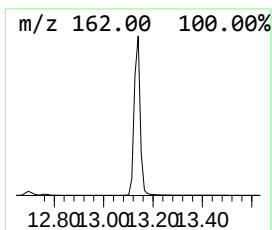
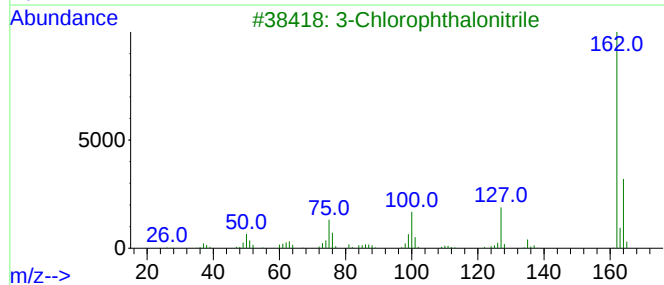
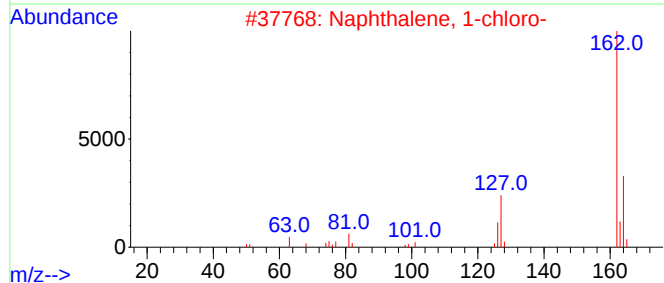
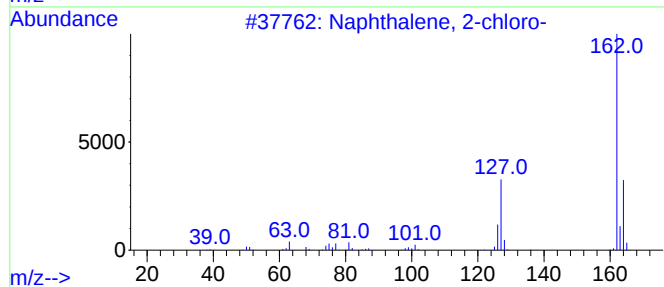
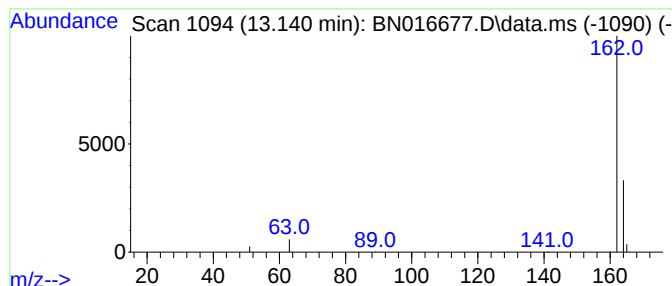
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Naphthalene, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.26 ng	131617	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 : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

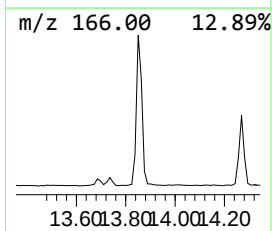
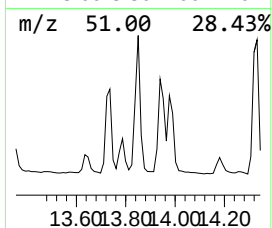
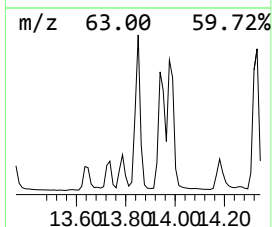
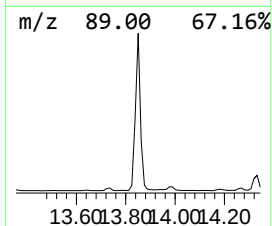
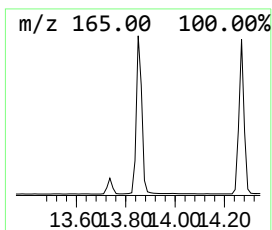
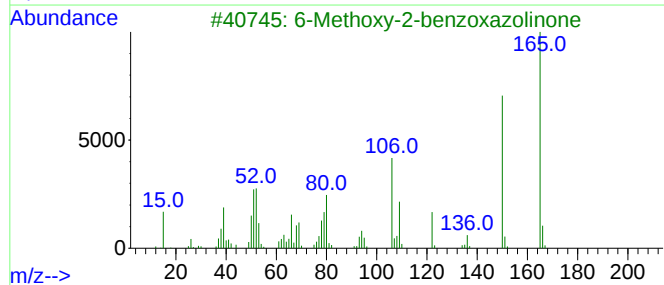
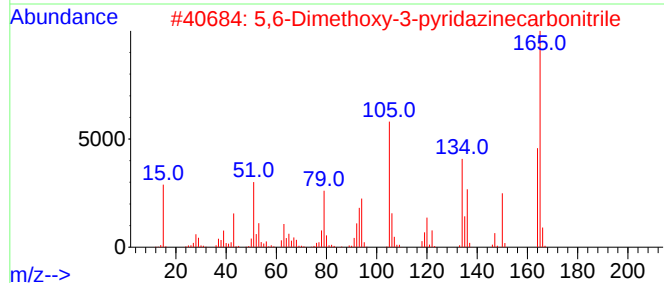
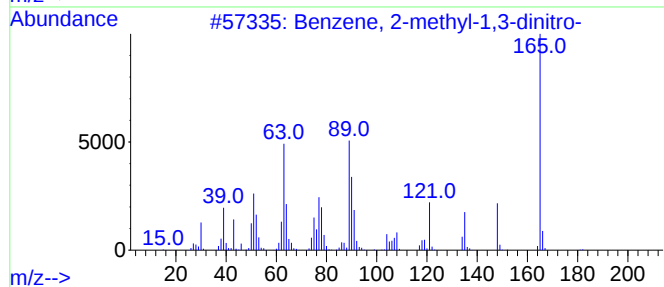
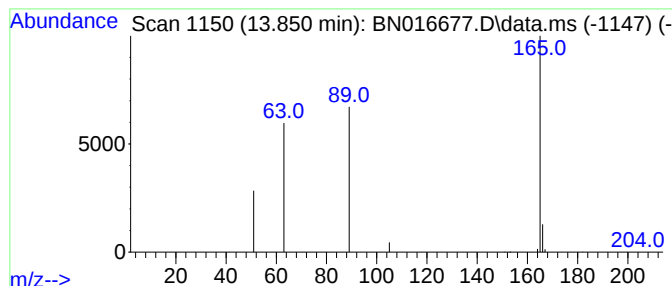
