

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016686.D
 Acq On : 03 Oct 2021 00:22
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 54 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: BN016686.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	6405	9292	1.70%	0.109%
2	3.281	20	22	42	rVB	5076	24802	4.54%	0.291%
3	3.594	51	56	77	rVB	6357	30129	5.52%	0.353%
4	5.263	231	237	254	rVB	14908	58162	10.66%	0.682%
5	6.821	401	406	418	rBV	25907	64664	11.85%	0.758%
6	6.978	418	423	429	rVV	18559	40313	7.39%	0.473%
7	7.080	429	434	440	rVV	34904	71233	13.05%	0.835%
8	7.199	440	447	460	rVB	12456	33335	6.11%	0.391%
9	7.522	478	482	489	rVB	6513	14390	2.64%	0.169%
10	7.642	490	495	512	rVB2	47551	116204	21.29%	1.363%
11	7.956	524	529	538	rVB2	46126	104523	19.15%	1.226%
12	8.168	547	552	557	rVB2	2942	7079	1.30%	0.083%
13	8.429	571	577	585	rBV3	23841	55104	10.10%	0.646%
14	8.695	595	598	601	rBV	4418	8332	1.53%	0.098%
15	8.784	601	605	606	rBV	37677	71885	13.17%	0.843%
16	8.822	606	608	616	rVB	31246	58658	10.75%	0.688%
17	9.342	645	649	652	rBV	55676	91210	16.71%	1.070%
18	9.519	660	663	666	rBV	3732	7238	1.33%	0.085%
19	9.595	666	669	678	rVB	9552	17034	3.12%	0.200%
20	9.836	685	688	700	rVB	16377	28875	5.29%	0.339%
21	10.051	702	705	715	rVB	4538	10061	1.84%	0.118%
22	10.406	729	733	735	rBV	104207	190717	34.95%	2.237%
23	10.457	735	737	740	rVV	106761	174431	31.96%	2.046%
24	10.571	743	746	756	rVV	32304	68578	12.57%	0.804%
25	10.748	756	760	763	rVB	31769	55018	10.08%	0.645%
26	11.306	801	804	812	rBV	2730	6582	1.21%	0.077%
27	11.709	852	865	891	rBV	16021	29314	5.37%	0.344%
28	12.002	921	931	939	rBV	57797	93315	17.10%	1.095%
29	12.078	939	948	972	rVV	127466	206349	37.81%	2.420%
30	12.296	987	997	1019	rVV	126576	198979	36.46%	2.334%
31	12.695	1056	1059	1062	rBV	20289	33680	6.17%	0.395%
32	12.771	1062	1065	1071	rVB	14056	29069	5.33%	0.341%
33	12.885	1071	1074	1078	rBV	116194	195355	35.80%	2.291%
34	13.139	1089	1094	1097	rBV	78299	131746	24.14%	1.545%
35	13.736	1138	1141	1143	rBV	12881	18212	3.34%	0.214%
36	13.850	1147	1150	1153	rVB	22781	33366	6.11%	0.391%

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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

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37	13.939	1155	1157	1158	rBV	5747	9296	1.70%	0.109%
38	13.989	1158	1161	1164	rVB	102400	167388	30.67%	1.963%
39	14.268	1180	1183	1185	rBV	139759	199501	36.56%	2.340%
40	14.332	1185	1188	1191	rVB	166807	245086	44.91%	2.875%
41	14.636	1209	1212	1220	rBV2	19323	49108	9.00%	0.576%
42	14.814	1224	1226	1230	rBV	6542	11623	2.13%	0.136%
43	14.903	1230	1233	1236	rBV	9015	13333	2.44%	0.156%
44	15.106	1246	1249	1252	rBV	9739	12598	2.31%	0.148%
45	15.321	1263	1266	1270	rBV2	233668	357641	65.54%	4.195%
46	15.410	1271	1273	1280	rVV2	2517	6304	1.16%	0.074%
47	15.537	1280	1283	1287	rVV	40748	67867	12.44%	0.796%
48	15.613	1287	1289	1298	rVV2	47668	74013	13.56%	0.868%
49	15.766	1298	1301	1311	rVB2	15932	26828	4.92%	0.315%
50	16.226	1334	1338	1341	rBV2	61873	94852	17.38%	1.113%
51	16.323	1343	1346	1350	rVB	45942	71818	13.16%	0.842%
52	16.506	1358	1361	1372	rBV	26315	42825	7.85%	0.502%
53	16.676	1372	1375	1384	rBV	26742	46292	8.48%	0.543%
54	17.017	1400	1403	1405	rBV	100768	166010	30.42%	1.947%
55	17.066	1405	1407	1410	rVV	152093	220238	40.36%	2.583%
56	17.151	1411	1414	1434	rVB	125445	199376	36.53%	2.338%
57	17.431	1434	1437	1453	rBV	98182	156049	28.60%	1.830%
58	18.015	1482	1485	1498	rVB	7110	9999	1.83%	0.117%
59	19.068	1686	1697	1699	rBV	127234	174692	32.01%	2.049%
60	19.097	1699	1703	1731	rVB	198975	276083	50.59%	3.238%
61	19.460	1767	1776	1798	rBV	205634	277249	50.80%	3.252%
62	19.678	1813	1820	1842	rBV	117935	150417	27.56%	1.764%
63	20.377	1918	1921	1924	rBV	88723	107054	19.62%	1.256%
64	21.163	1993	1995	1998	rBV	91113	131790	24.15%	1.546%
65	21.216	1998	2000	2003	rVV2	239615	466385	85.46%	5.470%
66	21.270	2003	2005	2016	rVB	221089	287914	52.76%	3.377%
67	22.055	2076	2079	2091	rVB	139853	182133	33.37%	2.136%
68	22.321	2101	2104	2108	rBV	3876	6099	1.12%	0.072%
69	22.806	2217	2229	2235	rBV	148174	241385	44.23%	2.831%
70	22.851	2235	2242	2287	rVB2	151864	274778	50.35%	3.223%
71	23.385	2385	2398	2416	rBV	107619	234343	42.94%	2.749%
72	23.484	2416	2427	2472	rVB	109983	224449	41.13%	2.633%
73	24.087	2592	2603	2624	rBV	11939	23929	4.38%	0.281%
74	24.857	2816	2828	2847	rVB	10983	25906	4.75%	0.304%
75	25.774	3066	3096	3172	rBV4	142912	545719	100.00%	6.401%
76	26.459	3272	3296	3348	rBV	75970	246413	45.15%	2.890%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	26.825	3387	3403	3431	rVB	2549	8262	1.51%	0.097%
78	28.088	3750	3772	3798	rBV2	1402	5531	1.01%	0.065%

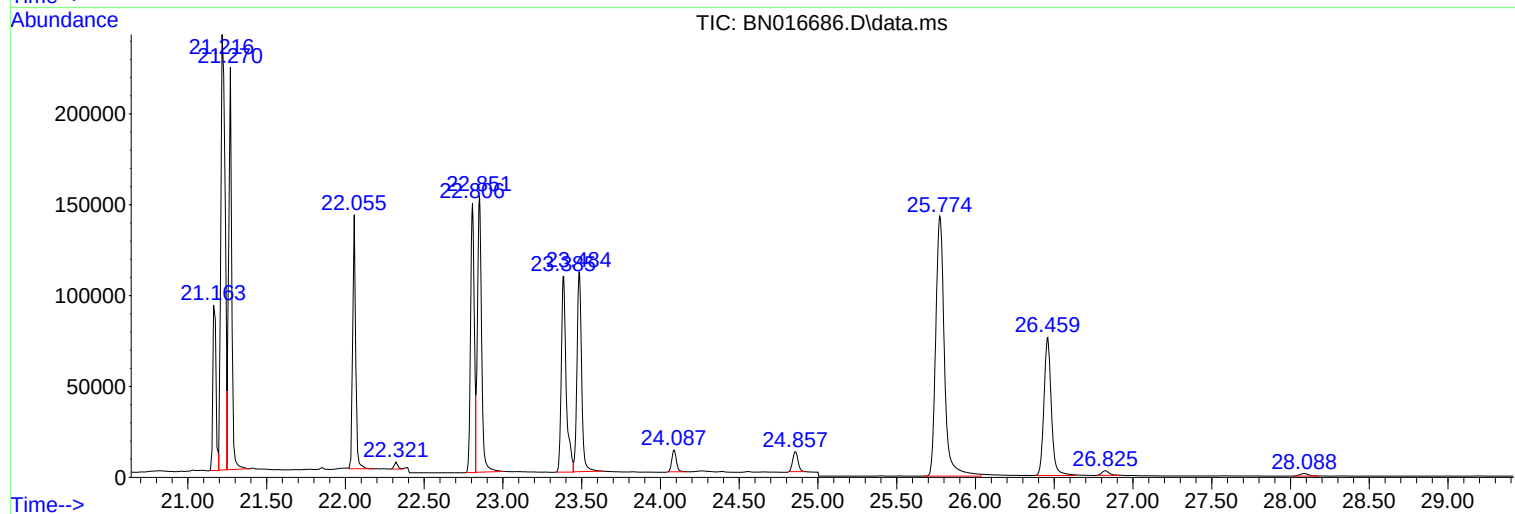
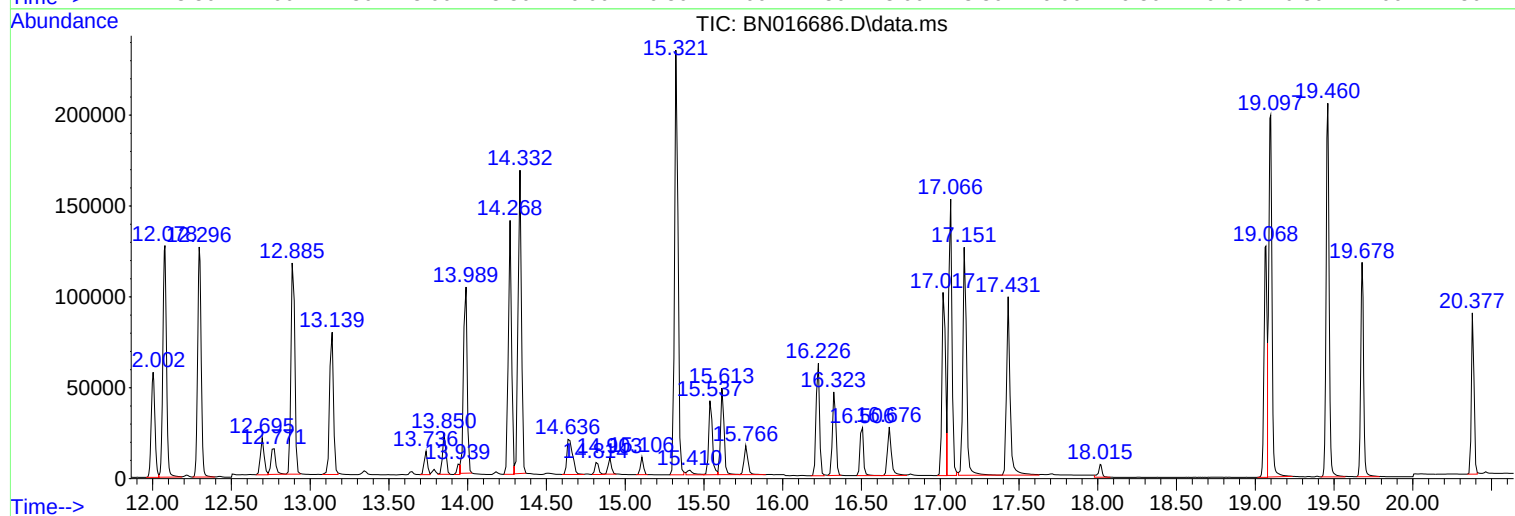
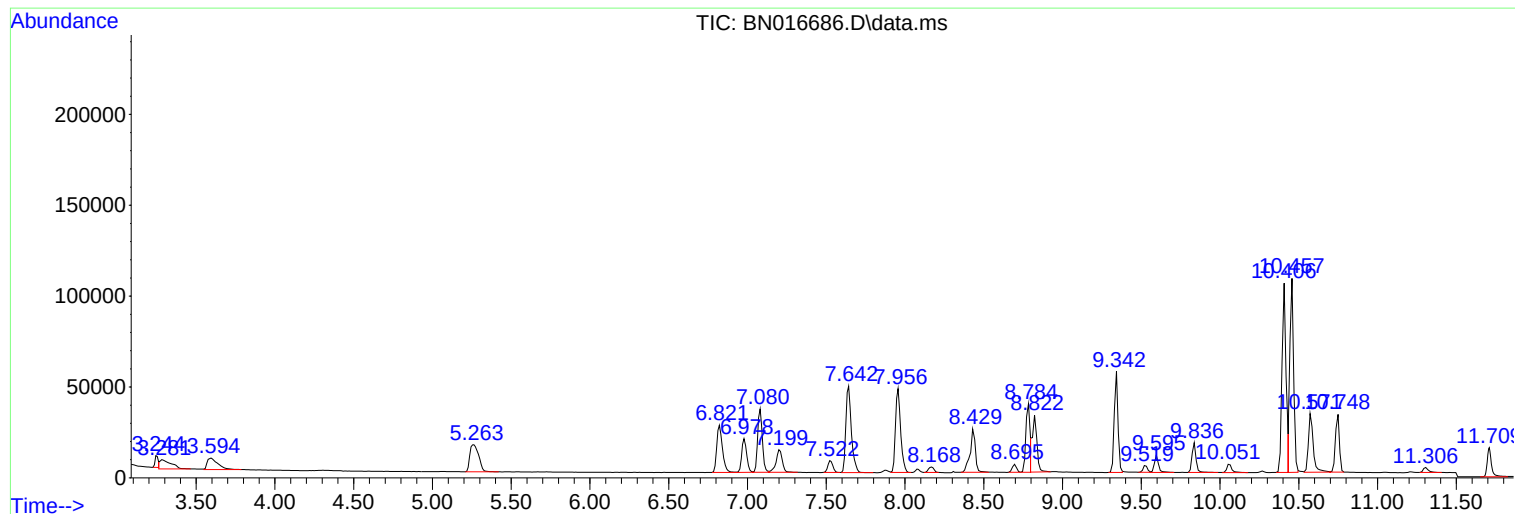
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Instrument :
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 54 Sample Multiplier: 1

