

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016669.D
 Acq On : 02 Oct 2021 14:08
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 37 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: BN016669.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	6062	8961	2.06%	0.122%
2	3.281	20	22	43	rVB	5320	24616	5.66%	0.334%
3	3.595	51	56	78	rVB	6236	28416	6.54%	0.386%
4	5.254	231	236	254	rBV	13866	52239	12.02%	0.709%
5	6.822	401	406	418	rBV	22516	57479	13.23%	0.780%
6	6.979	418	423	429	rVV	15086	33160	7.63%	0.450%
7	7.080	429	434	440	rVV	34096	69672	16.03%	0.946%
8	7.200	440	447	458	rVB	11599	30453	7.01%	0.413%
9	7.523	478	482	489	rVB	6712	14237	3.28%	0.193%
10	7.642	490	495	510	rVB2	47002	115014	26.46%	1.562%
11	7.956	524	529	538	rVB2	44937	103231	23.75%	1.402%
12	8.168	547	552	557	rBV	2992	7372	1.70%	0.100%
13	8.430	571	577	590	rBV3	20424	47278	10.88%	0.642%
14	8.696	594	598	601	rBV	4821	8854	2.04%	0.120%
15	8.784	601	605	606	rBV	30599	59642	13.72%	0.810%
16	8.823	606	608	616	rVB	25713	47939	11.03%	0.651%
17	9.342	645	649	652	rBV	41892	72222	16.62%	0.981%
18	9.520	660	663	666	rBV	3100	5947	1.37%	0.081%
19	9.596	666	669	680	rVB	7872	14550	3.35%	0.198%
20	9.836	684	688	702	rBV	14683	26652	6.13%	0.362%
21	10.052	702	705	715	rVB	3801	8186	1.88%	0.111%
22	10.407	729	733	735	rBV	100741	188547	43.38%	2.560%
23	10.457	735	737	741	rVV	99502	167666	38.58%	2.277%
24	10.571	743	746	756	rVV	25001	54805	12.61%	0.744%
25	10.749	756	760	763	rVB	30367	53751	12.37%	0.730%
26	11.307	801	804	818	rVB	1796	4921	1.13%	0.067%
27	11.709	853	865	895	rBV	12241	23823	5.48%	0.323%
28	12.003	921	931	939	rBV	54566	88486	20.36%	1.201%
29	12.074	939	947	972	rVV	121051	198343	45.64%	2.693%
30	12.296	987	997	1021	rVV	120902	190825	43.91%	2.591%
31	12.696	1056	1059	1062	rBV	16032	27124	6.24%	0.368%
32	12.759	1062	1064	1071	rVB	11380	23491	5.41%	0.319%
33	12.886	1071	1074	1078	rBV	116390	189880	43.69%	2.578%
34	13.140	1088	1094	1097	rBV	72400	126853	29.19%	1.722%
35	13.736	1138	1141	1143	rBV	11102	16102	3.71%	0.219%
36	13.850	1147	1150	1153	rVB	18530	26705	6.14%	0.363%

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Integrator: RTE

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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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.939	1155	1157	1158	rBV	5167	8315	1.91%	0.113%
38	13.990	1158	1161	1164	rVB	86160	146478	33.70%	1.989%
39	14.269	1180	1183	1185	rBV	132158	189694	43.65%	2.576%
40	14.332	1185	1188	1191	rVB	158414	232748	53.56%	3.160%
41	14.637	1209	1212	1220	rBV3	15970	41621	9.58%	0.565%
42	14.814	1224	1226	1230	rVV	5233	8930	2.05%	0.121%
43	14.903	1230	1233	1243	rVB	7176	12067	2.78%	0.164%
44	15.106	1246	1249	1252	rBV	8361	10836	2.49%	0.147%
45	15.322	1263	1266	1270	rBV2	220629	340104	78.26%	4.618%
46	15.411	1270	1273	1280	rVV2	3115	8517	1.96%	0.116%
47	15.538	1280	1283	1287	rVV	36270	60137	13.84%	0.817%
48	15.614	1287	1289	1298	rVV2	40608	62502	14.38%	0.849%
49	15.766	1298	1301	1311	rVB2	12776	21670	4.99%	0.294%
50	16.227	1334	1338	1341	rBV2	55800	88683	20.41%	1.204%
51	16.324	1343	1346	1349	rVV	46602	70422	16.20%	0.956%
52	16.506	1358	1361	1372	rBV	18646	32473	7.47%	0.441%
53	16.677	1372	1375	1384	rBV	19337	33778	7.77%	0.459%
54	17.018	1400	1403	1405	rBV	97629	157297	36.19%	2.136%
55	17.066	1405	1407	1410	rVV	139853	211296	48.62%	2.869%
56	17.151	1411	1414	1434	rVB	108923	179358	41.27%	2.435%
57	17.431	1434	1437	1452	rBV	80095	132043	30.38%	1.793%
58	18.016	1482	1485	1508	rVB8	5183	6928	1.59%	0.094%
59	19.063	1685	1696	1699	rBV	110352	154723	35.60%	2.101%
60	19.093	1699	1702	1746	rVB	176841	252990	58.21%	3.435%
61	19.460	1767	1776	1806	rBV	180195	246292	56.67%	3.344%
62	19.679	1813	1820	1853	rBV	107812	137064	31.54%	1.861%
63	20.378	1918	1921	1924	rBV	46814	56928	13.10%	0.773%
64	21.164	1993	1995	1998	rBV	40907	61577	14.17%	0.836%
65	21.227	1998	2001	2003	rVV2	192451	389822	89.70%	5.293%
66	21.270	2003	2005	2017	rVB	195653	268546	61.79%	3.646%
67	22.056	2076	2079	2082	rBV	61446	74471	17.14%	1.011%
68	22.807	2217	2229	2236	rBV	118037	199397	45.88%	2.707%
69	22.851	2236	2242	2288	rVB	126409	229015	52.70%	3.110%
70	23.385	2385	2398	2416	rBV	75658	168801	38.84%	2.292%
71	23.488	2416	2428	2484	rVB	89631	195229	44.92%	2.651%
72	24.087	2595	2603	2622	rVB2	3864	7238	1.67%	0.098%
73	24.857	2818	2828	2846	rVB2	3783	8045	1.85%	0.109%
74	25.774	3067	3096	3166	rBV3	110338	434594	100.00%	5.901%
75	26.459	3273	3296	3362	rBV2	61641	206724	47.57%	2.807%

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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