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.850	0.06 ng	27825	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	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9
3	6-Methoxy-2-benzoxazolinone		165	C8H7NO3	000532-91-2	9
4	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
5	Furo[3,4-c]pyridin-1(3H)-one, 7-...		165	C8H7NO3	004753-19-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139503BS

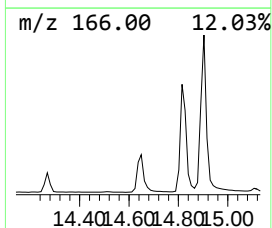
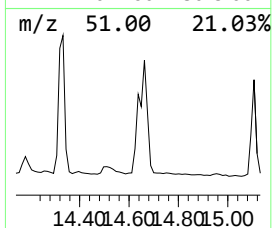
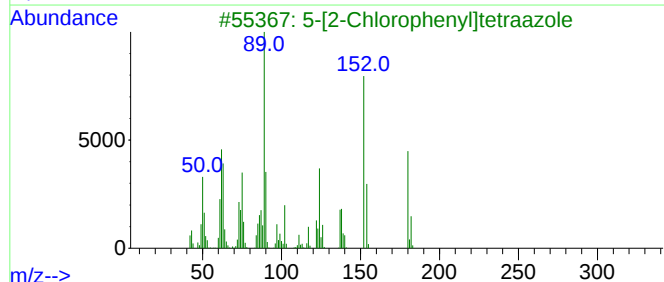
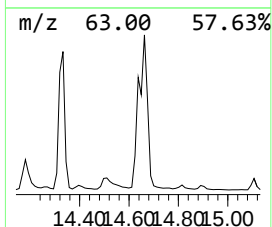
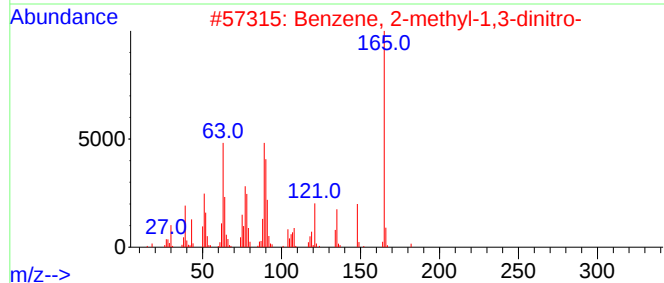
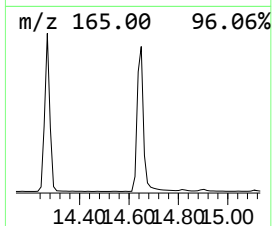
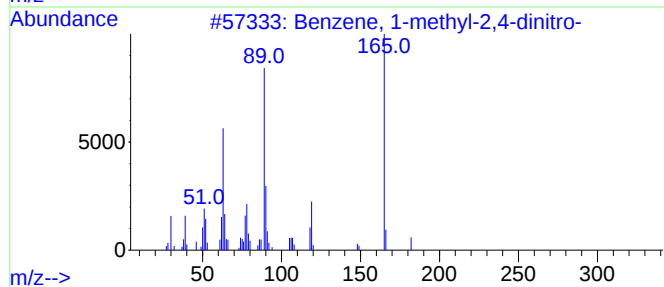
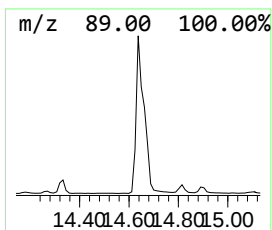
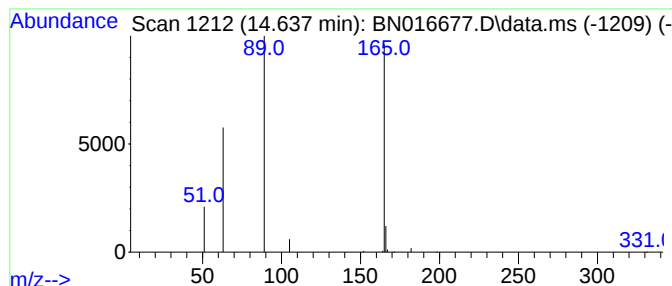
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	43109	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]tetraazole	180	C7H5ClN4	050907-46-5	9