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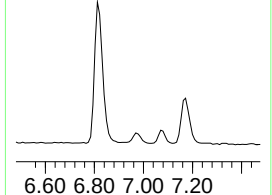
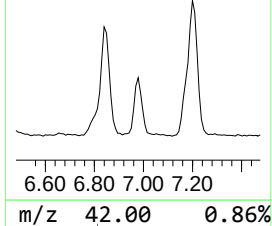
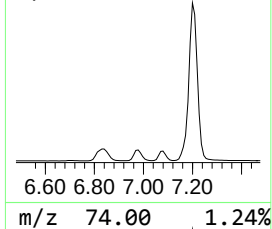
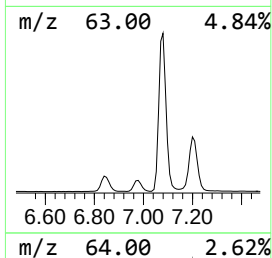
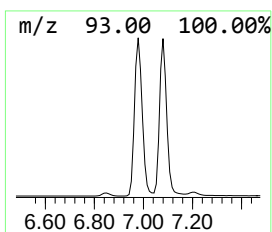
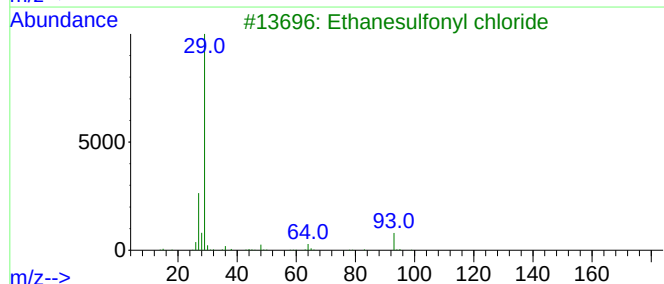
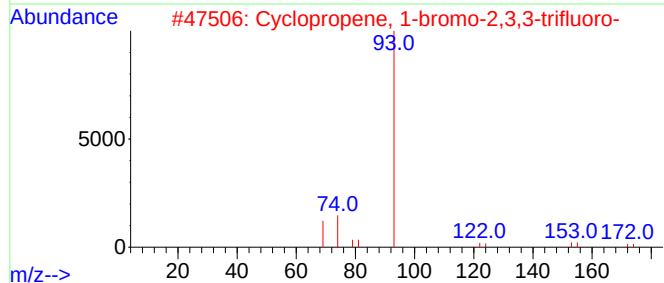
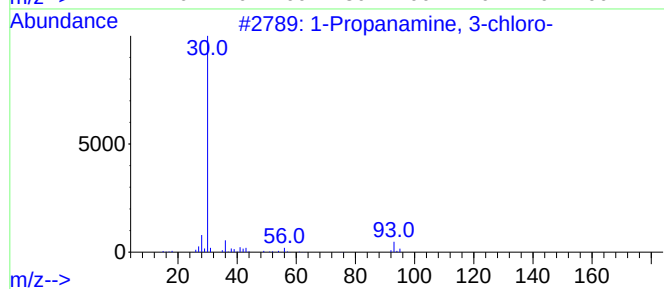
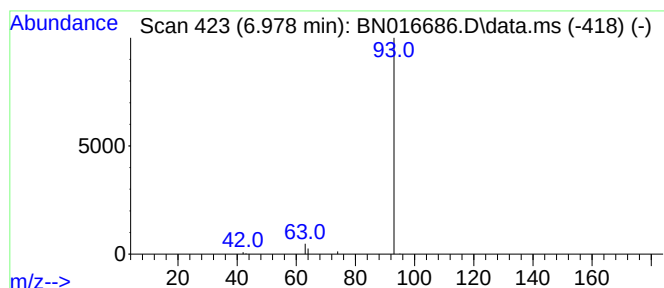
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
6.978	0.14 ng	40313	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 : 54 Sample Multiplier: 1

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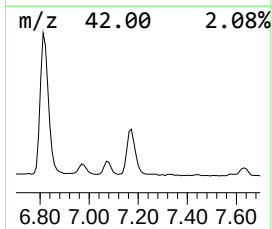
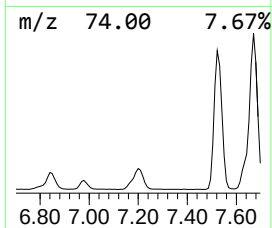
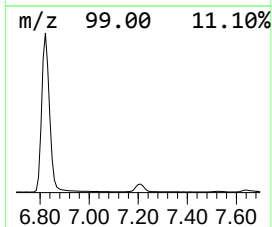
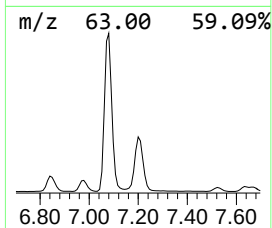
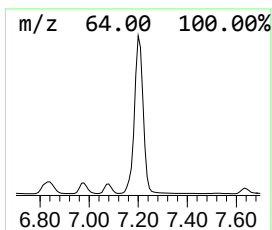
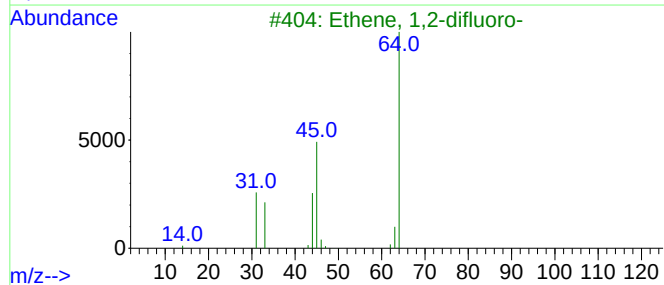
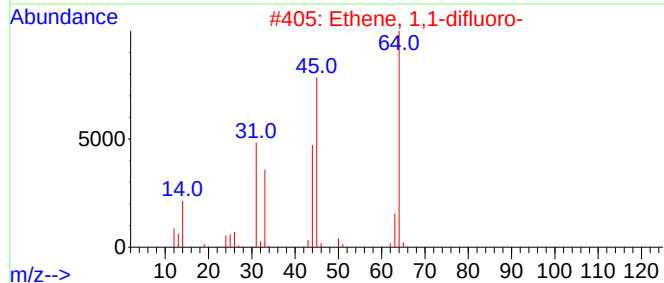
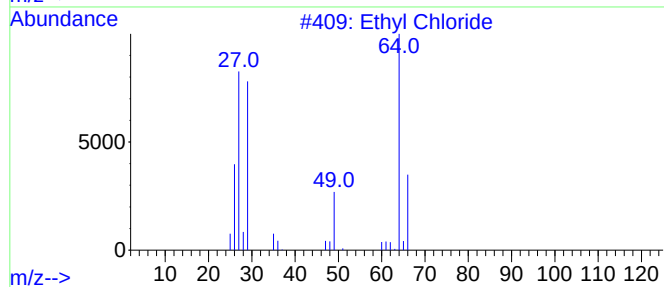
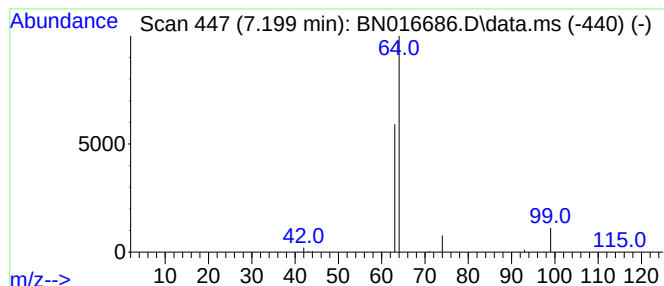
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethyl Chloride Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.199	0.11 ng	33335	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
2			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	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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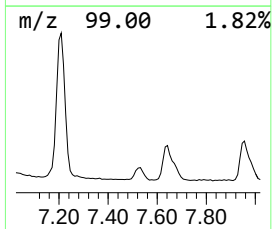
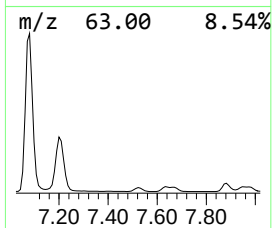
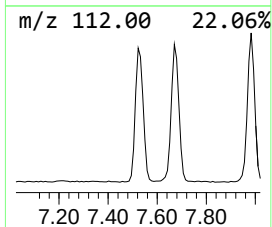
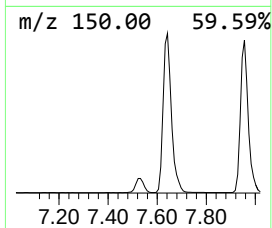
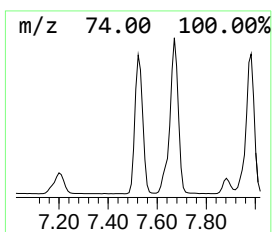
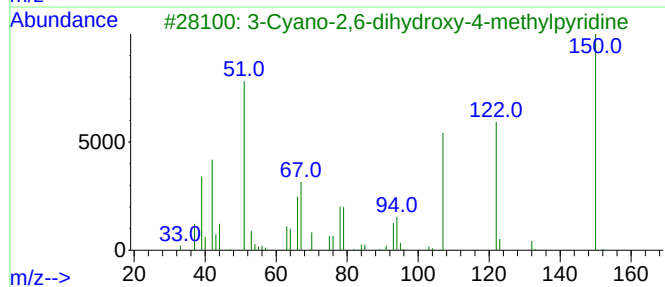
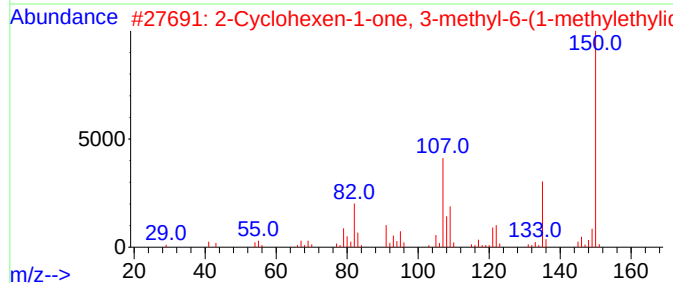
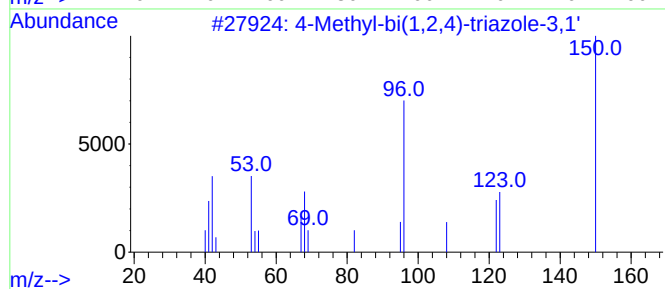
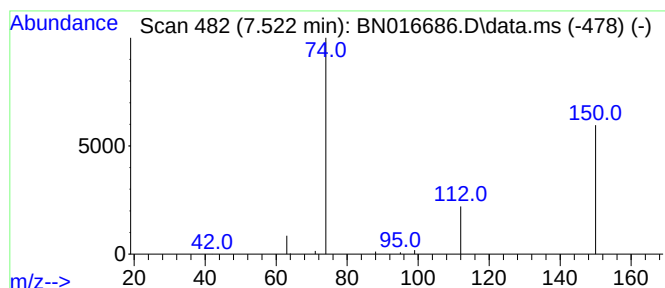
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	14390	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		2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
3		3-Cyano-2,6-dihydroxy-4-methylpy...	150	C7H6N2O2	005444-02-0	2
4		3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
5		N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2