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Peak separation: 5

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

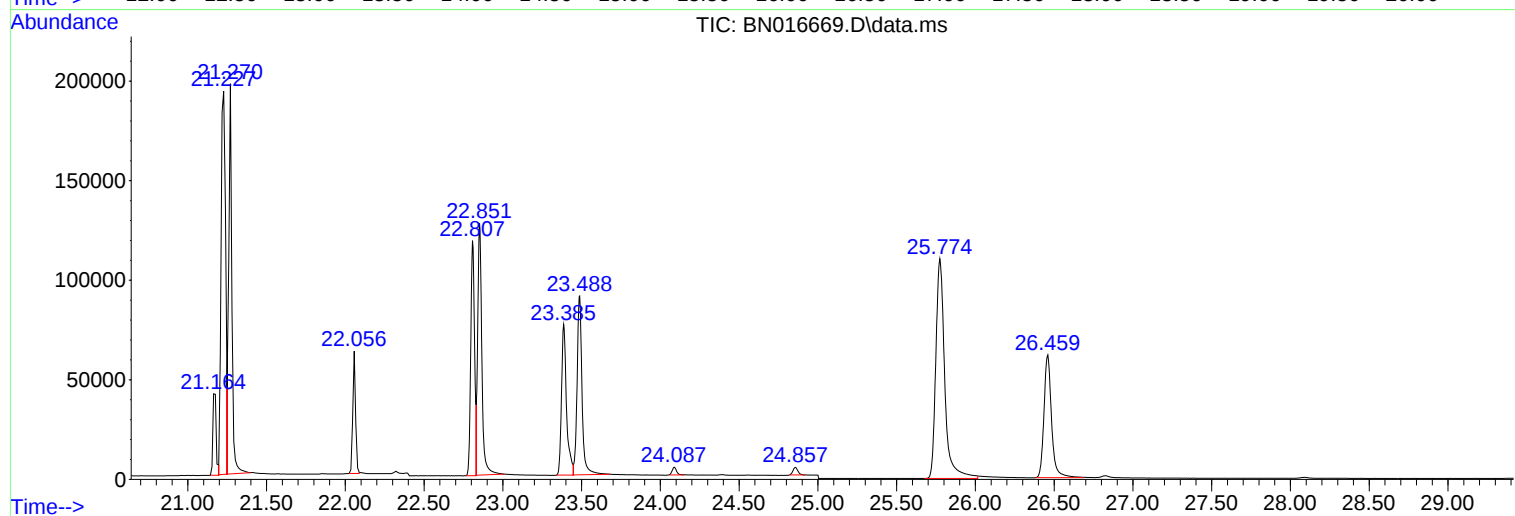
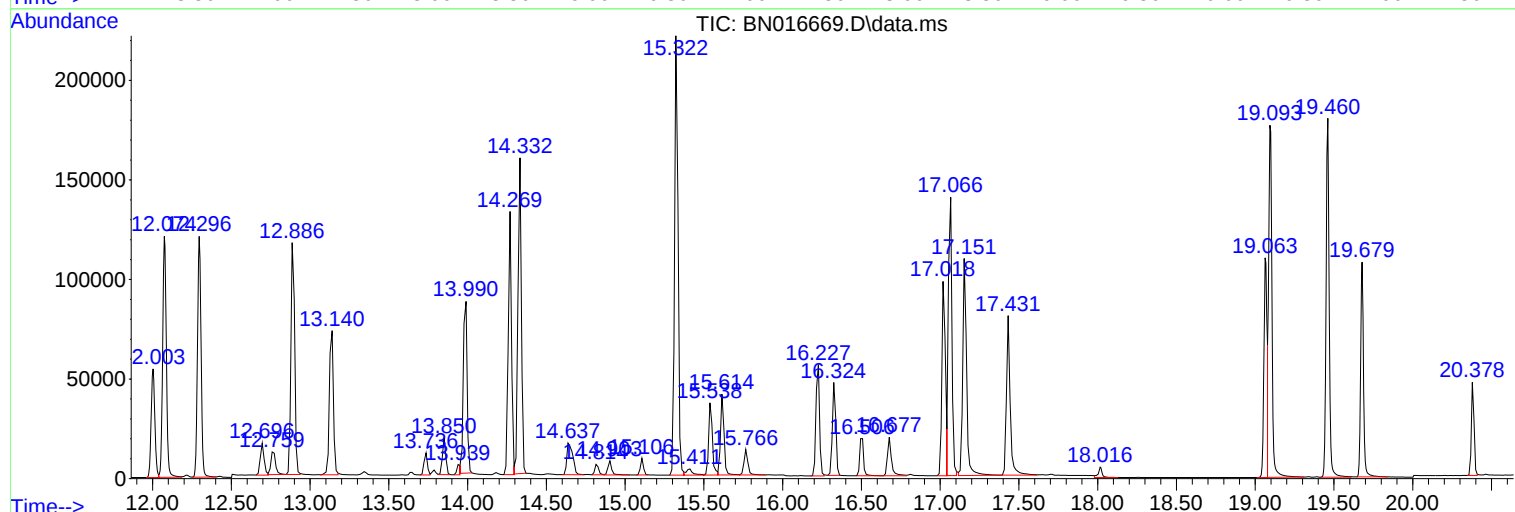
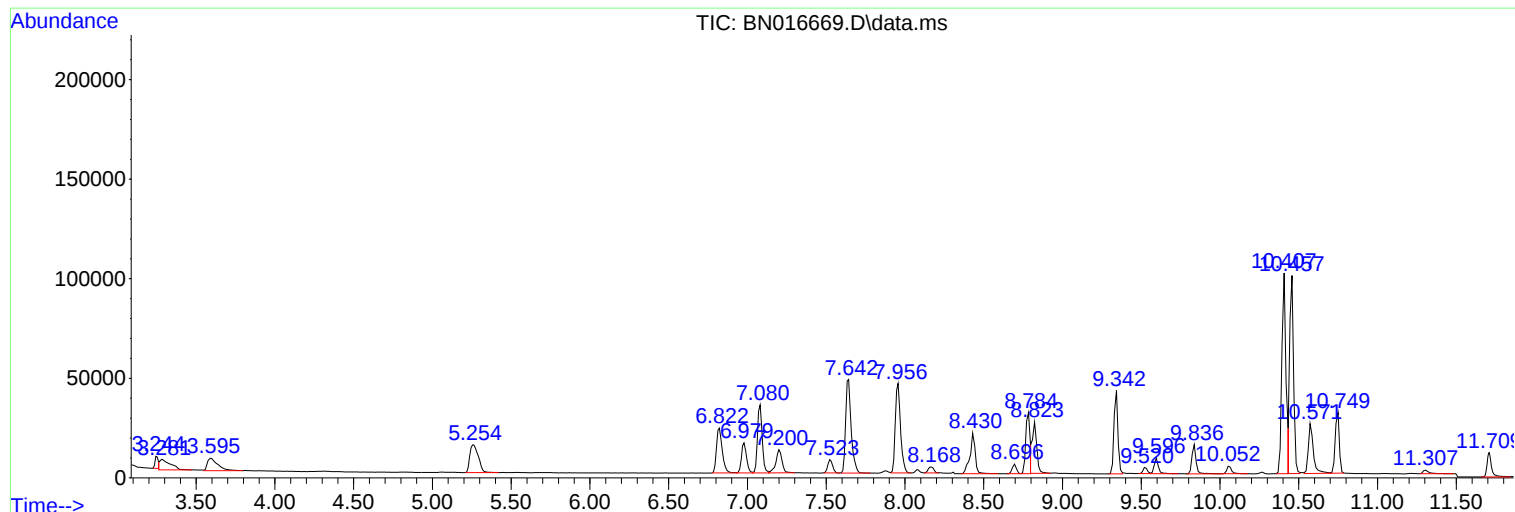
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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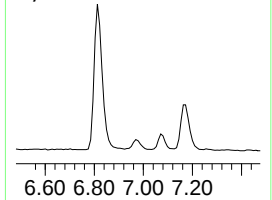
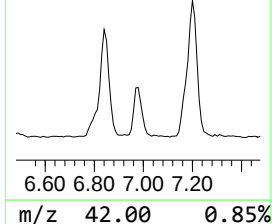
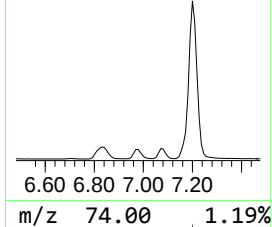
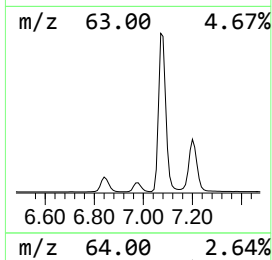
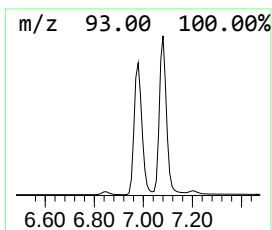
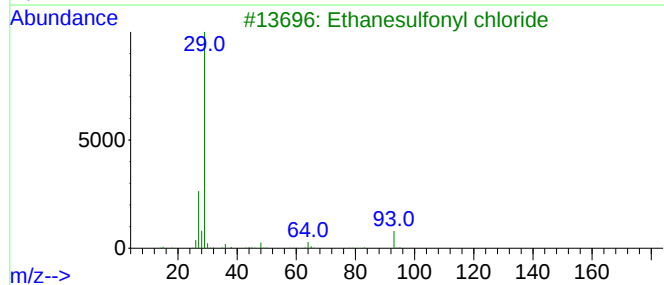
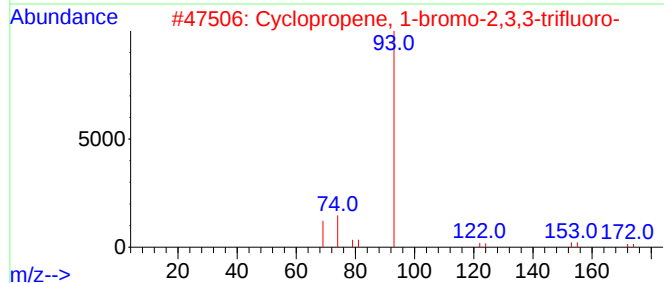
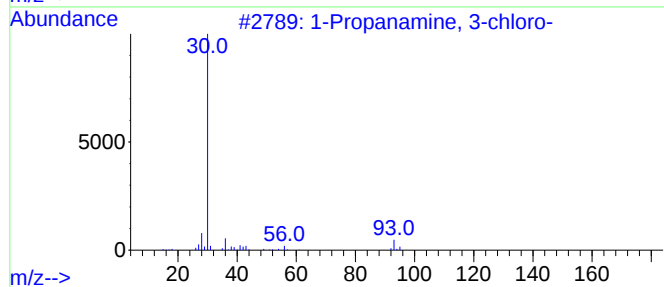
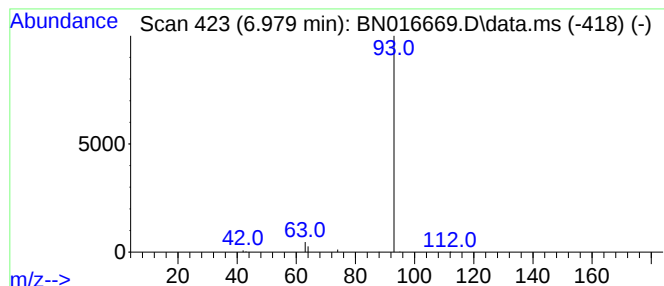
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.12 ng	33160	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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ALS Vial : 37 Sample Multiplier: 1

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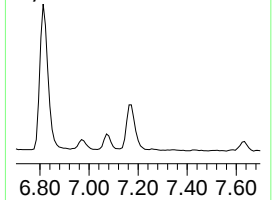
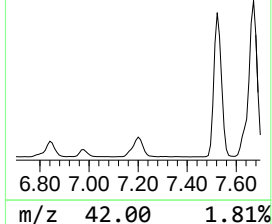
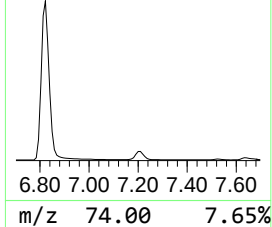
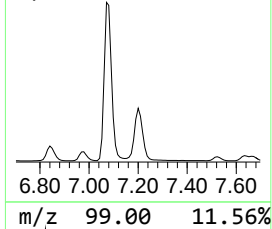
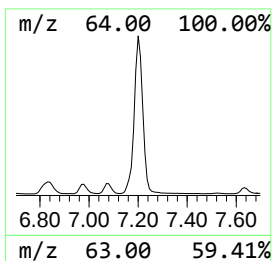
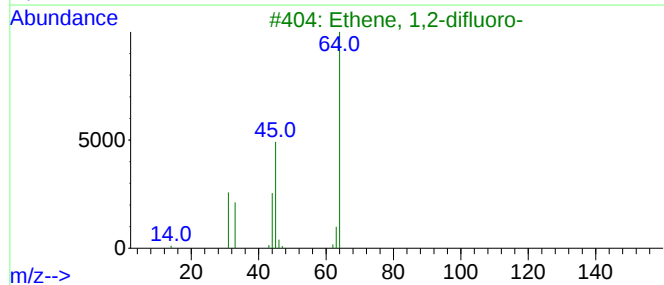
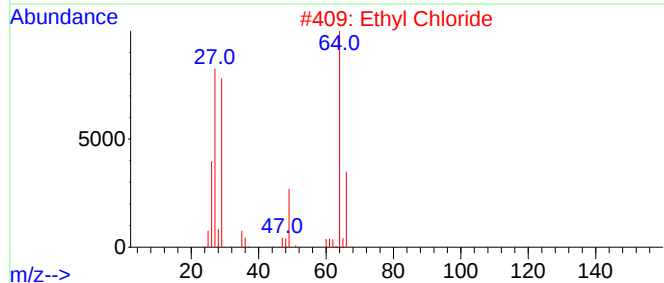
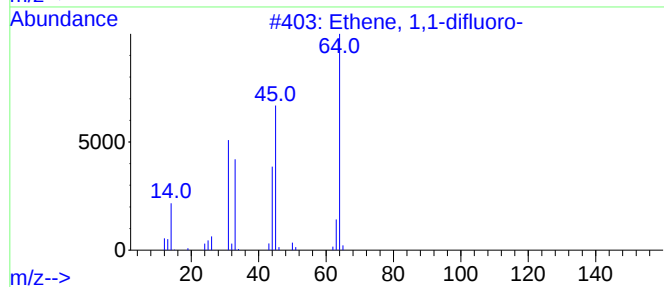
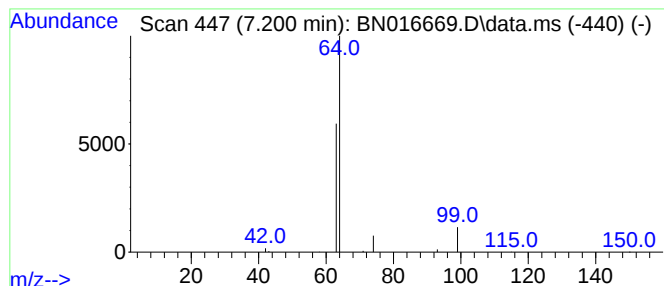
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	30453	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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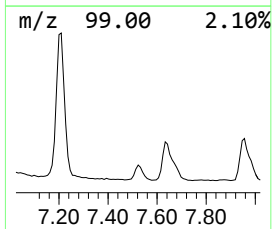
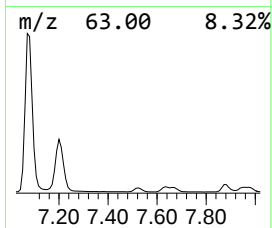
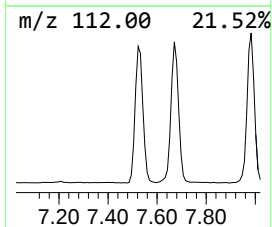
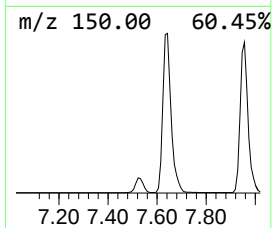
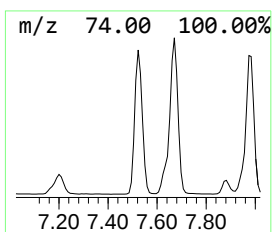
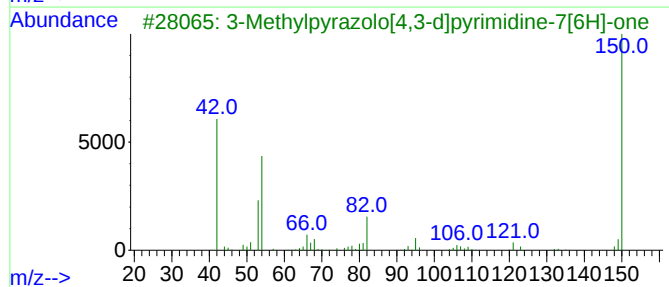
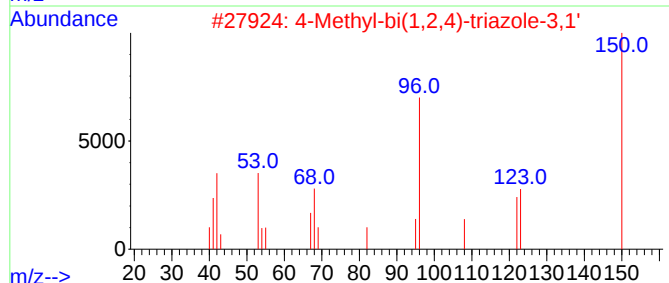
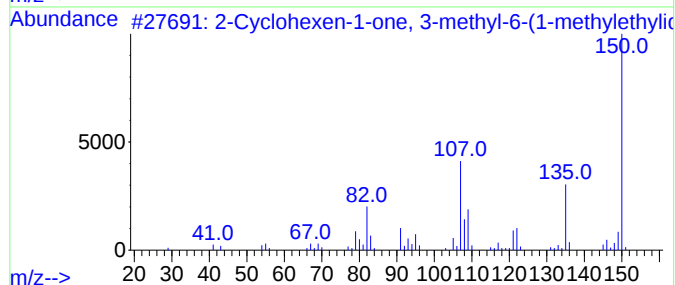
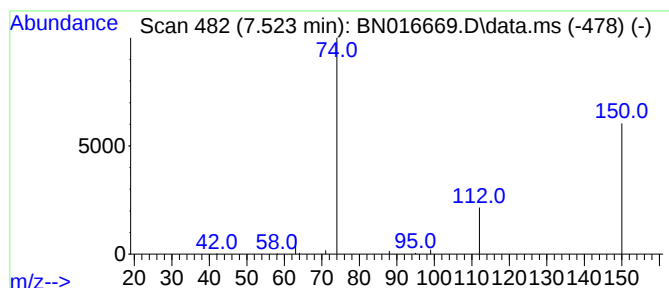
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Cyclohexen-1-one, 3-methy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	14237	1,4-Dichlorobenzene-d4	7.642