4			Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	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 : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139503BS

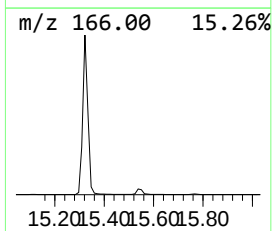
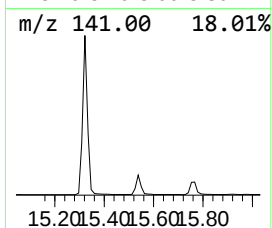
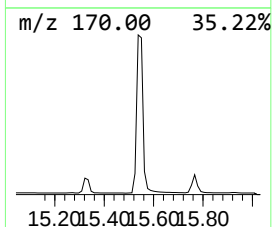
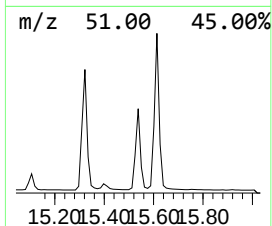
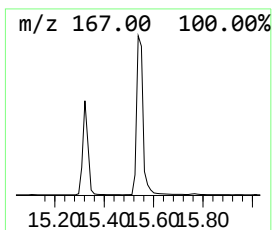
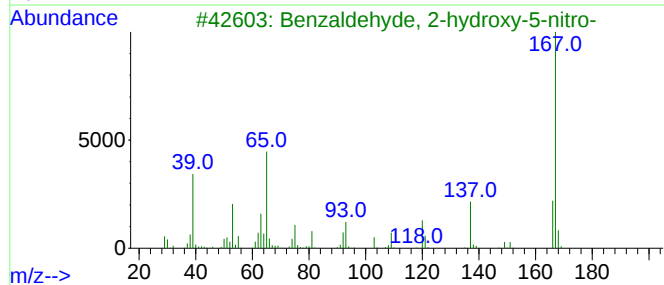
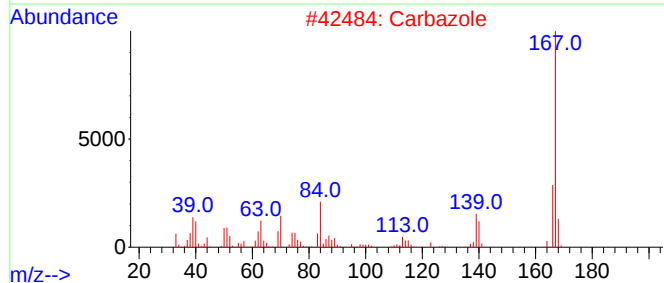
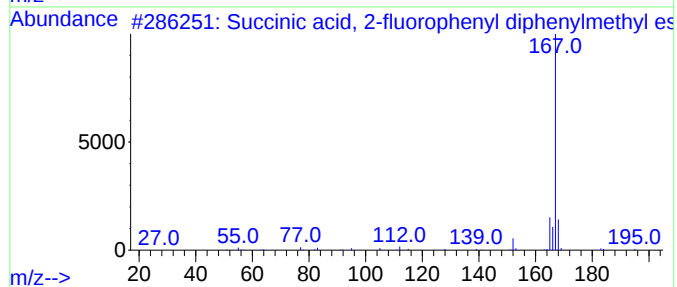
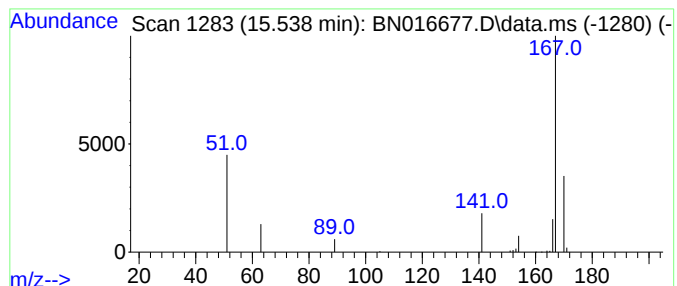
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	64058	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			Indol-2-one, 5-chloro-1,3-dihydro-	167	C8H6ClNO	017630-75-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
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Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