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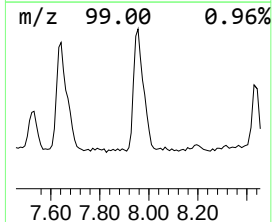
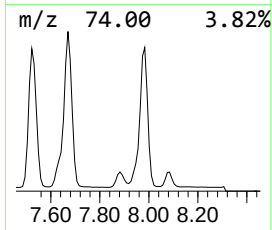
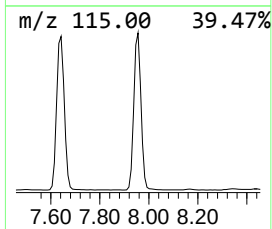
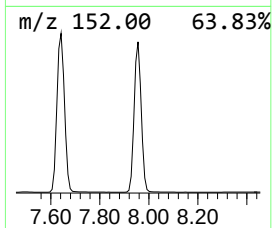
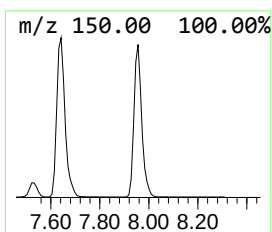
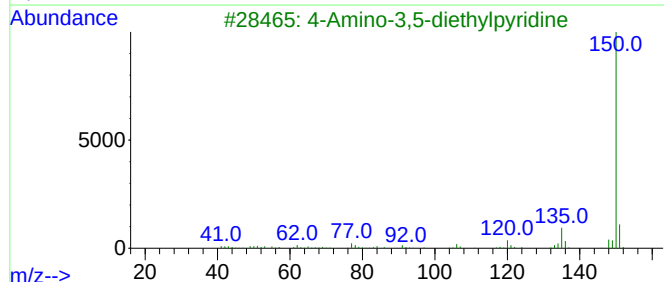
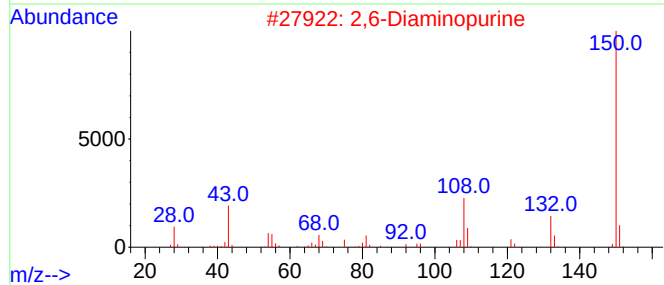
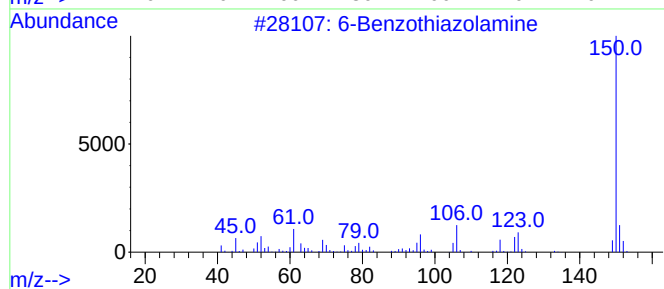
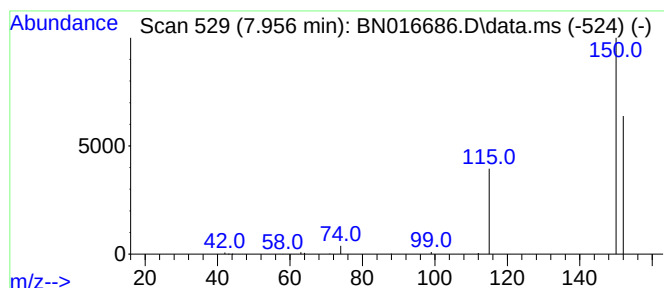
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	104523	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 : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
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Instrument :
BNA_N
LabSampleId :
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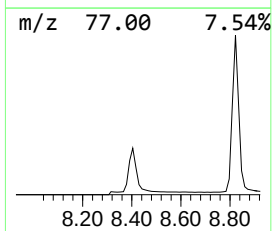
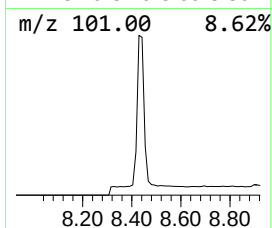
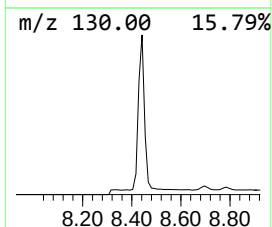
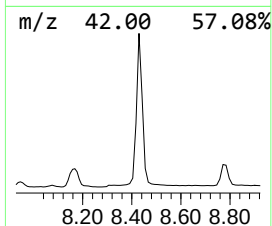
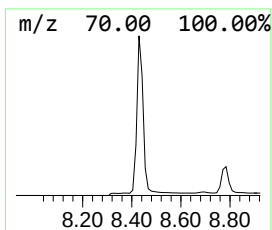
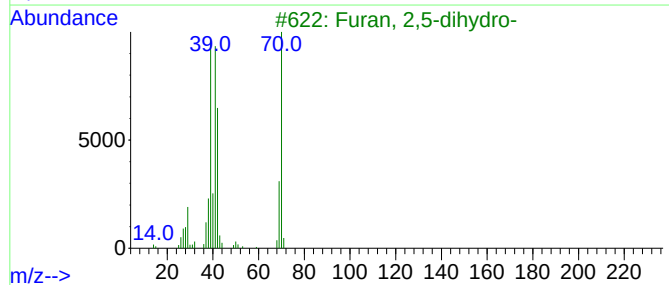
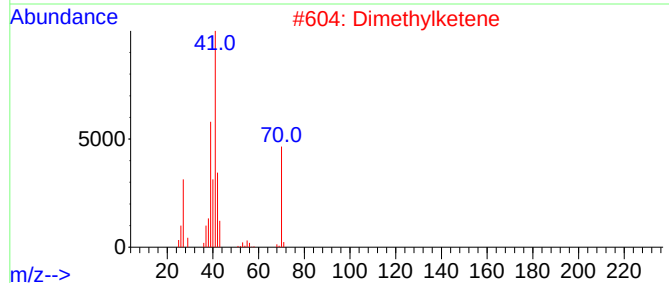
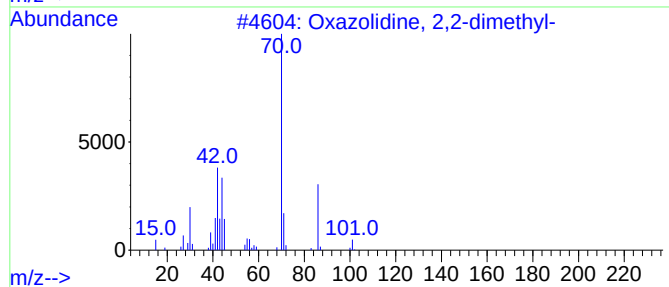
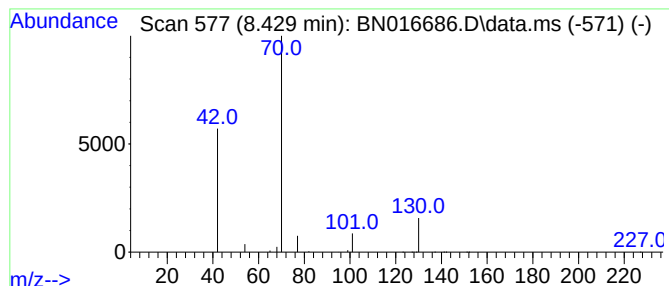
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Oxazolidine, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.19 ng	55104	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
2			Dimethylketene	70	C4H6O	000598-26-5	5
3			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	4
4			1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4
5			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4