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



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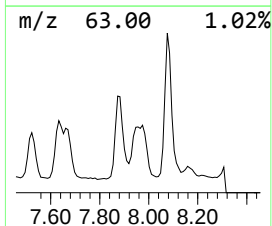
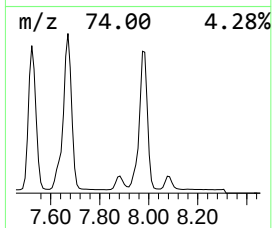
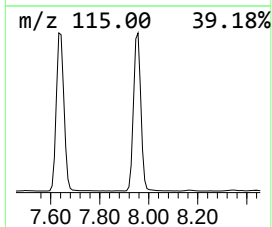
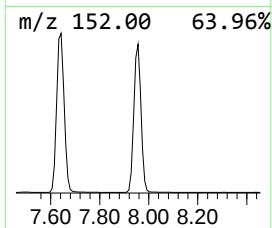
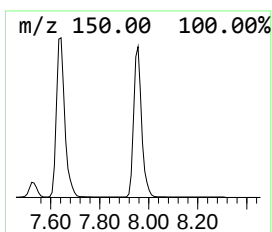
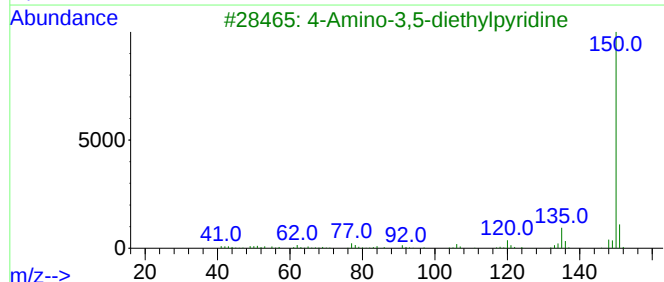
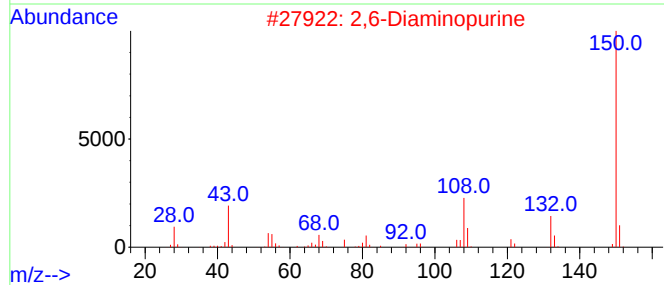
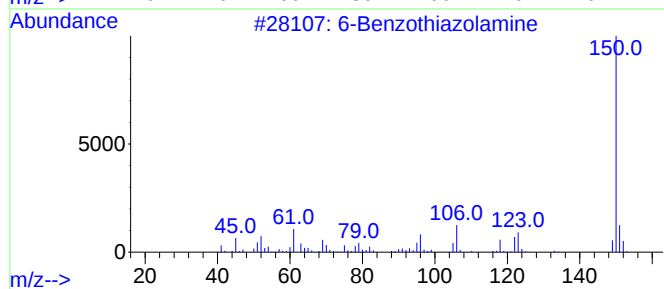
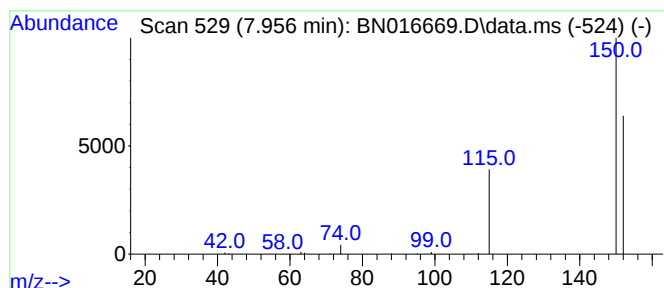
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	103231	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 : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

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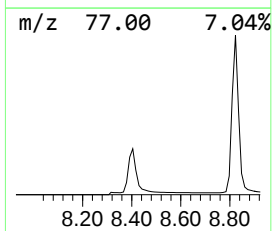
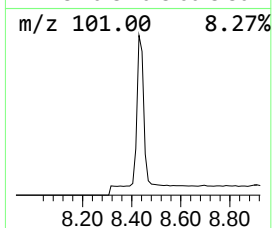
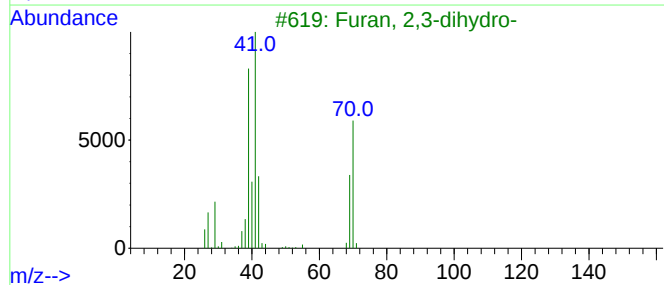
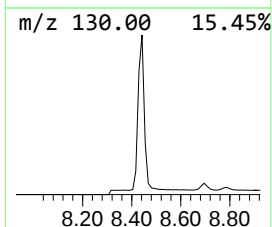
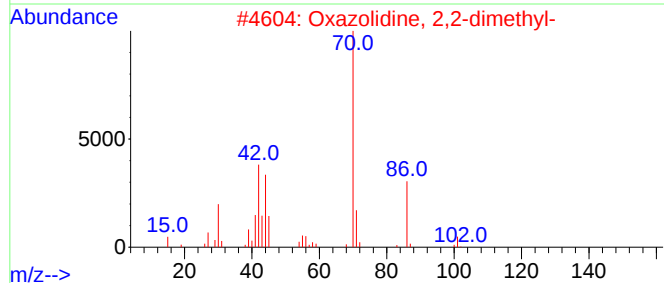
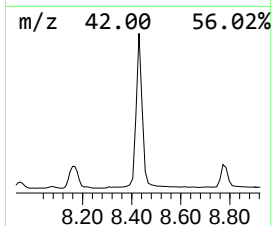
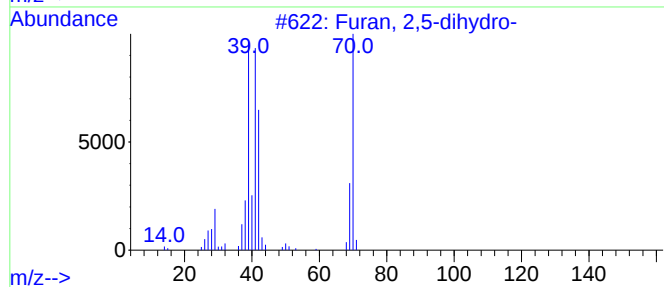
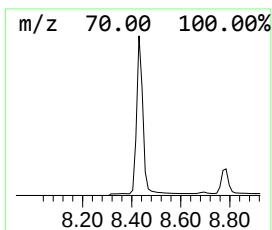
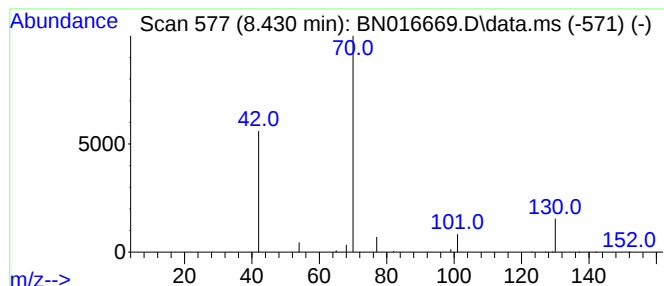
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
8.430	0.16 ng	47278	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 : BN016669.D
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Misc :
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Instrument :
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LabSampleId :
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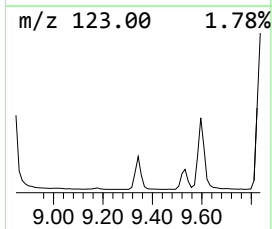
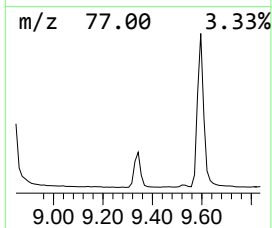
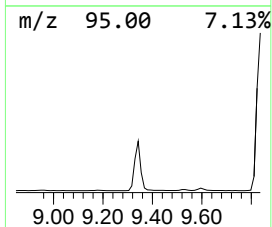
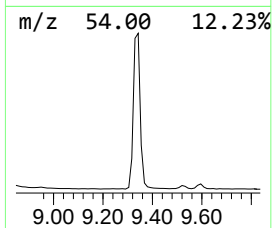
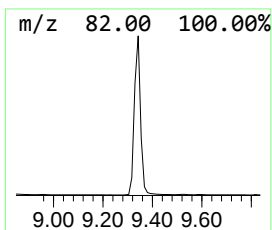
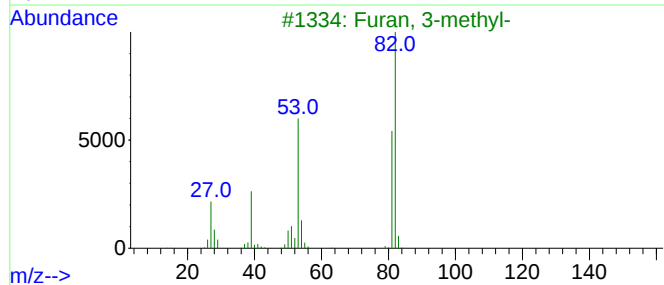
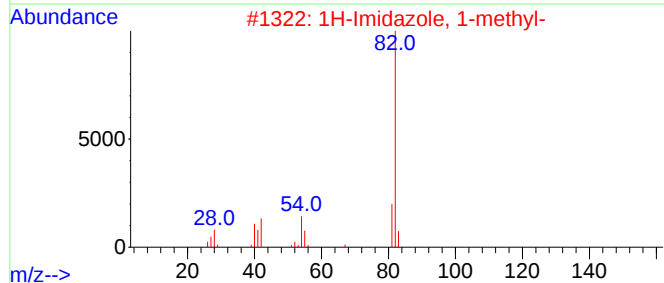
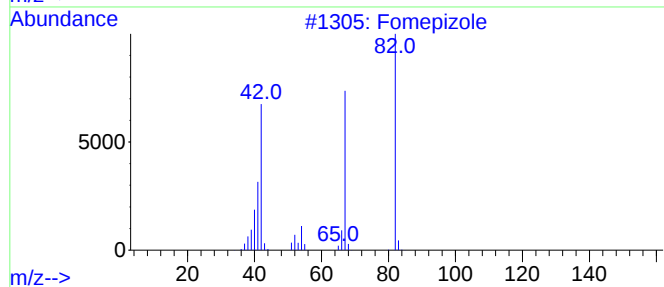
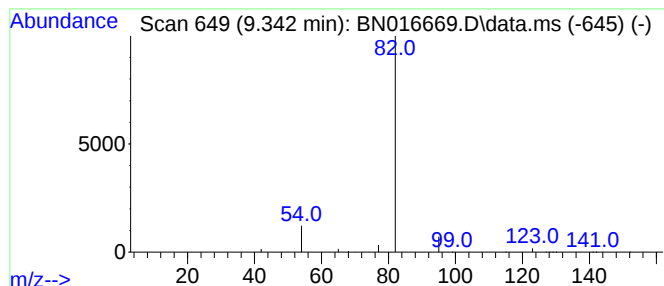
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.15 ng	72222	Naphthalene-d8	10.407