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ClientSampleId :
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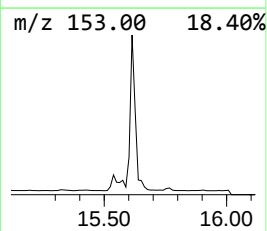
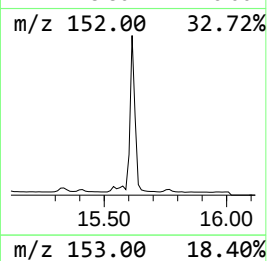
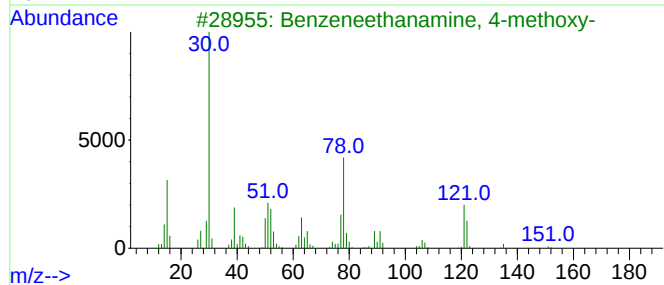
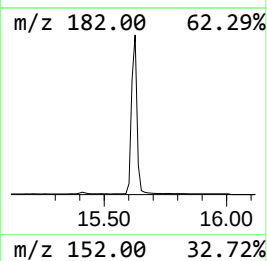
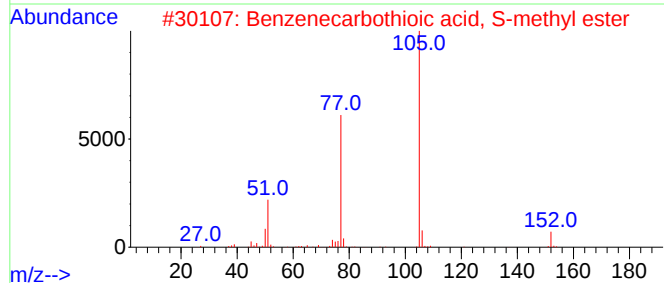
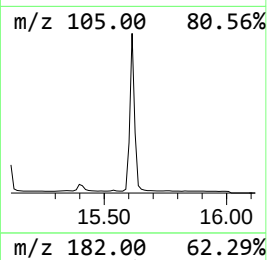
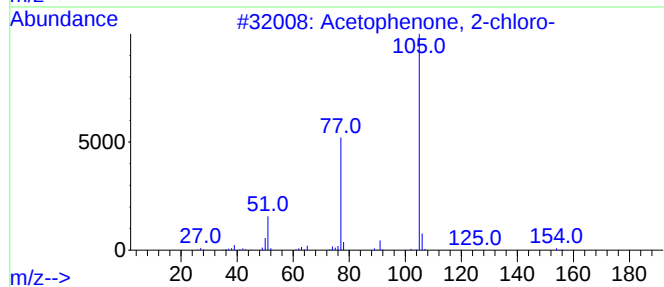
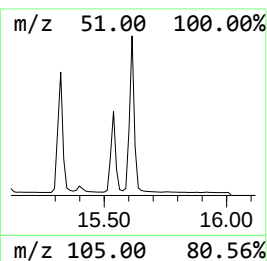
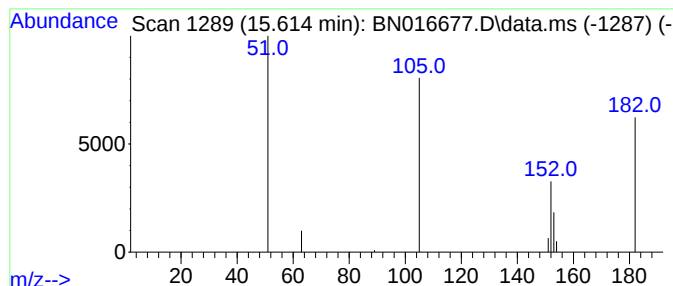
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Acetophenone, 2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	65436	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139503BS

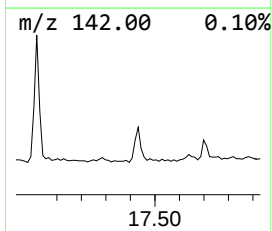
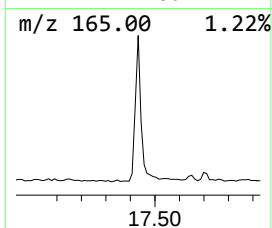
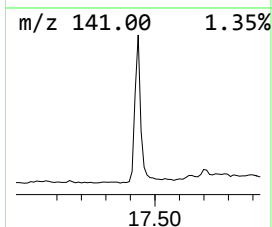
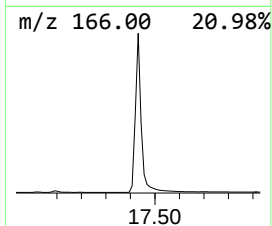
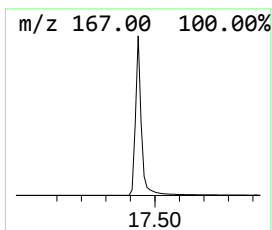