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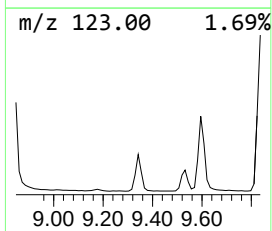
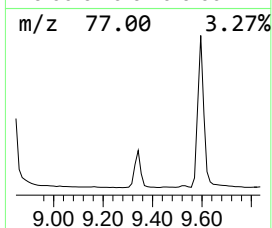
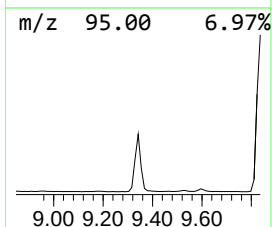
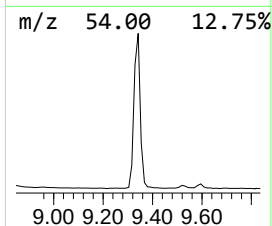
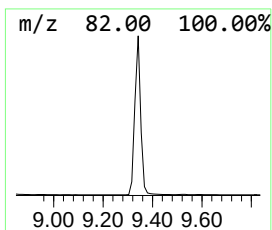
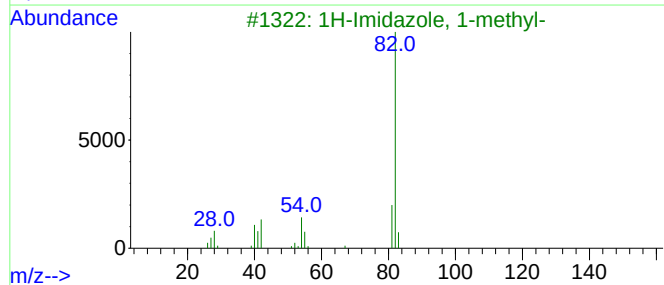
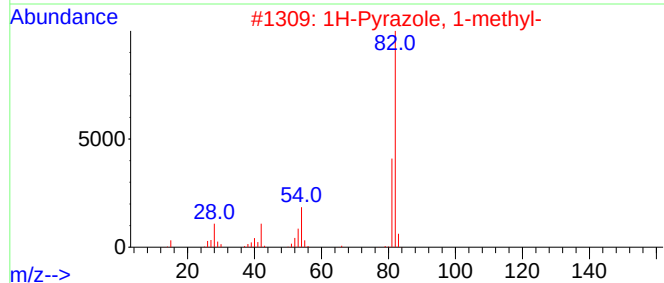
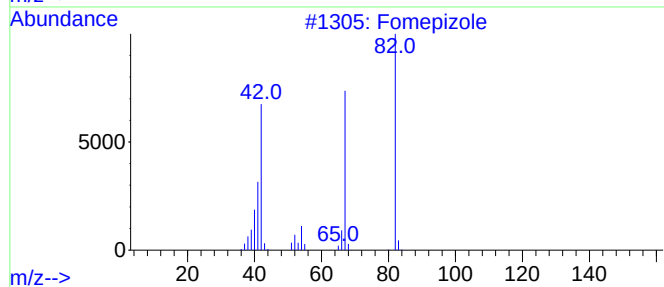
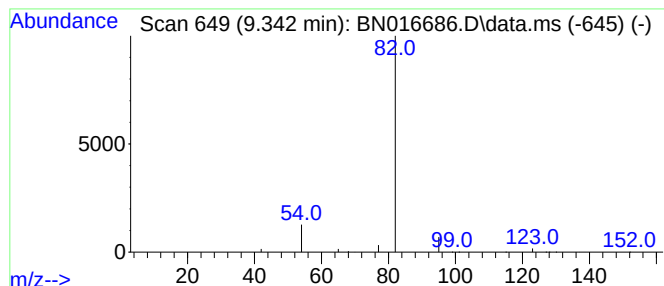
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.19 ng	91210	Naphthalene-d8	10.406

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 : BN016686.D
Acq On : 03 Oct 2021 00:22
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Misc :
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LabSampleId :
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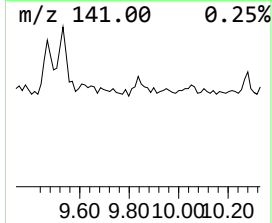
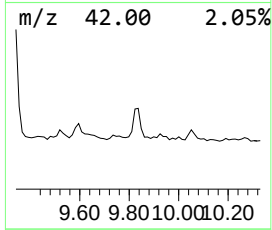
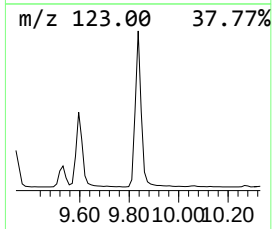
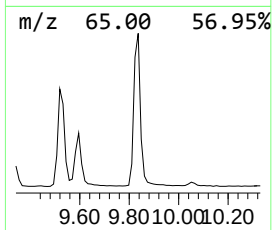
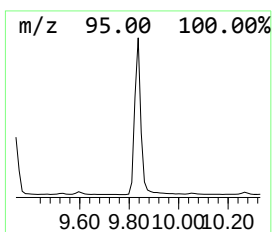
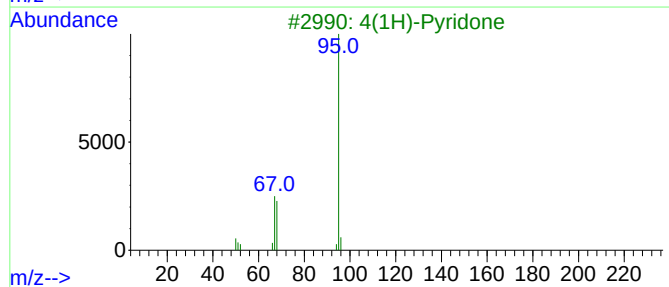
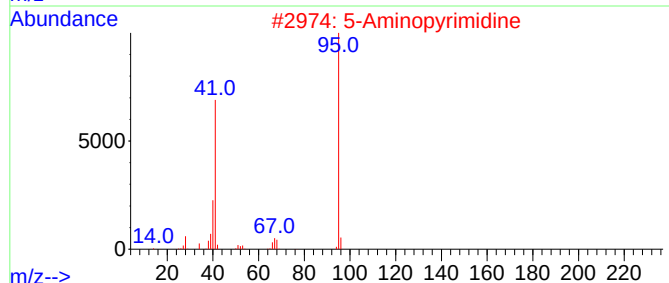
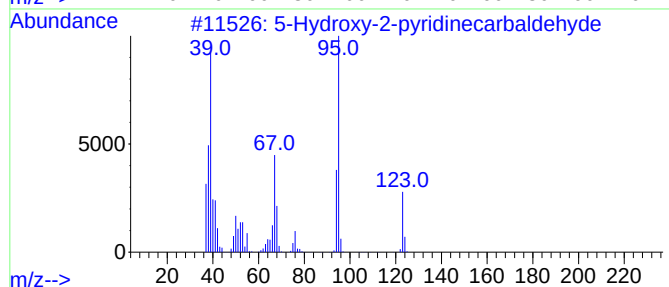
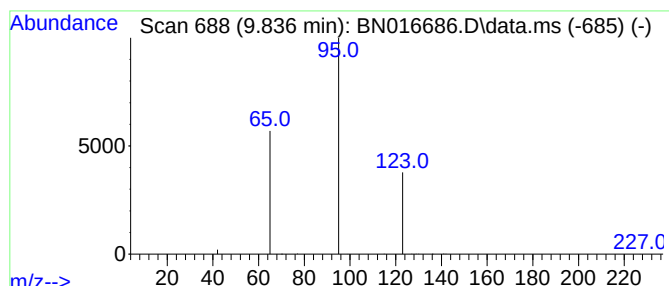
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Hydroxy-2-pyridinecarbal... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	28875	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2		5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
3		4(1H)-Pyridone	95	C5H5NO	000108-96-3	2
4		Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
5		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2



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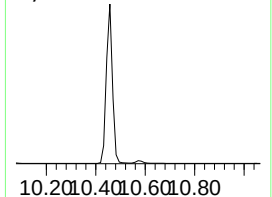
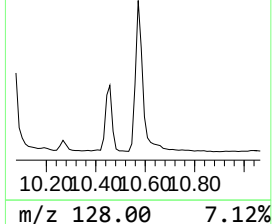
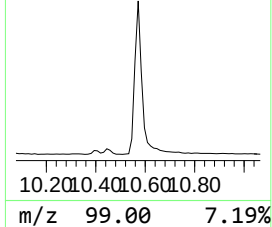
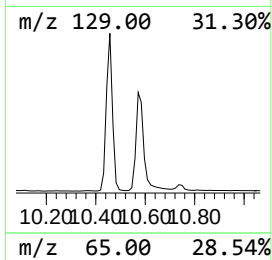
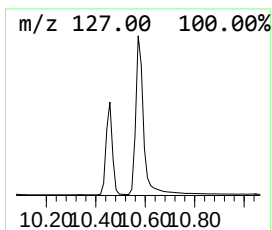
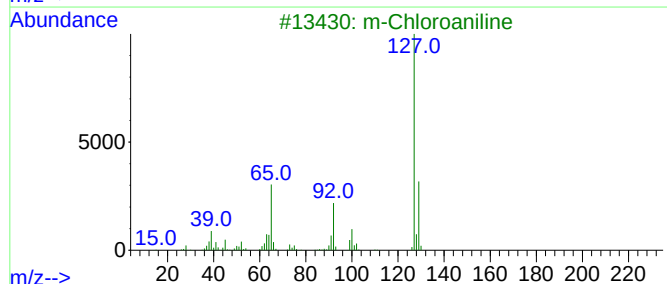
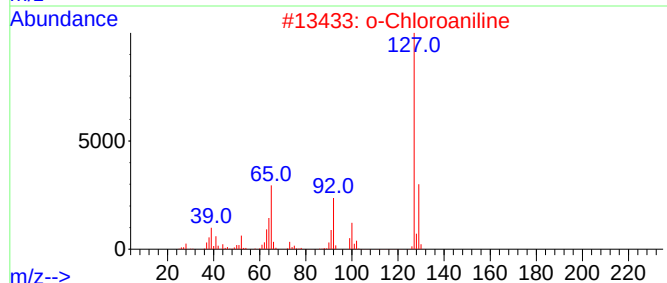
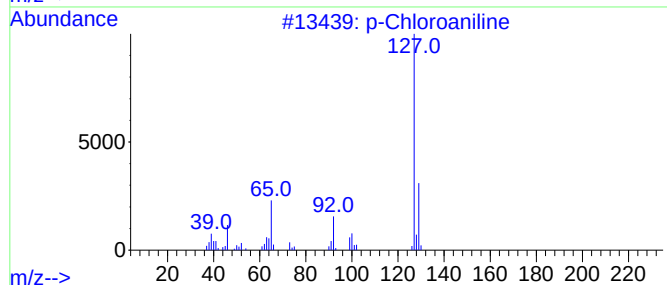
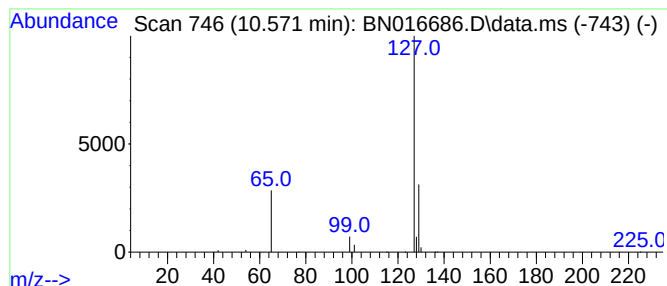
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.14 ng	68578	Naphthalene-d8	10.406