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 : BN016669.D
Acq On : 02 Oct 2021 14:08
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Misc :
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LabSampleId :
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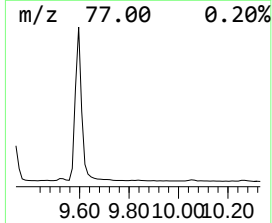
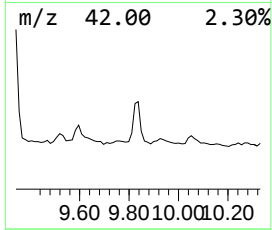
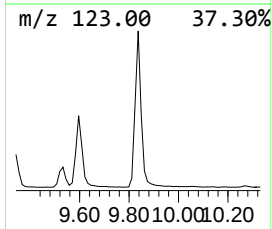
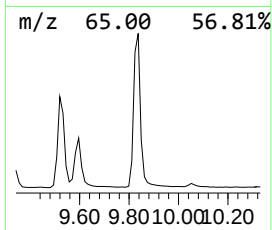
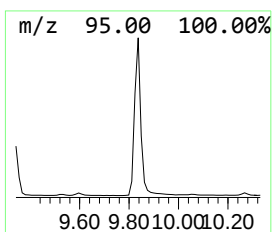
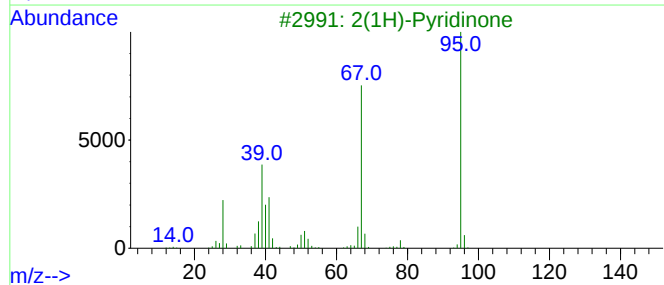
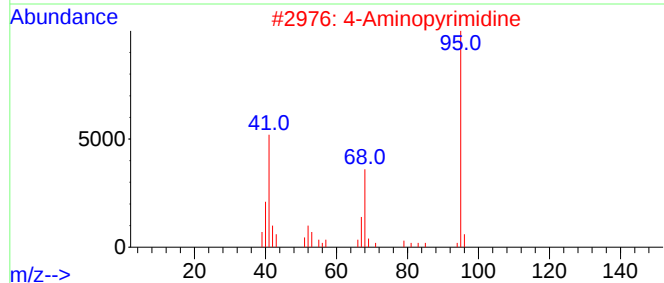
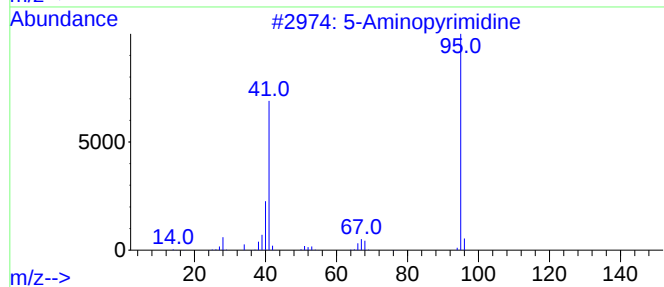
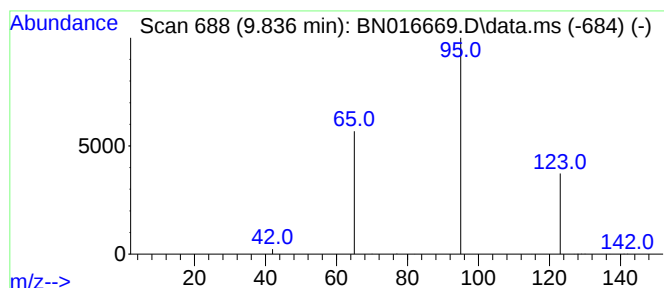
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Aminopyrimidine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	26652	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 : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
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Instrument :
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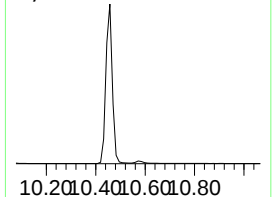
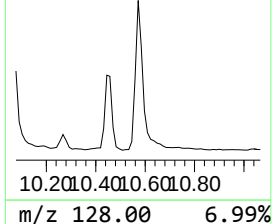
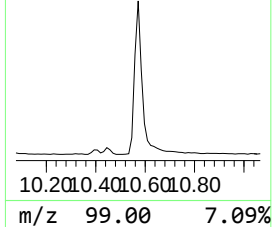
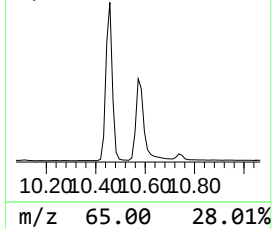
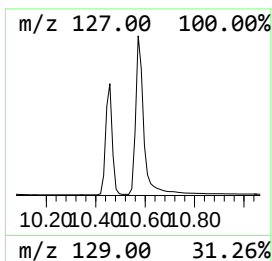
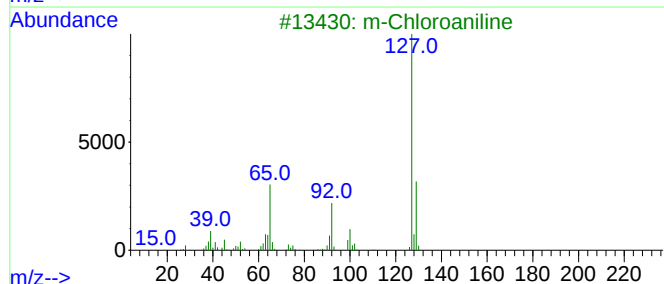
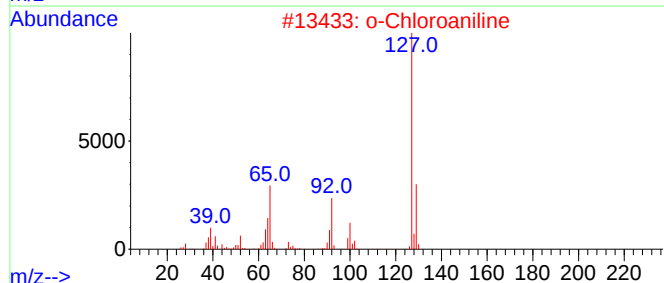
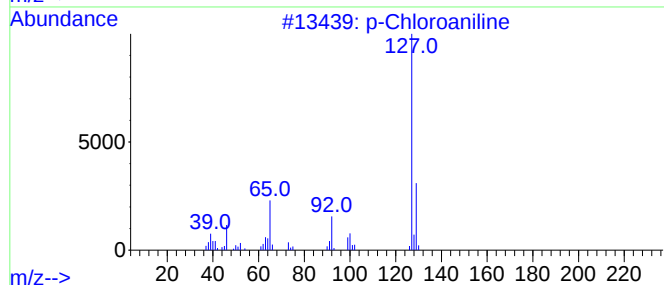
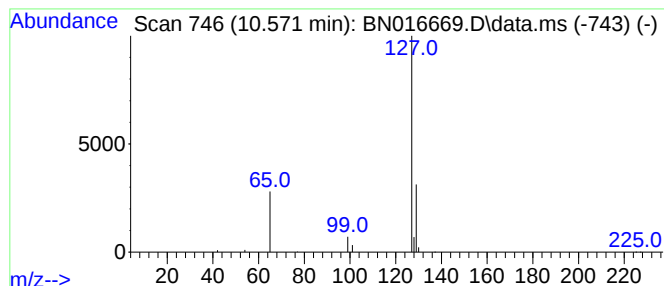
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.12 ng	54805	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			2-Chloromethylpyridine	127	C6H6ClN	004377-33-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
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Misc :
ALS Vial : 37 Sample Multiplier: 1