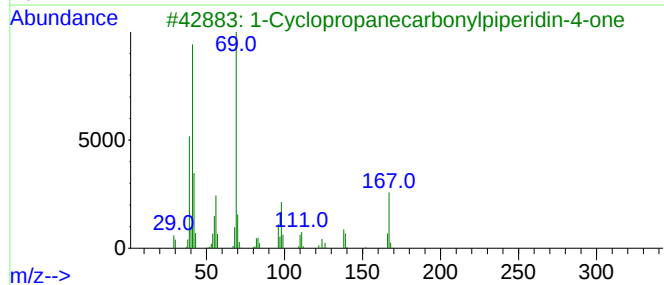
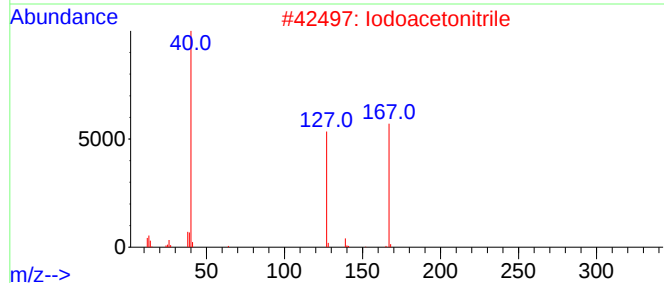
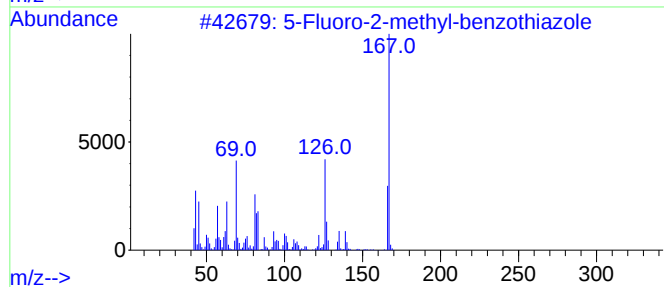
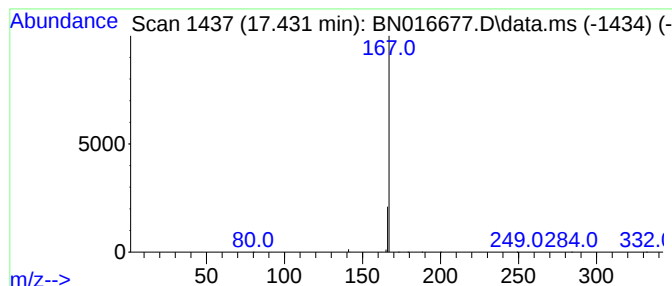
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	140736	Phenanthrene-d10	17.018

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		1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
4		1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
5		2(1H)-Pyrimidinone, 4-[(2-methyl...	167	C8H13N3O	119608-70-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016677.D
Acq On : 02 Oct 2021 18:57
Operator : CG/JU
Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139503BS

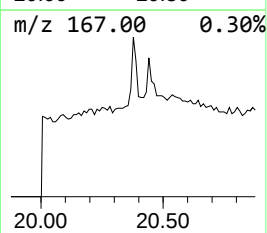
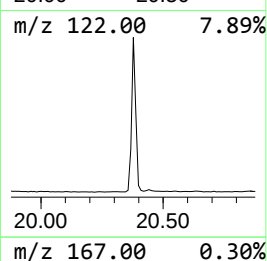
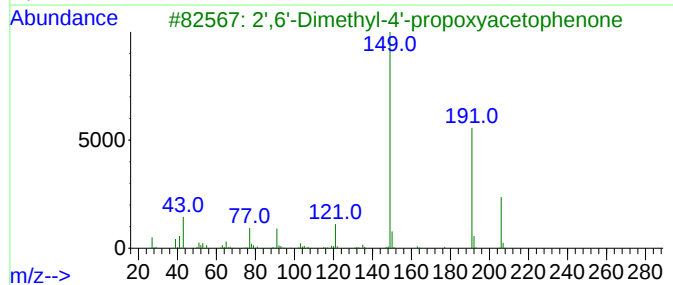
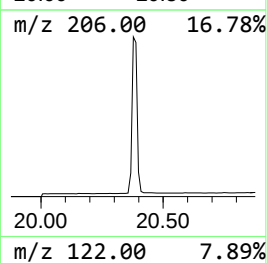
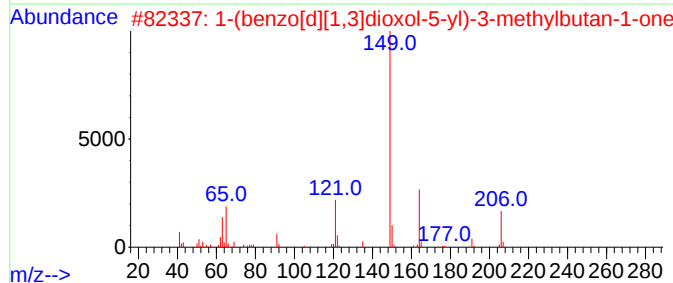
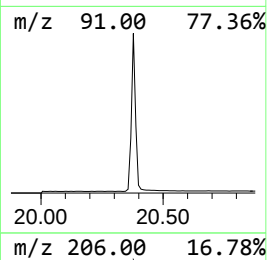