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			Picloxydine	474	C20H24Cl2N10	005636-92-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016686.D
Acq On : 03 Oct 2021 00:22
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Misc :
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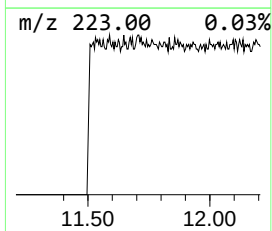
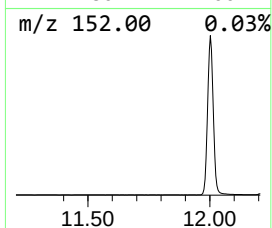
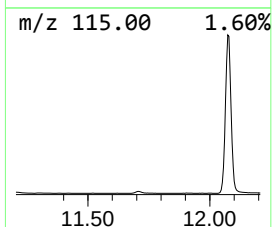
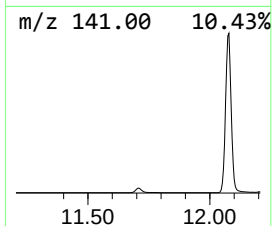
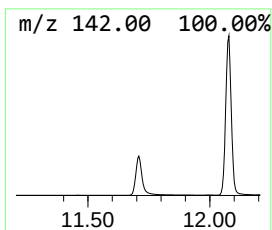
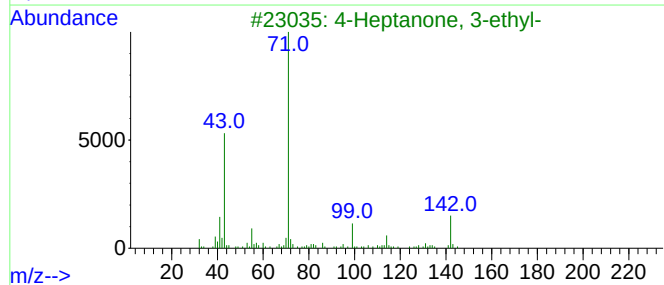
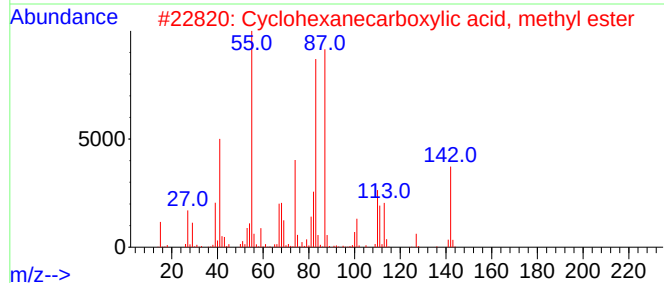
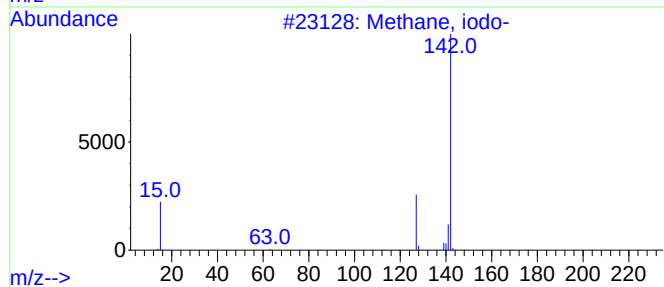
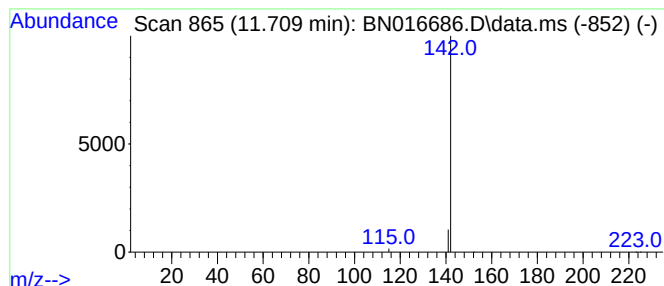
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Methane, iodo- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.06 ng	29314	Naphthalene-d8	10.406

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



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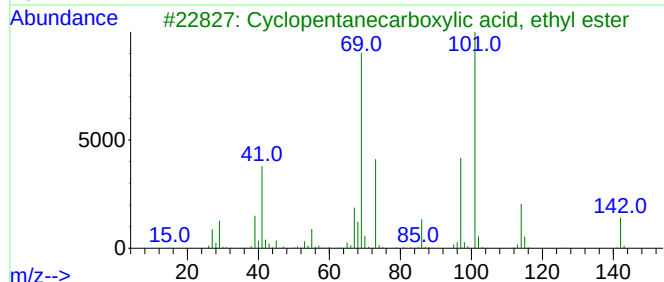
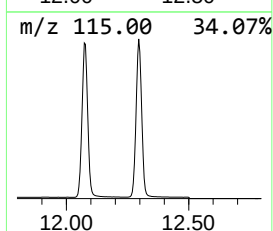
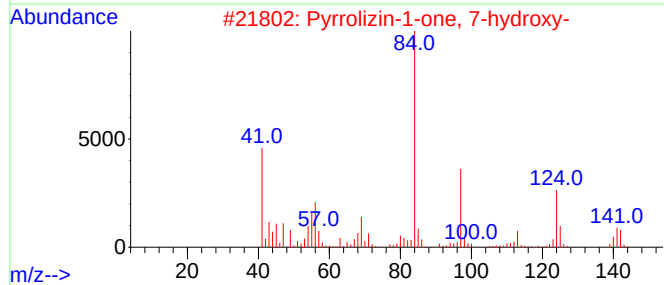
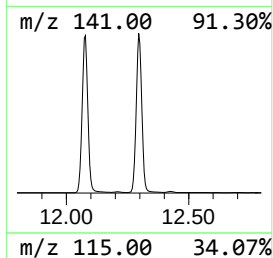
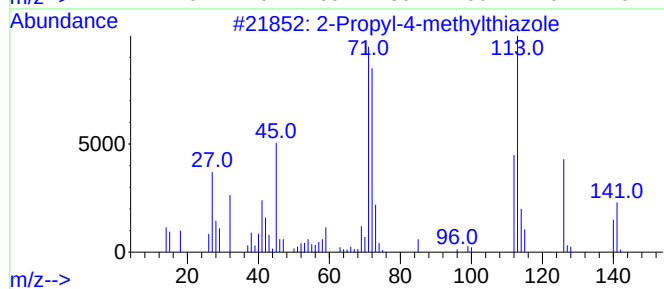
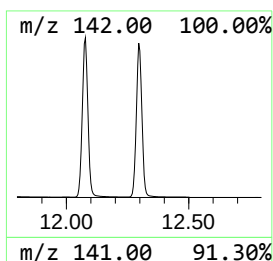
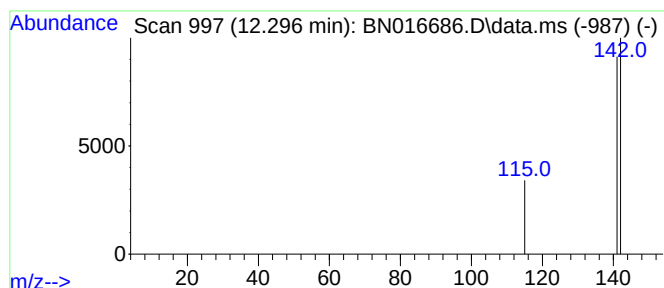
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.42 ng	198979	Naphthalene-d8	10.406	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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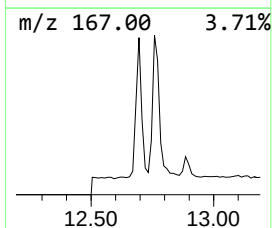
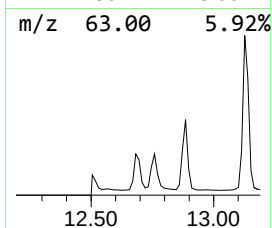
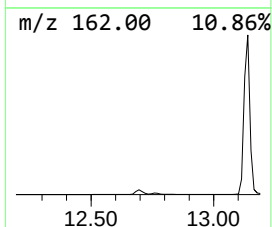
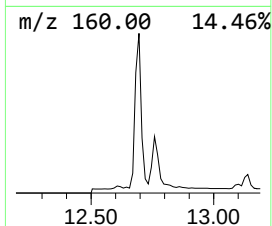
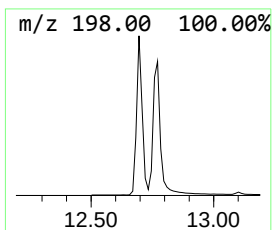
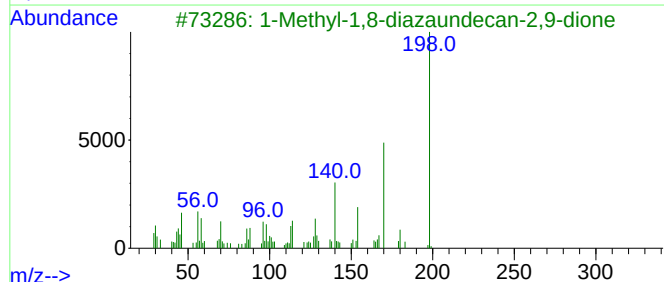
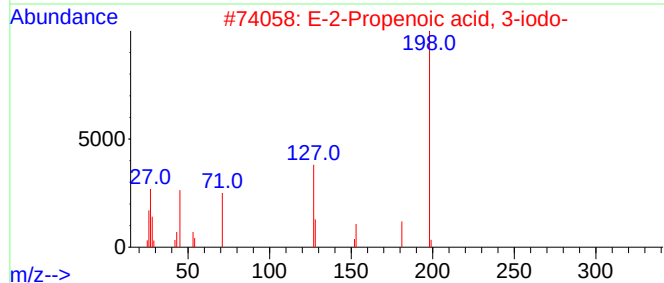
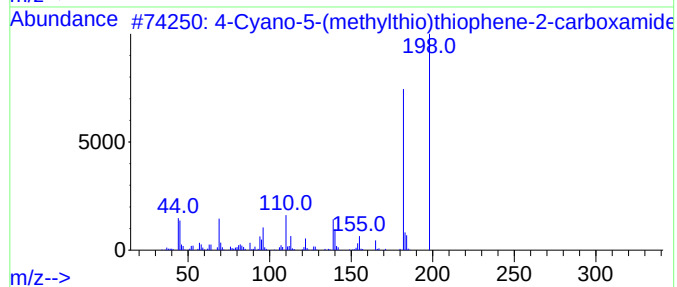
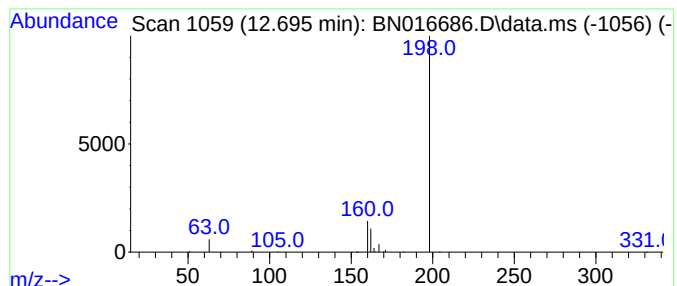
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LabSampleId :
SSTDCCC0.4

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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.	
12.695	0.07 ng	33680	Acenaphthene-d10		14.268	
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 : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