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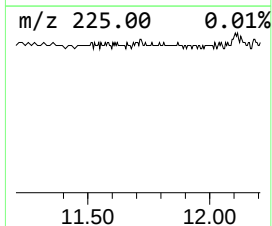
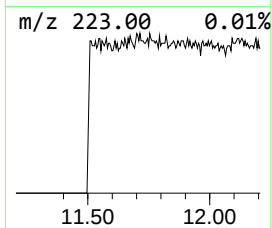
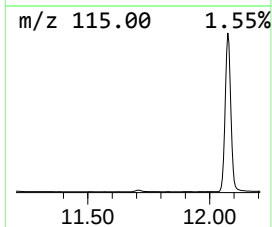
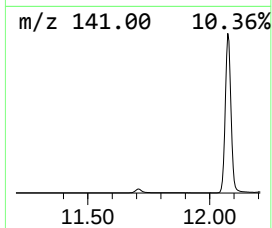
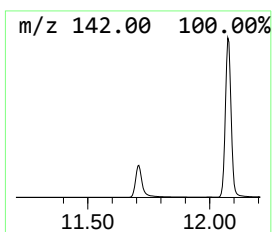
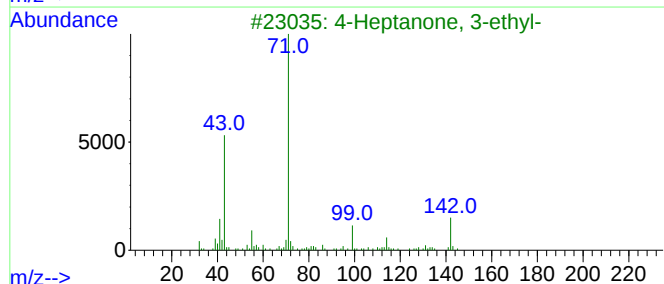
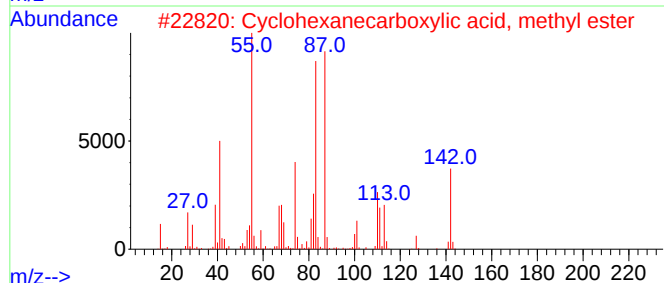
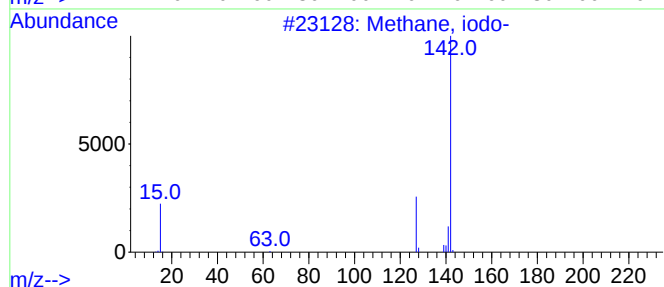
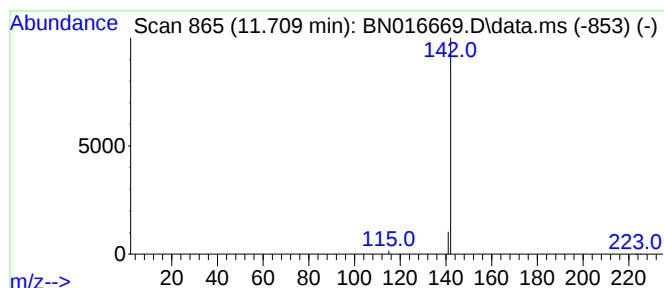
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	23823	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\
Data File : BN016669.D
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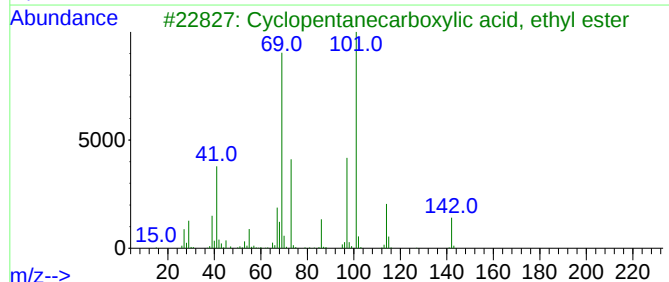
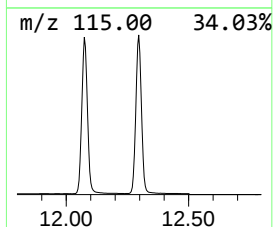
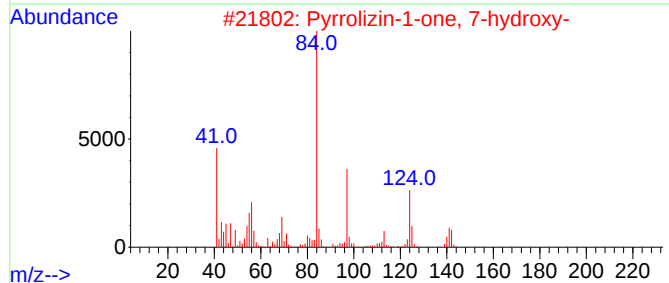
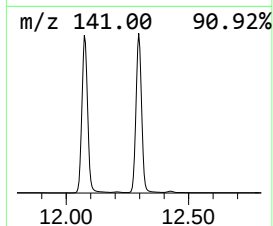
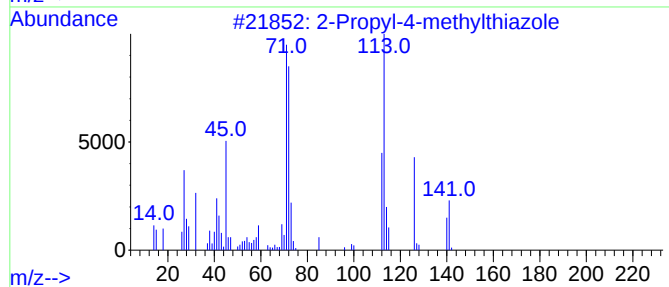
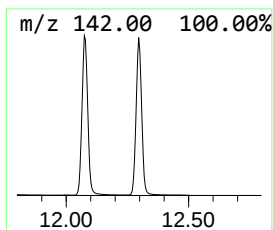
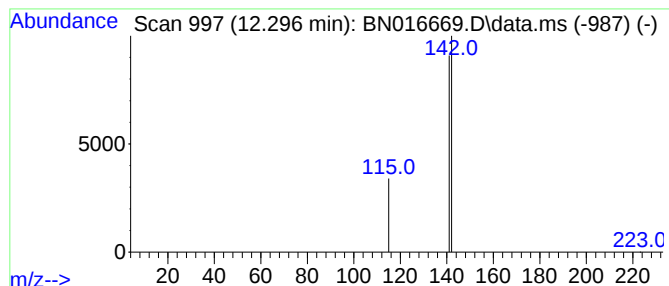
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.296	0.40 ng	190825	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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

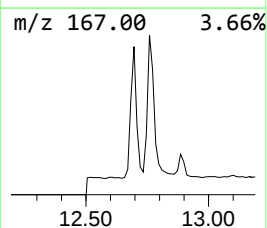
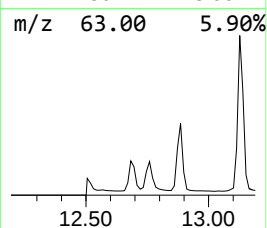
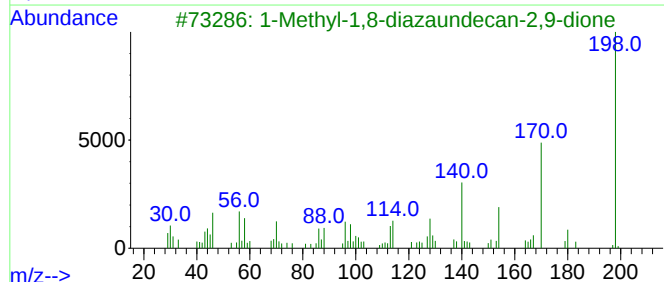
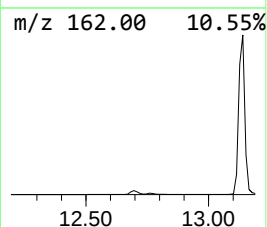
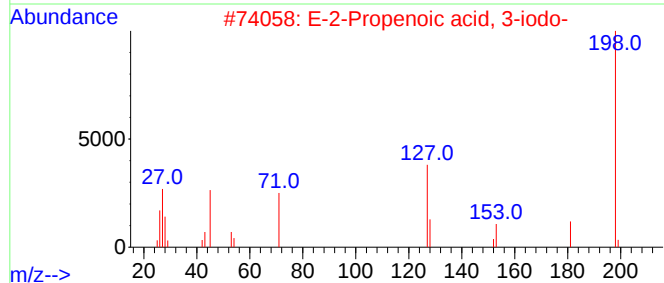
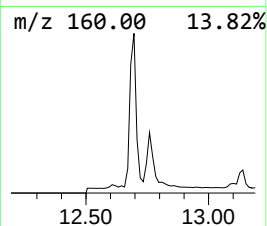
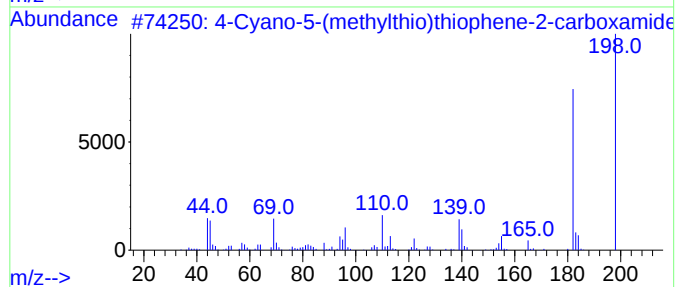
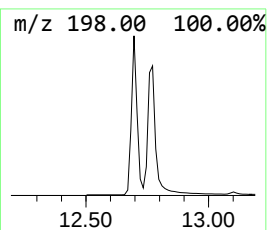
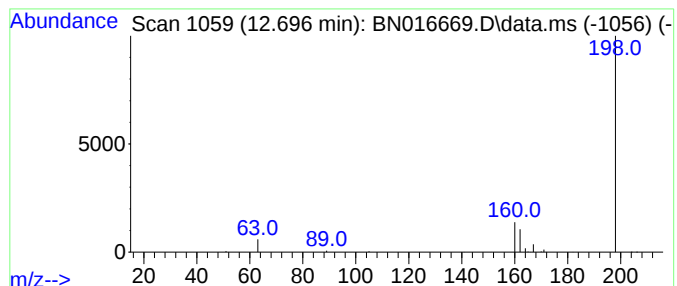
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.696	0.06 ng	27124	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 : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

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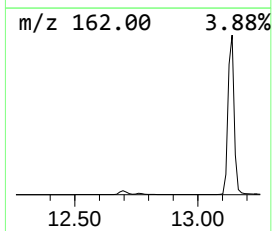
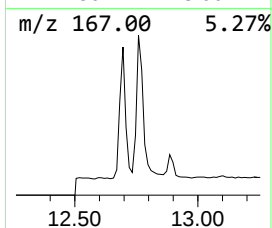
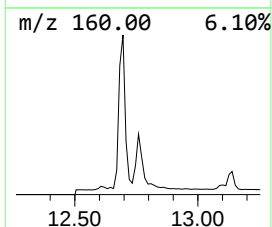
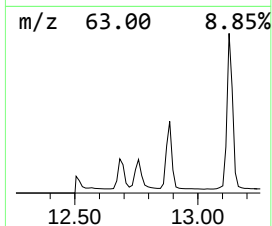
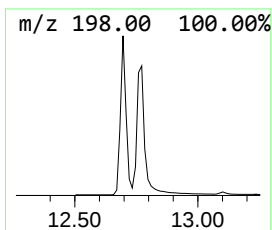
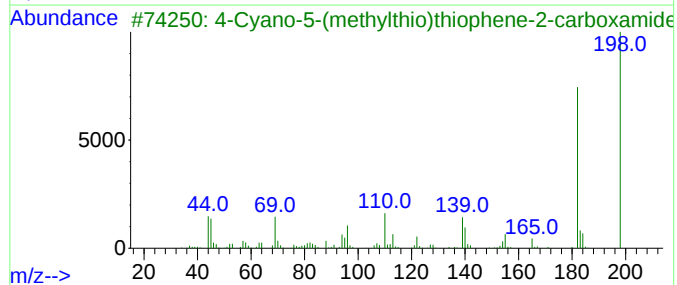
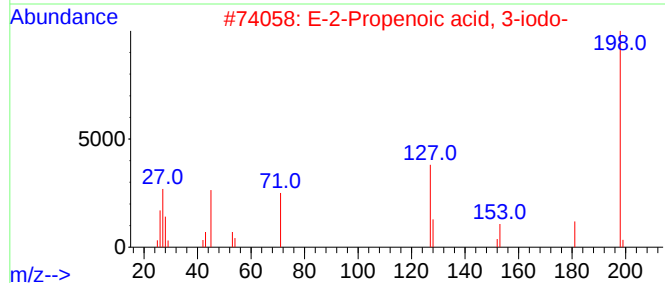
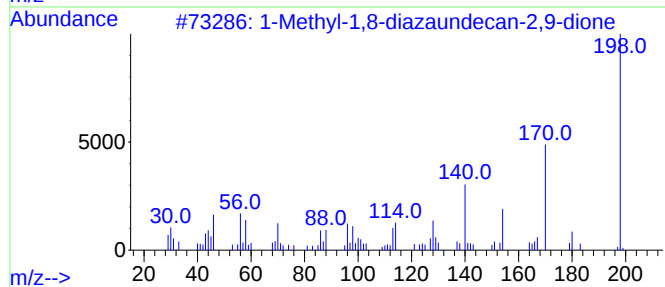
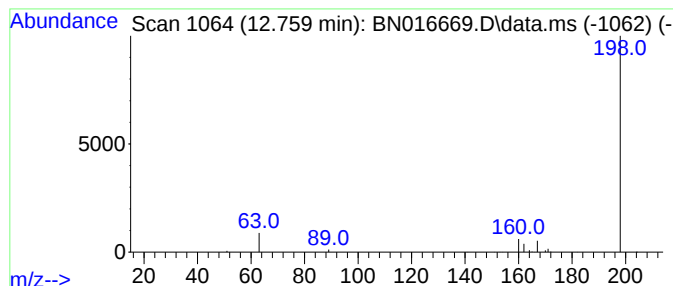
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Methyl-1,8-diazaundecan-2... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	23491	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	4
2			E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3			4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
4			Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
5			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