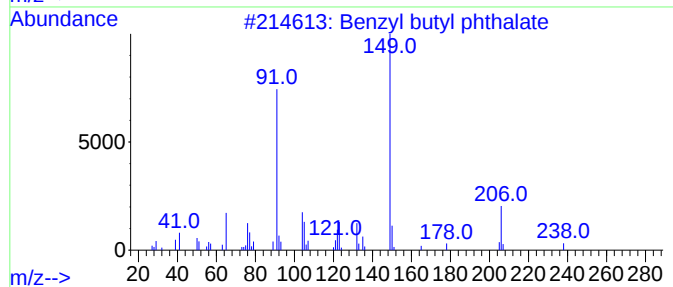
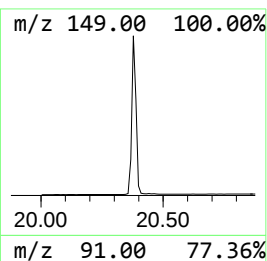
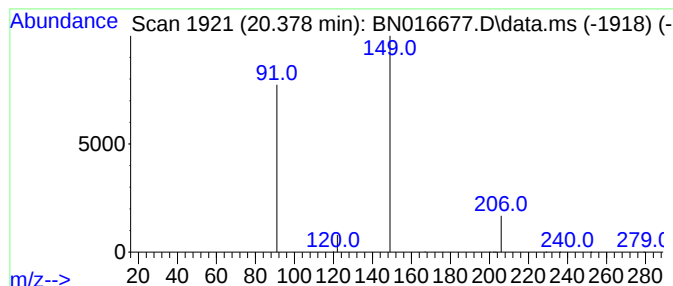
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	61736	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl butyl phthalate	312	C19H20O4	000085-68-7	40
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\
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Sample : PB139503BS
Misc :
ALS Vial : 45 Sample Multiplier: 1

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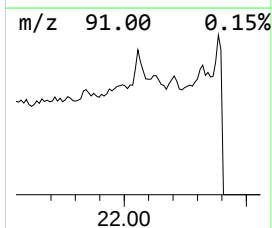
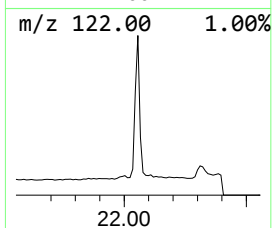
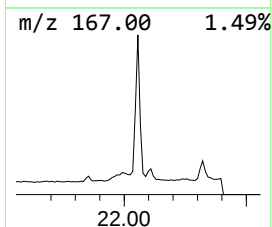
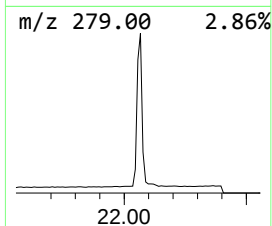
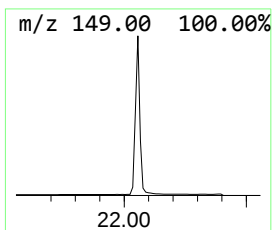
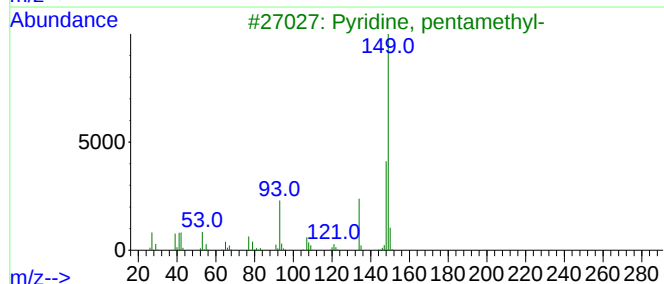
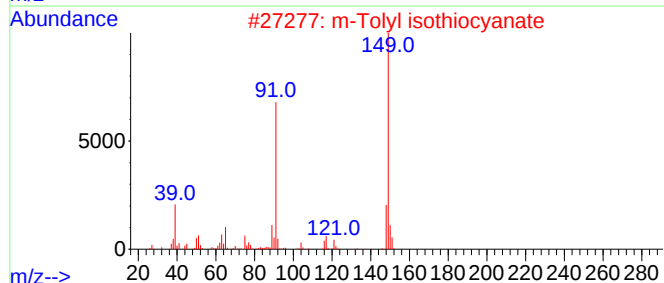
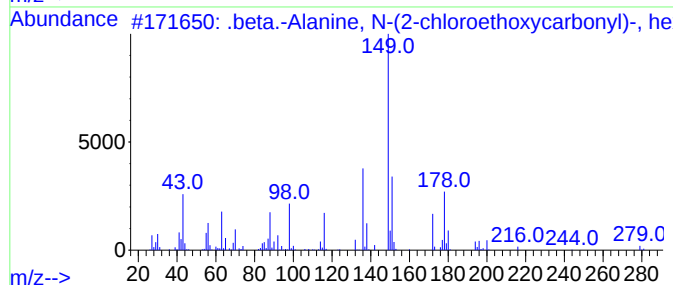
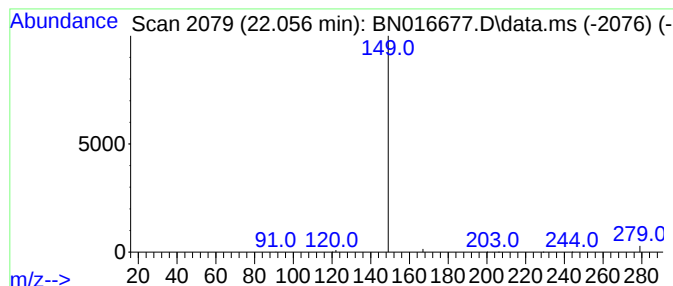