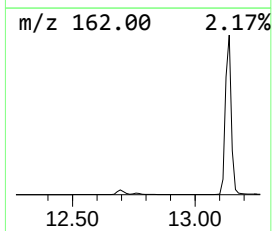
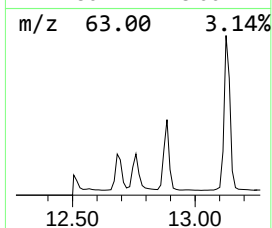
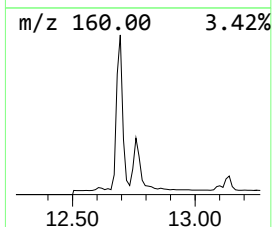
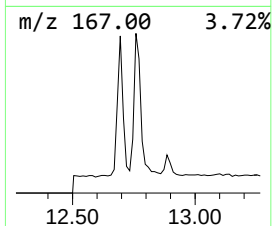
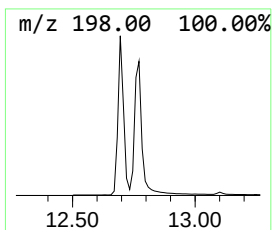
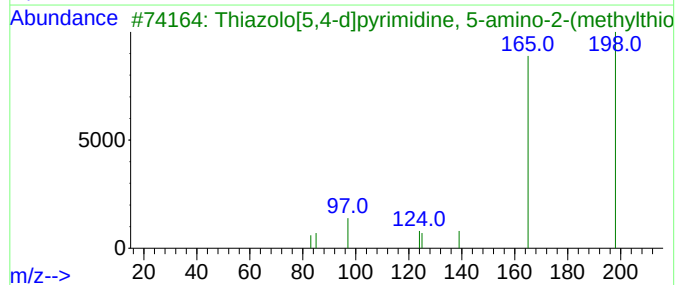
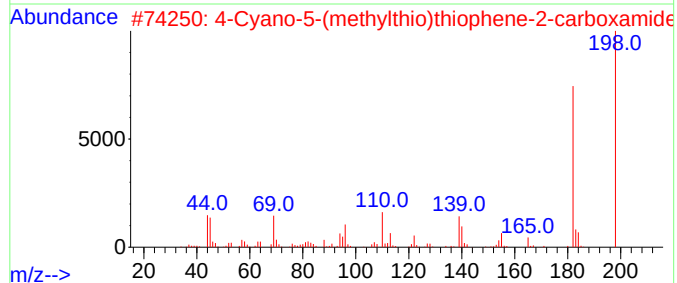
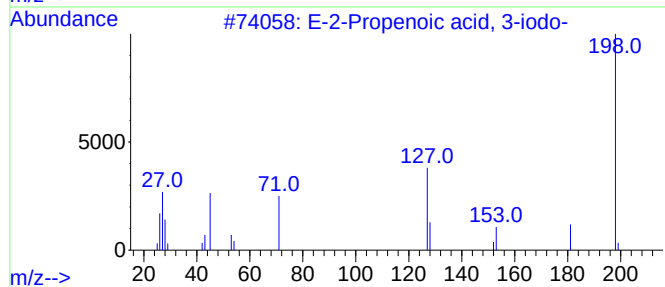
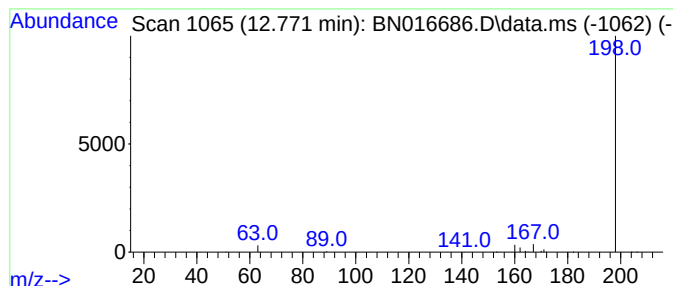
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.771	0.06 ng	29069	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
2			4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
3			Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
4			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5			Methyl 2-(dimethylhydrazono)-3,3...	198	C6H9F3N2O2	1000489-35-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

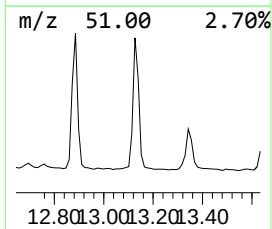
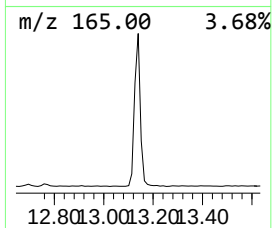
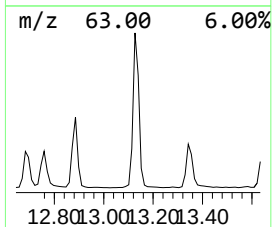
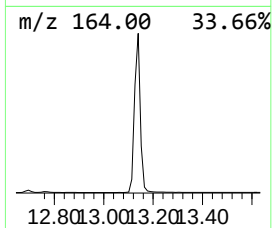
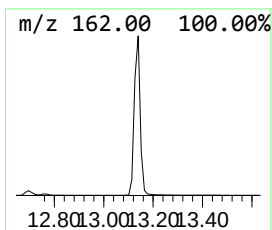
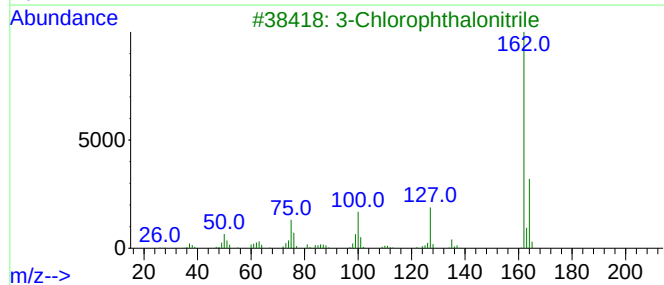
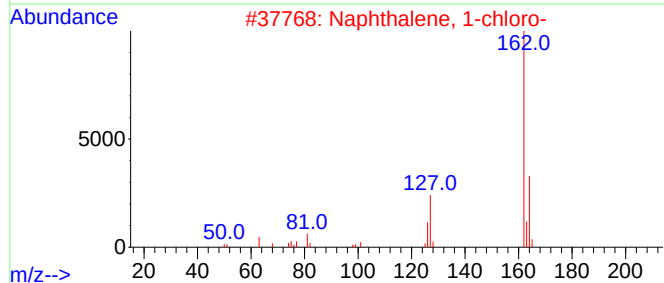
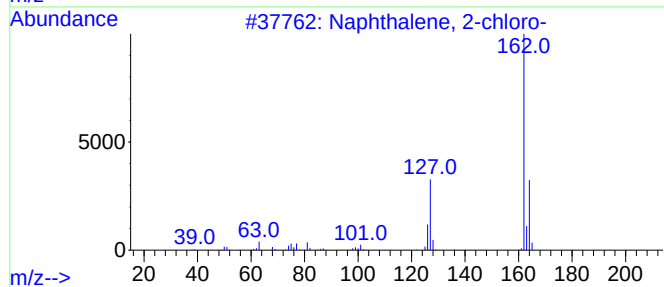
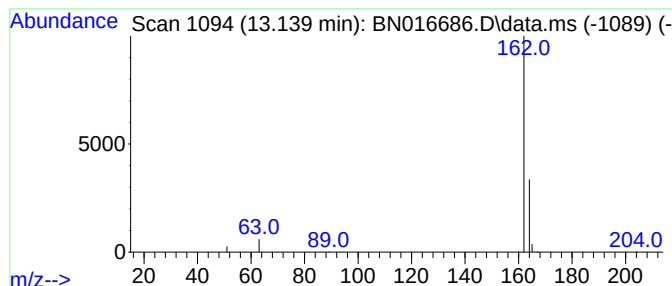
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.26 ng	131746	Acenaphthene-d10	14.268

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			3-Chloro-4-fluorothiophenol	162	C6H4ClFS	060811-23-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

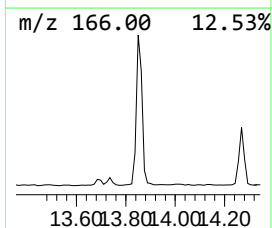
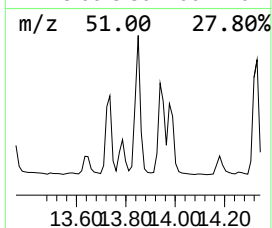
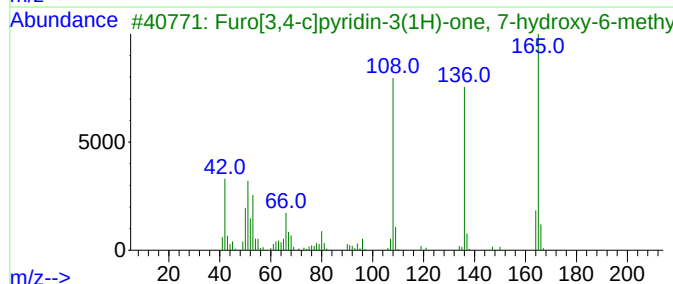
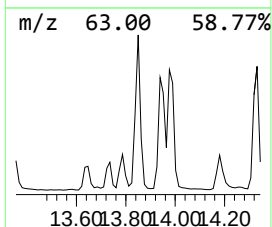
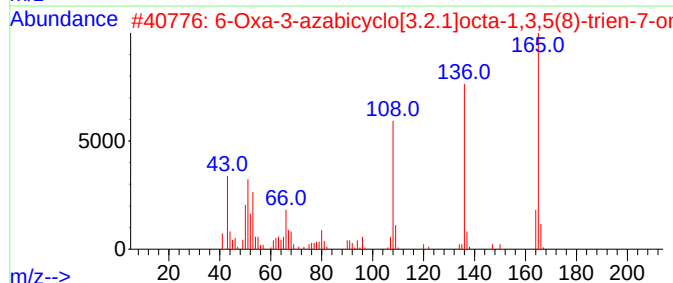
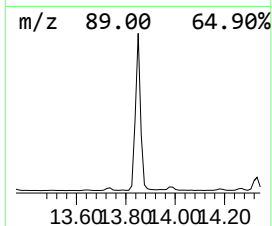
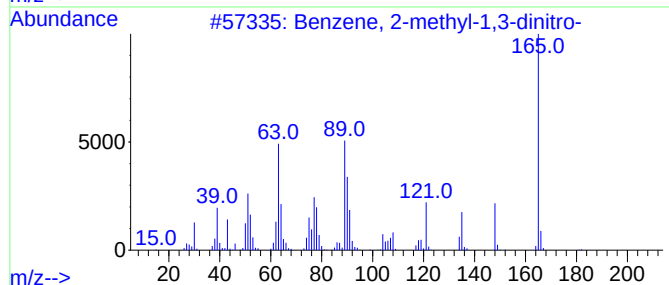
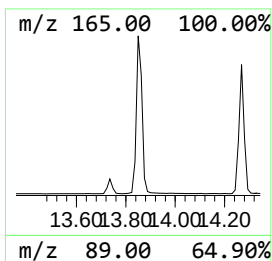
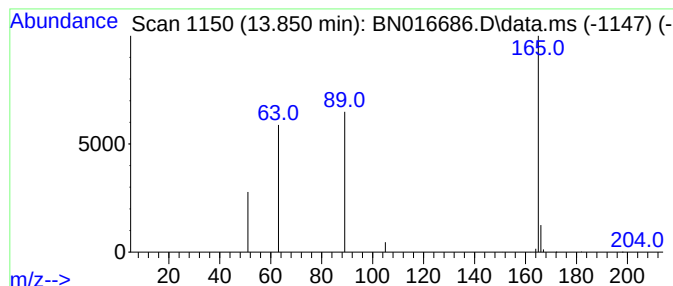
Instrument :
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.850	0.07 ng	33366	Acenaphthene-d10		14.268	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	83
2	6-Oxa-3-azabicyclo[3.2.1]octa-1,...		165	C8H7NO3	055255-96-4	9
3	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
4	Furo[3,4-c]pyridin-1(3H)-one, 7-...		165	C8H7NO3	004753-19-9	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