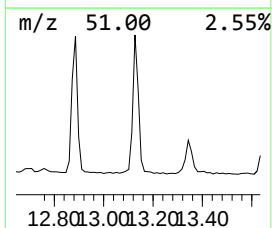
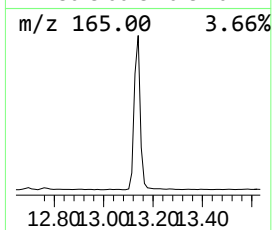
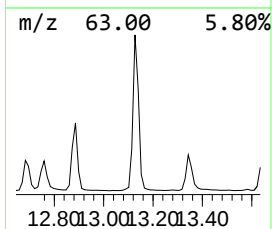
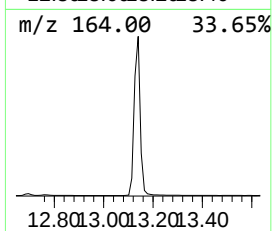
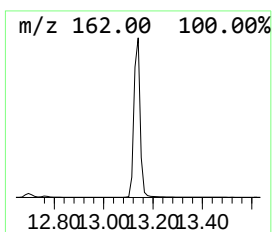
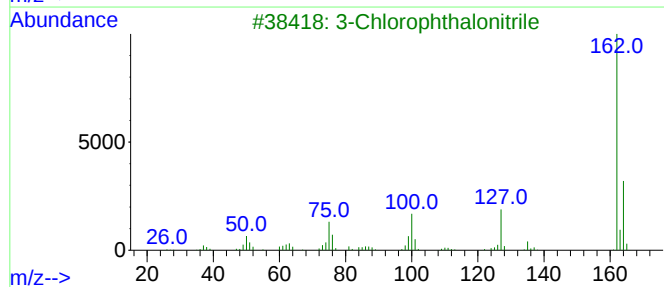
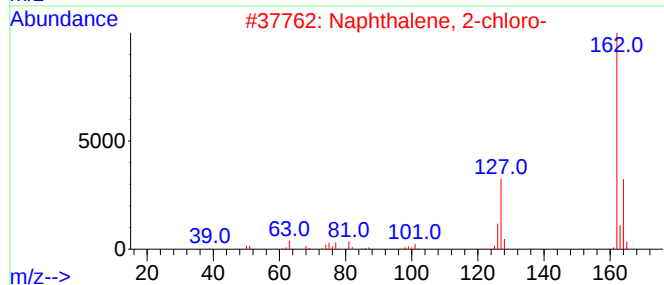
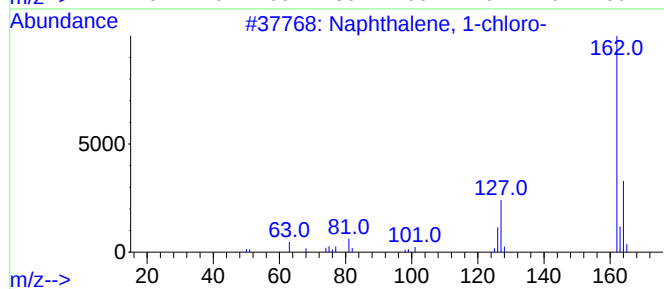
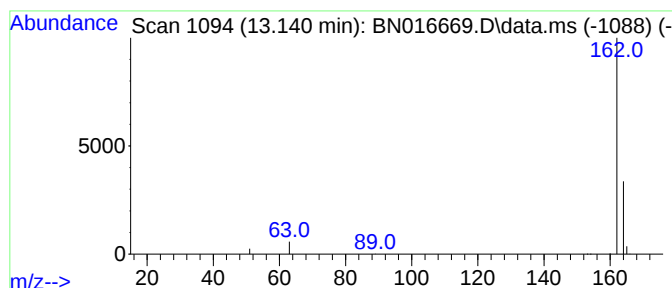
Instrument :
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LabSampleId :
SSTDCCC0.4

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, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.140	0.27 ng	126853	Acenaphthene-d10	14.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
2	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	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 : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

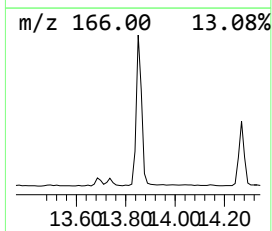
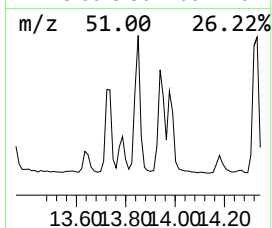
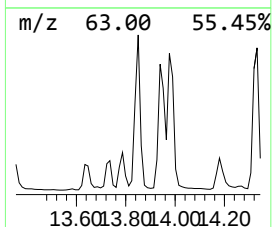
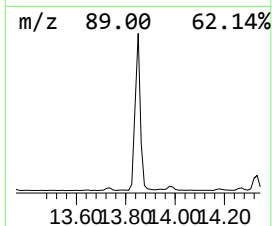
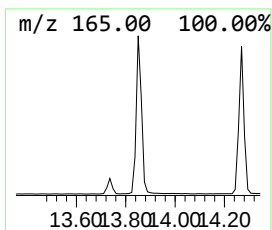
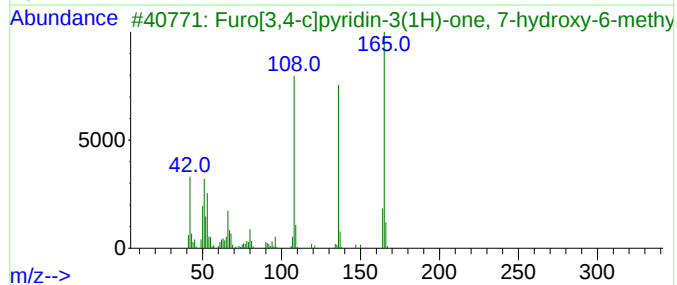
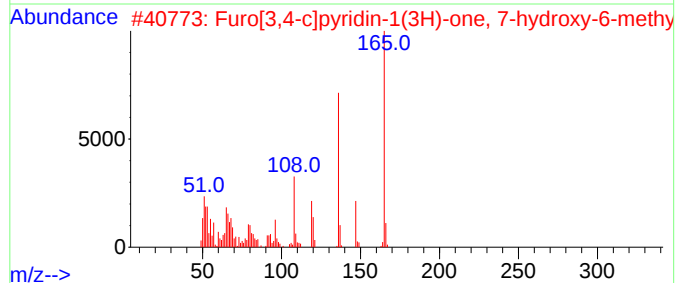
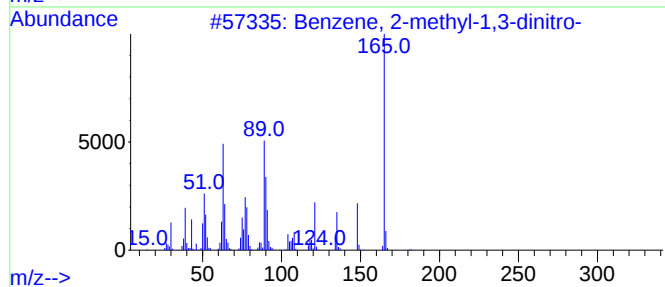
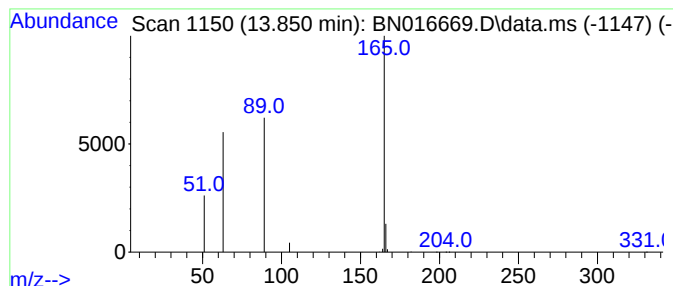
Instrument :
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.850	0.06 ng	26705	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	Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9
3	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
4	5,6-Dimethoxy-3-pyridazinecarbon...	165	C7H7N3O2	020552-46-9	9
5	7-Hydroxy-2,4-dihydro-1,4-benzox...	165	C8H7NO3	067193-97-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

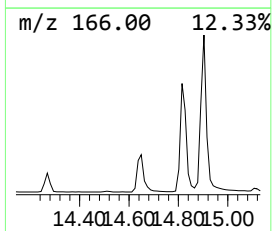
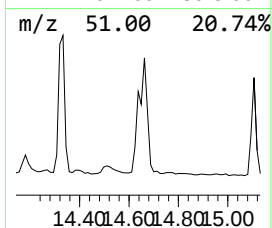
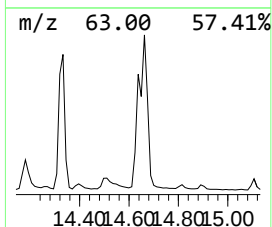
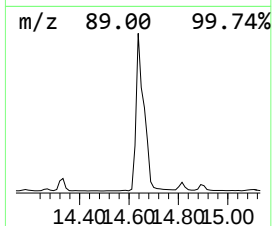
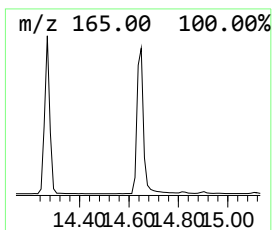
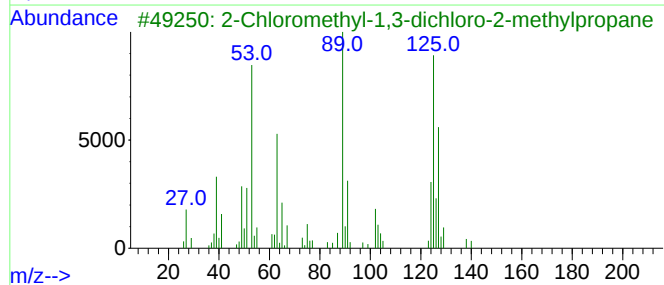
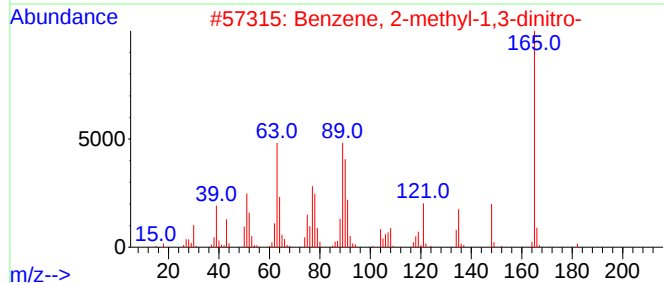
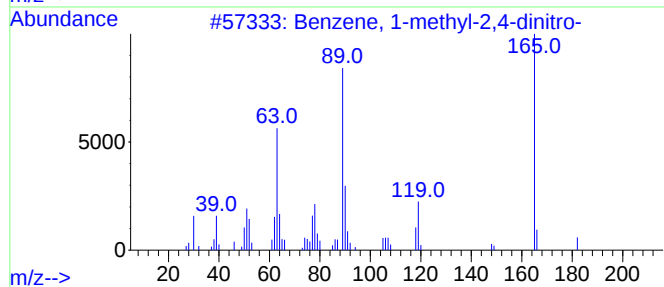
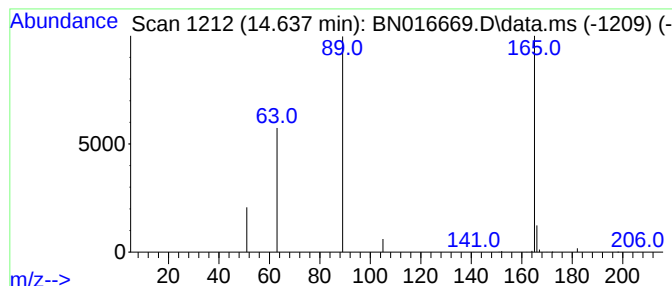
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.637	0.09 ng	41621	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	2-Chloromethyl-1,3-dichloro-2-me...		174	C5H9Cl3	001067-09-0	9
4	Ethanol, 1-(4-nitrophenyl)-2-[1-...		304	C17H24N2O3	1000264-75-7	9
5	5-[2-Chlorophenyl]tetraazole		180	C7H5ClN4	050907-46-5	9