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.09 ng	94217	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	m-Tolyl		isothiocyanate	149	C8H7NS	000621-30-7	4
3	Pyridine,		pentamethyl-	149	C10H15N	003748-83-2	4
4	Phthalic acid,		7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Benzene,		1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016677.D
 Acq On : 02 Oct 2021 18:57
 Operator : CG/JU
 Sample : PB139503BS
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139503BS

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, ...	6.979	0.1	ng	39454	1	7.642	124842	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	33431	1	7.642	124842	0.4
4-Methyl-bi(1,2...	7.523	0.0	ng	15538	1	7.642	124842	0.4
6-Benzothiazola...	7.956	0.4	ng	111301	1	7.642	124842	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	50722	1	7.642	124842	0.4
Fomepizole	9.342	0.2	ng	79873	2	10.407	201060	0.4
5-Aminopyrimidine	9.836	0.1	ng	28392	2	10.407	201060	0.4
p-Chloroaniline	10.572	0.1	ng	63712	2	10.407	201060	0.4
Methane, iodo-	11.709	0.1	ng	25629	2	10.407	201060	0.4
2-Propyl-4-meth...	12.296	0.4	ng	204114	2	10.407	201060	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	28539	3	14.269	198879	0.4
E-2-Propenoic a...	12.772	0.1	ng	24884	3	14.269	198879	0.4
Naphthalene, 2-...	13.140	0.3	ng	131617	3	14.269	198879	0.4
Benzene, 2-meth...	13.850	0.1	ng	27825	3	14.269	198879	0.4
Benzene, 1-meth...	14.637	0.1	ng	43109	3	14.269	198879	0.4
Succinic acid, ...	15.538	0.1	ng	64058	3	14.269	198879	0.4
Acetophenone, 2...	15.614	0.1	ng	65436	3	14.269	198879	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	140736	4	17.018	164510	0.4
Benzyl butyl ph...	20.378	0.1	ng	61736	5	21.227	435506	0.4
.beta.-Alanine,...	22.056	0.1	ng	94217	5	21.227	435506	0.4