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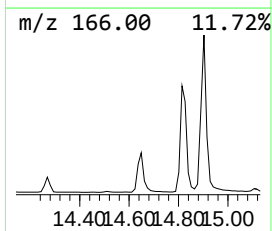
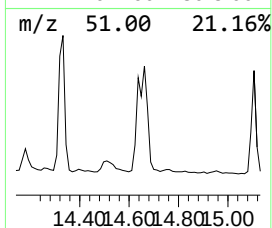
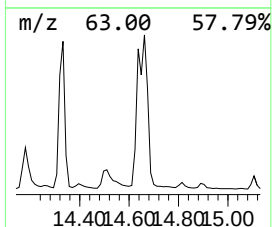
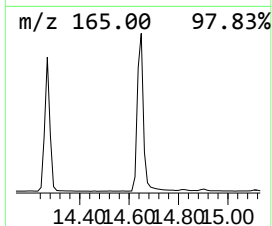
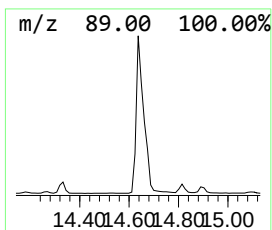
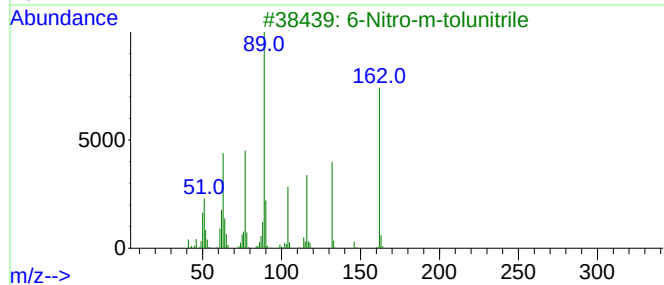
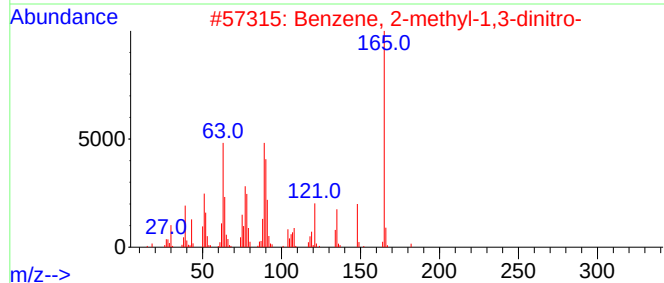
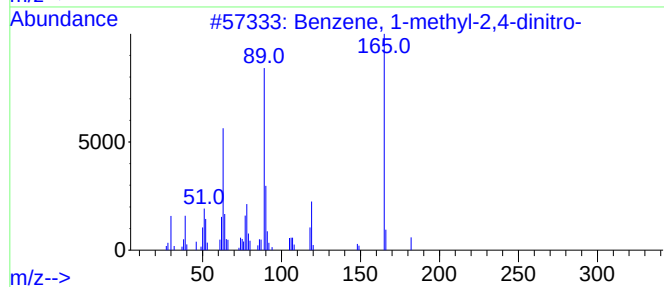
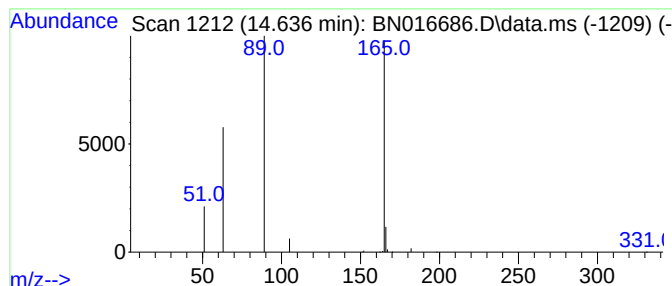
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.636	0.10 ng	49108	Acenaphthene-d10	14.268

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		6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9
4		5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	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 : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

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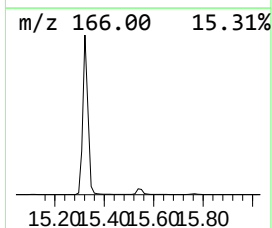
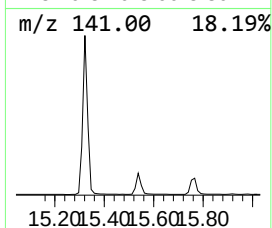
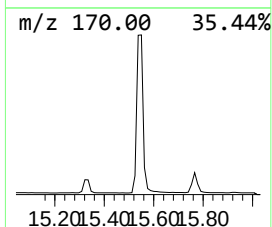
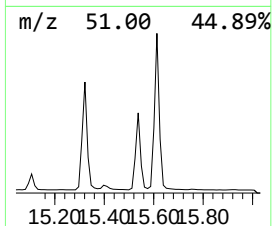
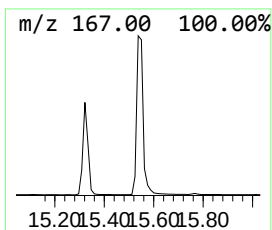
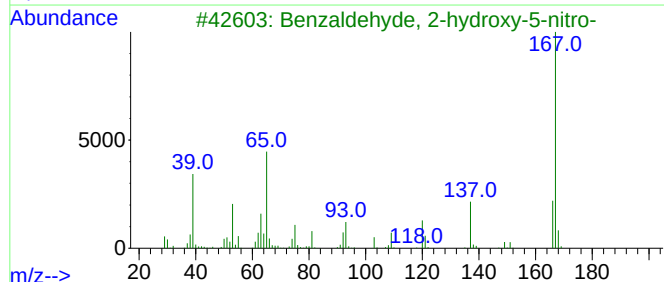
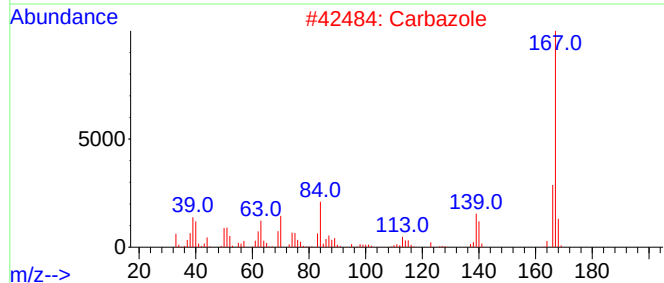
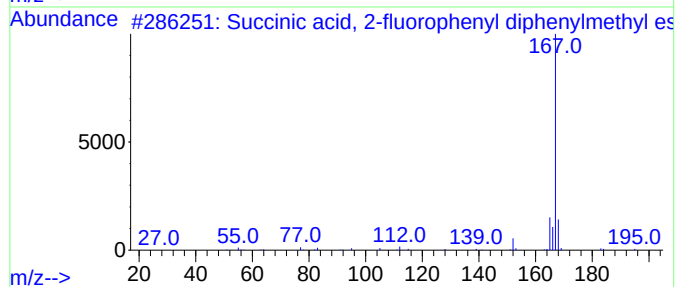
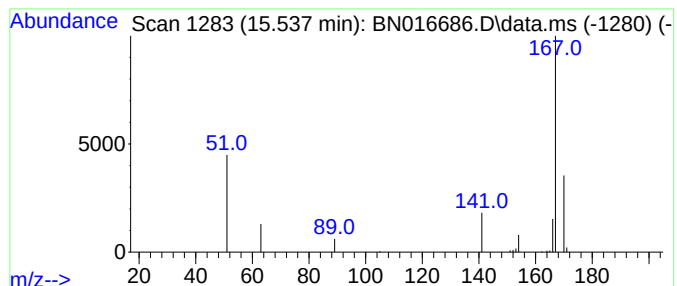
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.14 ng	67867	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19F04	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5N04	000097-51-8	5
4			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5			2-Azafluorene	167	C12H9N	000244-40-6	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016686.D
Acq On : 03 Oct 2021 00:22
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Misc :
ALS Vial : 54 Sample Multiplier: 1

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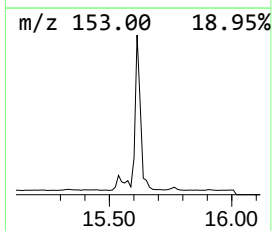
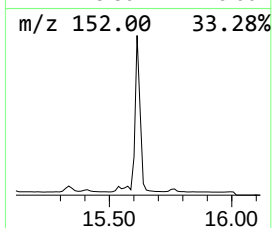
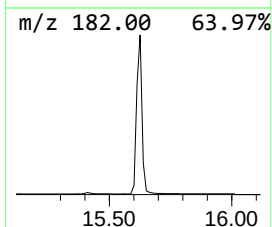
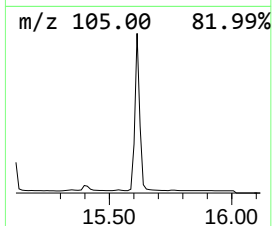
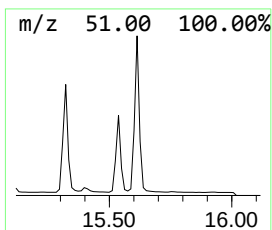
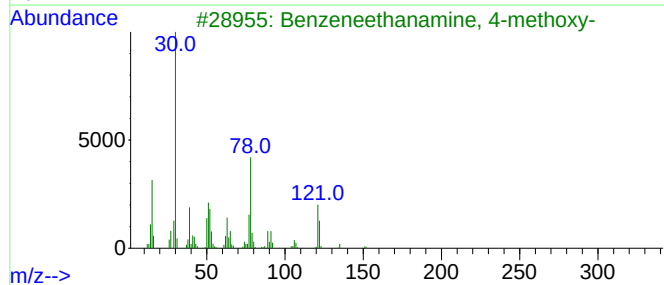
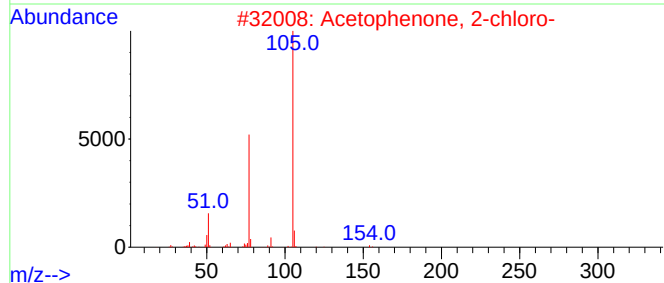
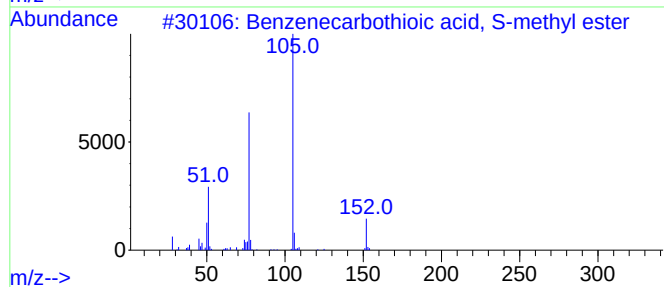
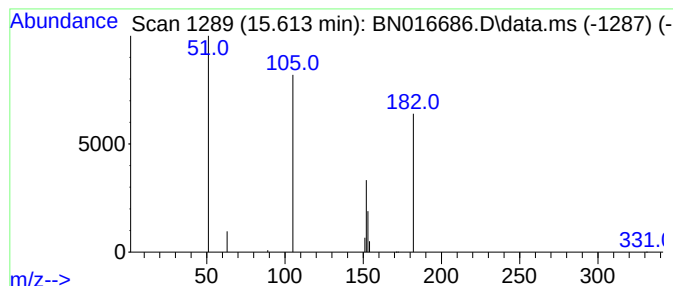
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzenecarbothioic acid, S-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.613	0.15 ng	74013	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	4
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	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



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Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