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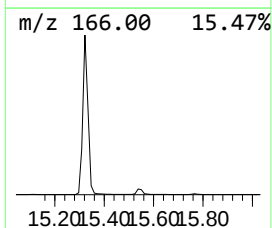
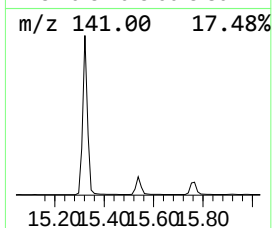
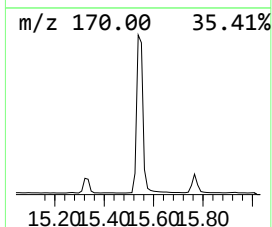
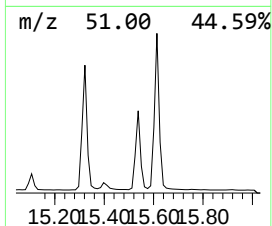
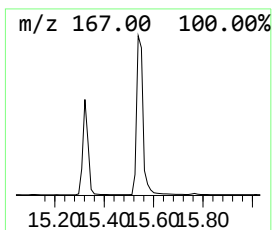
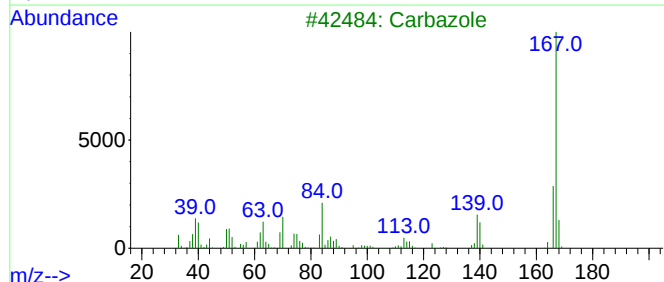
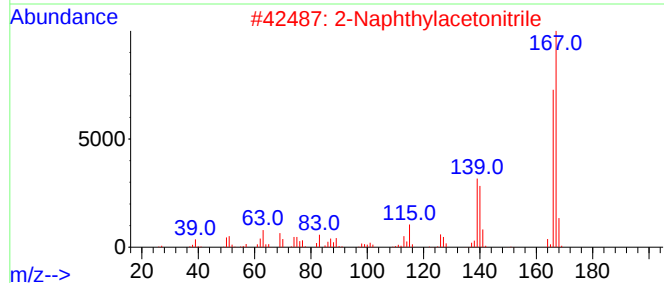
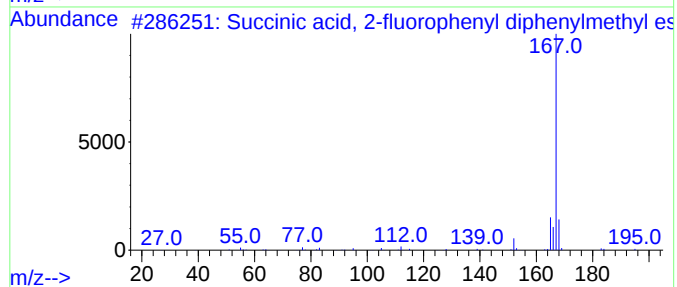
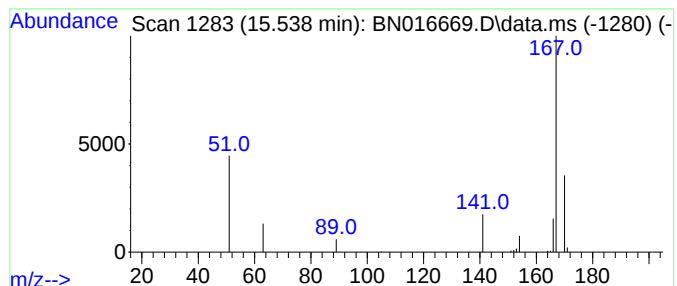
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	60137	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			2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
3			Carbazole	167	C12H9N	000086-74-8	7
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

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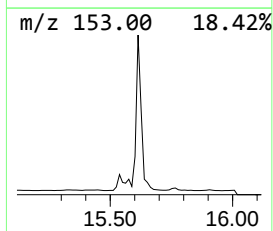
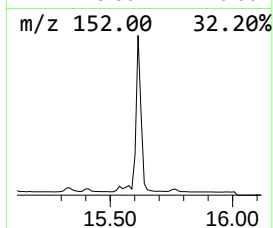
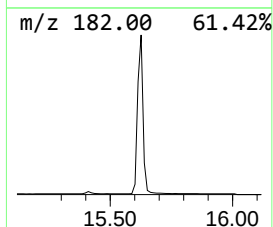
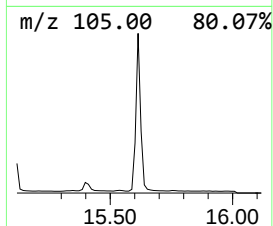
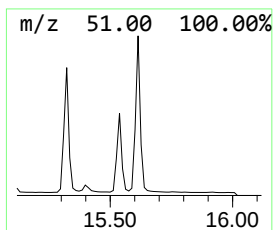
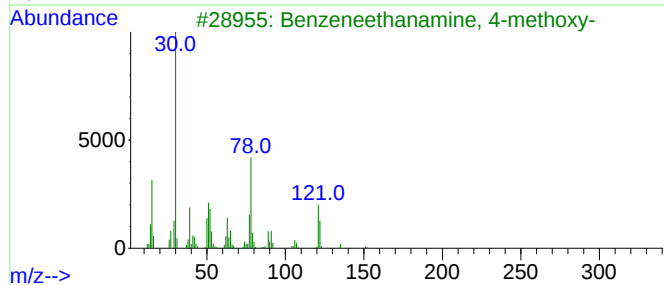
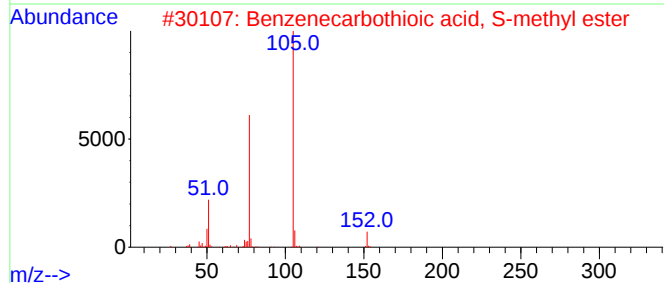
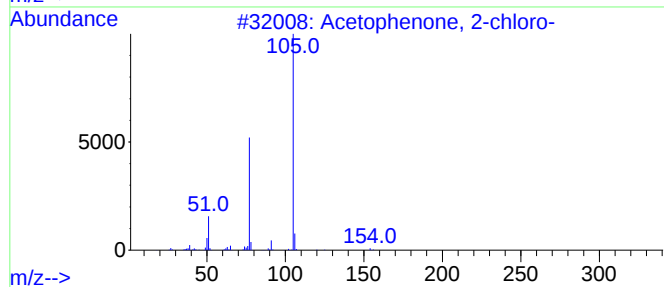
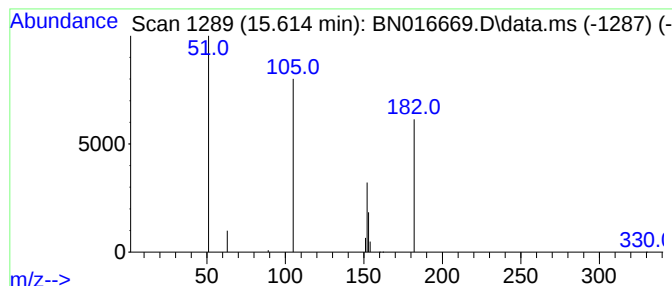
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	62502	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			Propiolonitrile	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 : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

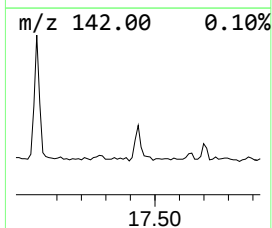
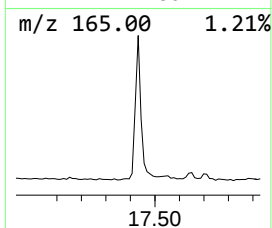
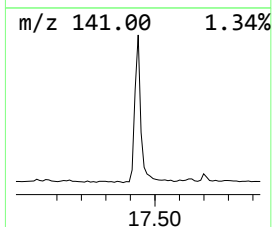
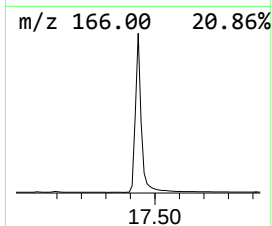
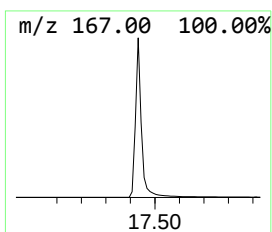
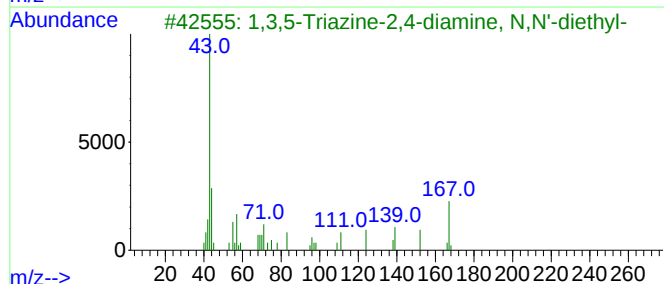
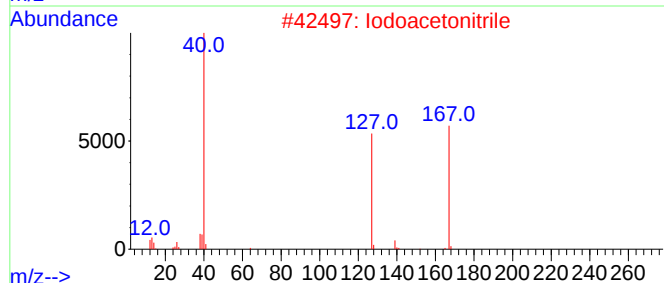
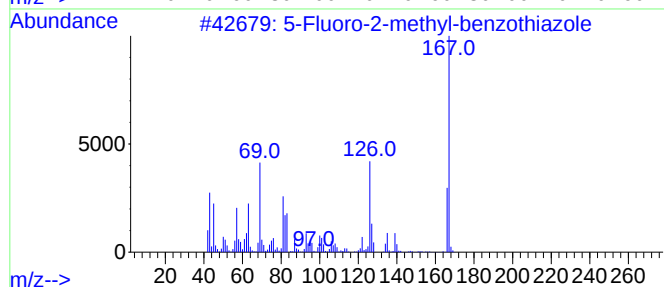
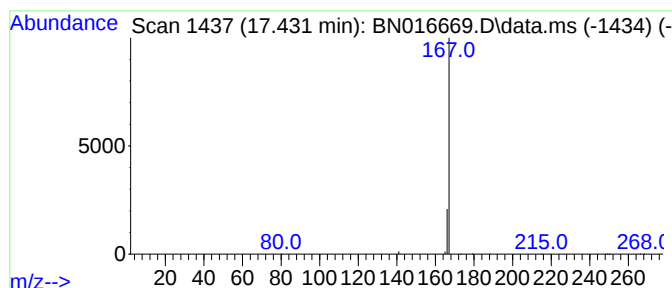
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.34 ng	132043	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		1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
4		1-Cyclopropanecarbonylpiperidin-...	167	C9H13N02	063463-43-4	4
5		2-propenoic acid, 2-methyl-, 2-(...	167	C7H9N3O2	1000404-53-2	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

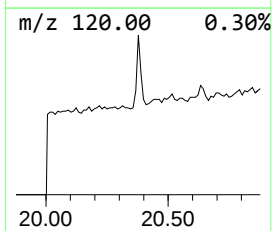
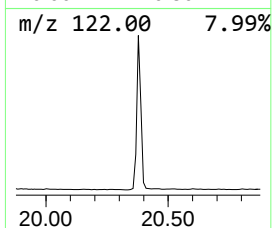
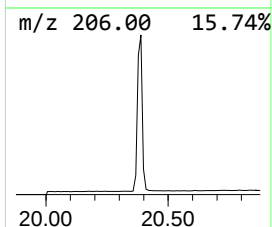
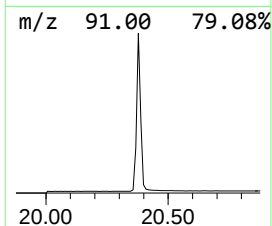
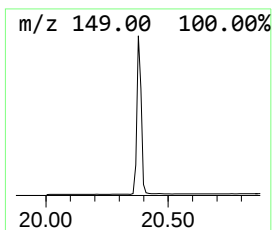
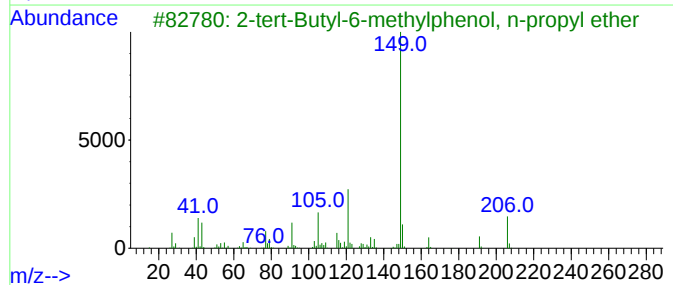
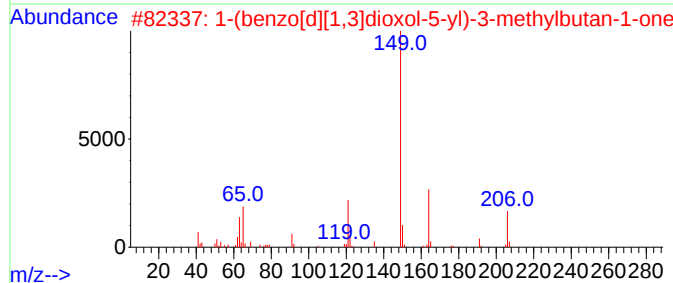
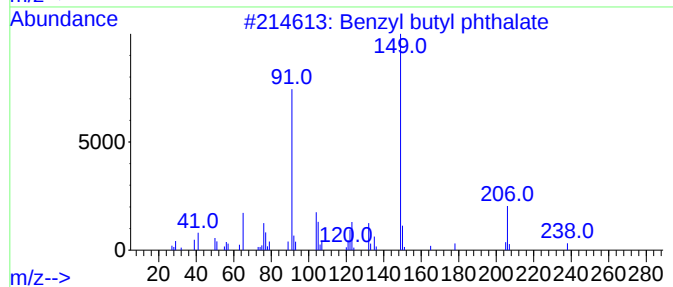
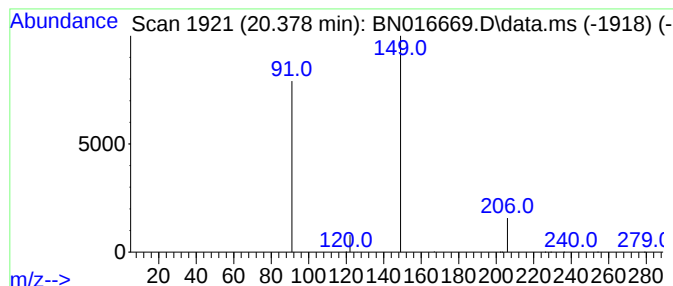
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	56928	Chrysene-d12	21.238

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-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
4			1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
5			2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

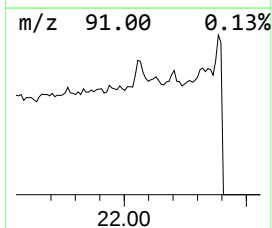
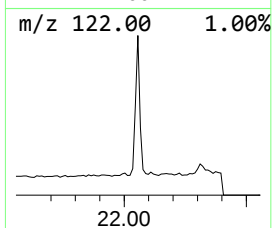
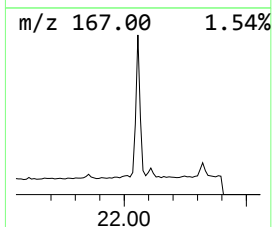
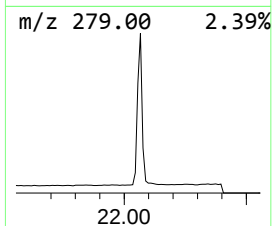
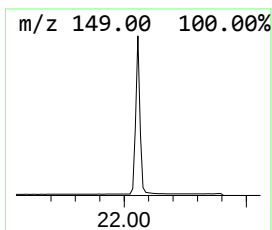
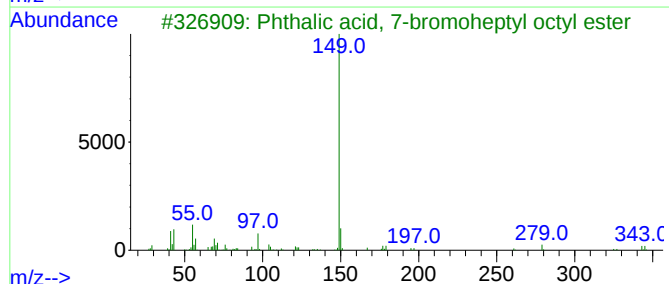
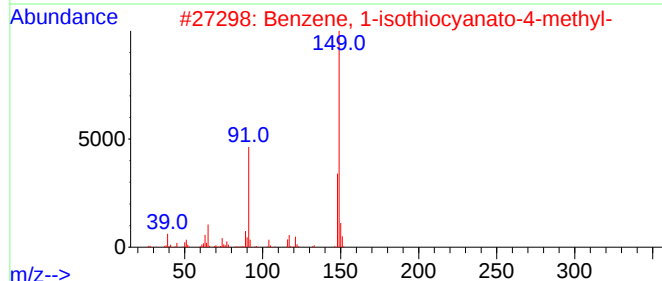
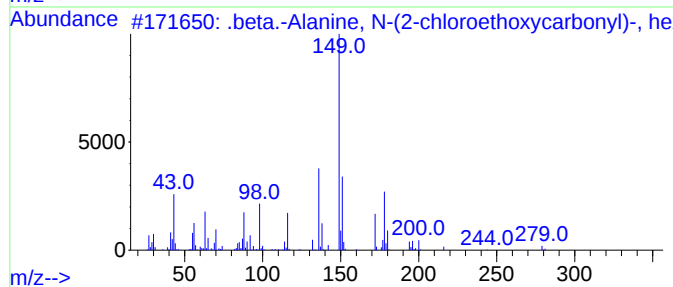
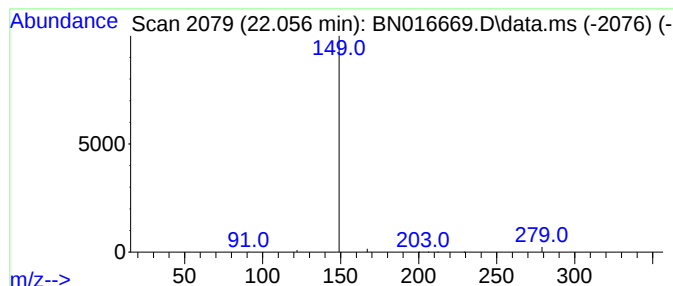
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	74471	Chrysene-d12	21.238

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		Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
4		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
5		m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016669.D
Acq On : 02 Oct 2021 14:08
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 37 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, ...	6.979	0.1	ng	33160	1	7.642	115014	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	30453	1	7.642	115014	0.4
2-Cyclohexen-1-...	7.523	0.0	ng	14237	1	7.642	115014	0.4
6-Benzothiazola...	7.956	0.4	ng	103231	1	7.642	115014	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	47278	1	7.642	115014	0.4
Fomepizole	9.342	0.2	ng	72222	2	10.407	188547	0.4
5-Aminopyrimidine	9.836	0.1	ng	26652	2	10.407	188547	0.4
p-Chloroaniline	10.572	0.1	ng	54805	2	10.407	188547	0.4
Methane, iodo-	11.709	0.1	ng	23823	2	10.407	188547	0.4
2-Propyl-4-meth...	12.296	0.4	ng	190825	2	10.407	188547	0.4
4-Cyano-5-(meth...	12.696	0.1	ng	27124	3	14.269	189694	0.4
1-Methyl-1,8-di...	12.759	0.0	ng	23491	3	14.269	189694	0.4
Naphthalene, 1-...	13.140	0.3	ng	126853	3	14.269	189694	0.4
Benzene, 2-meth...	13.850	0.1	ng	26705	3	14.269	189694	0.4
Benzene, 1-meth...	14.637	0.1	ng	41621	3	14.269	189694	0.4
Succinic acid, ...	15.538	0.1	ng	60137	3	14.269	189694	0.4
Acetophenone, 2...	15.614	0.1	ng	62502	3	14.269	189694	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	132043	4	17.018	157297	0.4
Benzyl butyl ph...	20.378	0.1	ng	56928	5	21.238	389822	0.4
.beta.-Alanine,...	22.056	0.1	ng	74471	5	21.238	389822	0.4