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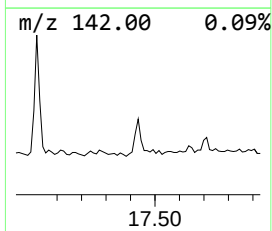
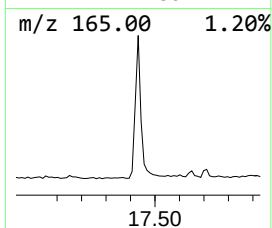
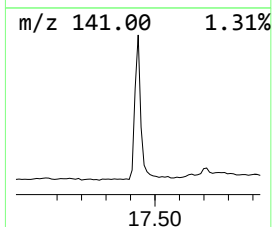
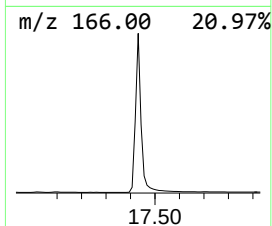
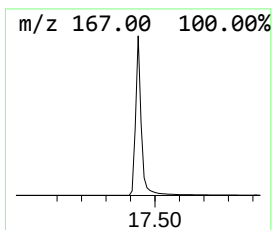
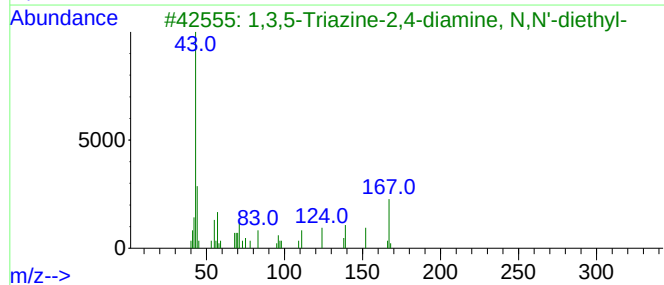
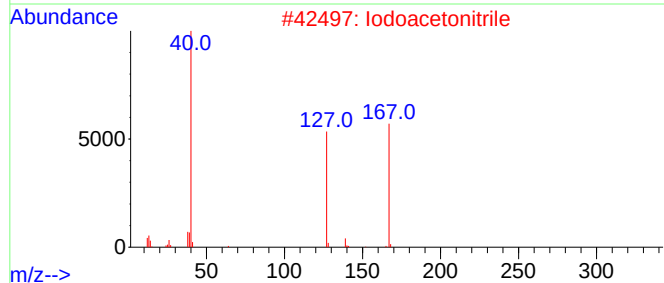
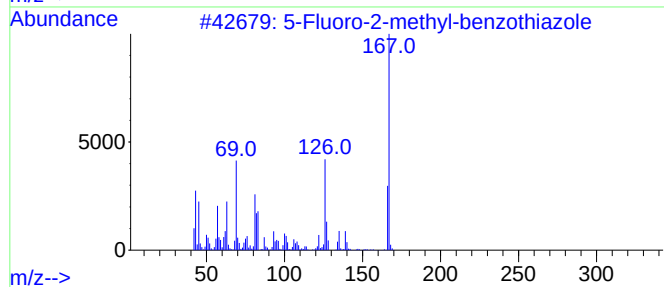
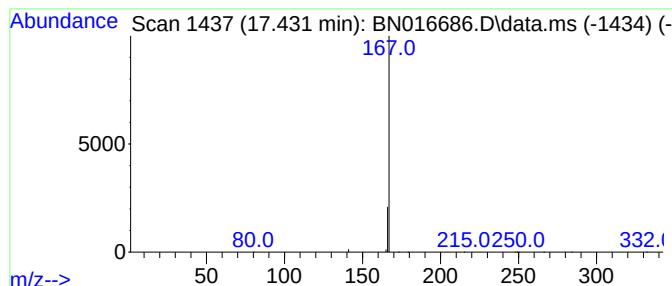
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.38 ng	156049	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Fluoro-2-methyl-benzothiazole	167	C8H6FN5	000399-75-7	5
2		Iodoacetoneitrile	167	C2H2IN	000624-75-9	4
3		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 : BN016686.D
Acq On : 03 Oct 2021 00:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

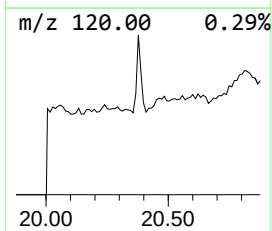
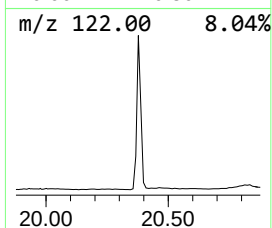
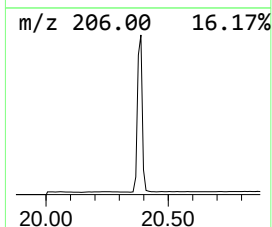
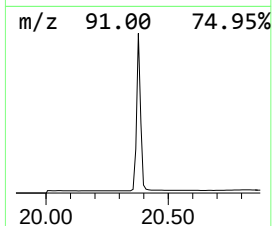
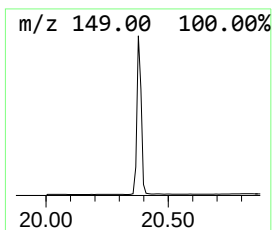
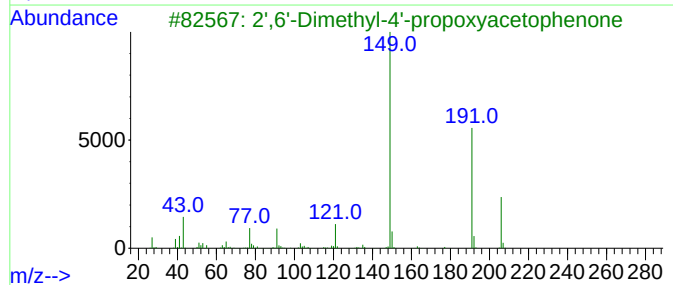
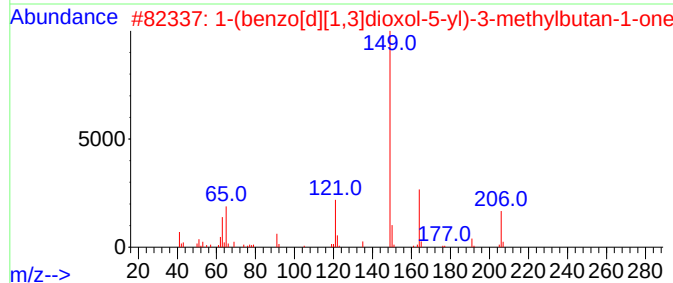
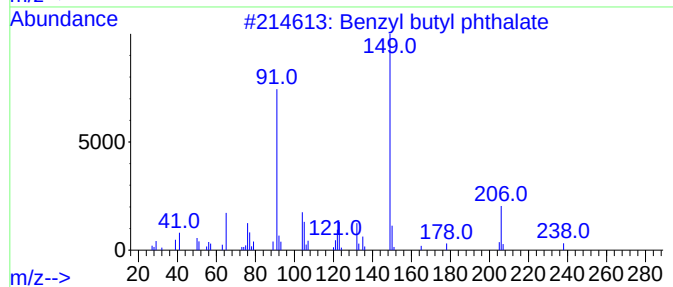
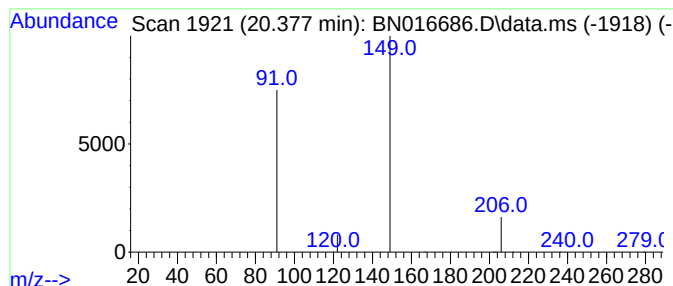
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.09 ng	107054	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',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4			2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	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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Misc :
ALS Vial : 54 Sample Multiplier: 1

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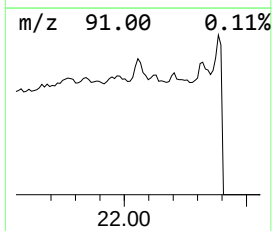
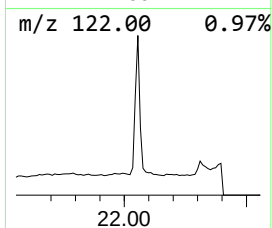
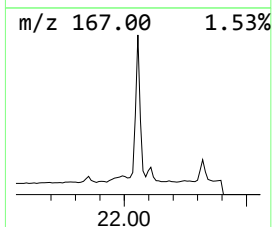
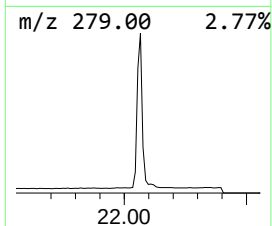
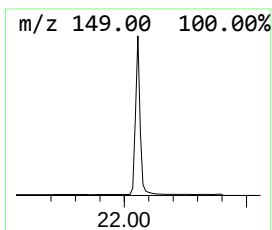
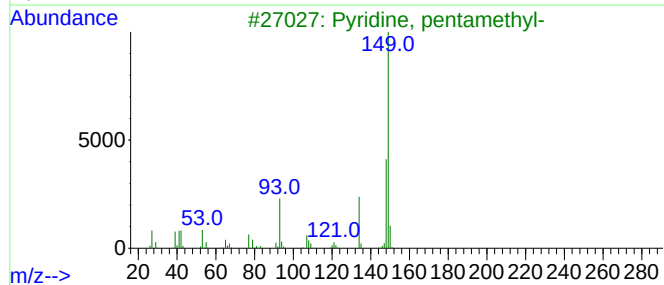
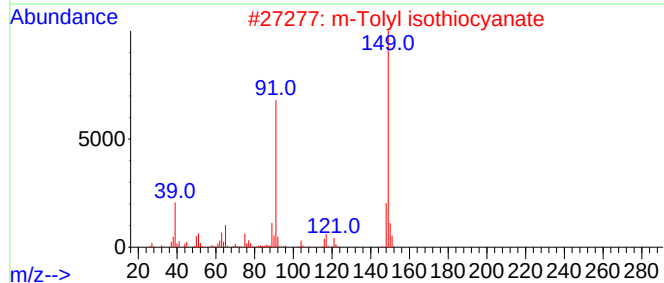
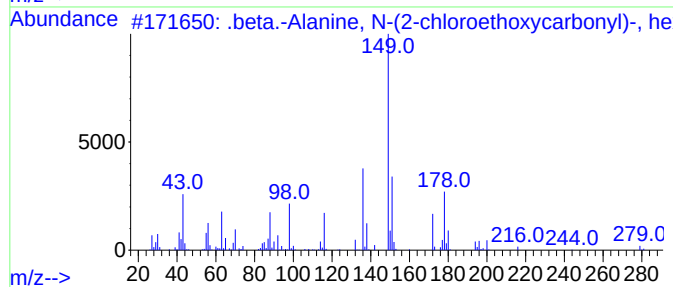
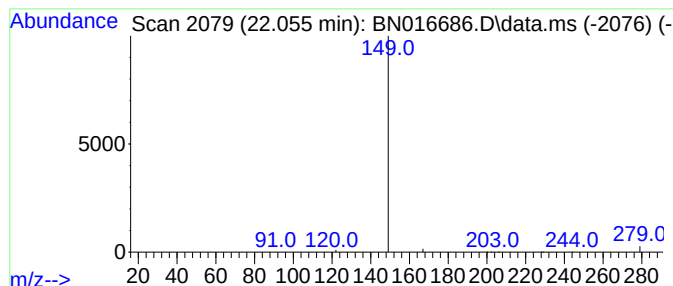
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.055	0.16 ng	182133	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		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



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 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 BNA_N
 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\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanamine, ...	6.978	0.1	ng	40313	1	7.642	116204	0.4
Ethyl Chloride	7.199	0.1	ng	33335	1	7.642	116204	0.4
4-Methyl-bi(1,2...	7.522	0.0	ng	14390	1	7.642	116204	0.4
6-Benzothiazola...	7.956	0.4	ng	104523	1	7.642	116204	0.4
Oxazolidine, 2,...	8.429	0.2	ng	55104	1	7.642	116204	0.4
Fomepizole	9.342	0.2	ng	91210	2	10.406	190717	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	28875	2	10.406	190717	0.4
p-Chloroaniline	10.571	0.1	ng	68578	2	10.406	190717	0.4
Methane, iodo-	11.709	0.1	ng	29314	2	10.406	190717	0.4
2-Propyl-4-meth...	12.296	0.4	ng	198979	2	10.406	190717	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	33680	3	14.268	199501	0.4
E-2-Propenoic a...	12.771	0.1	ng	29069	3	14.268	199501	0.4
Naphthalene, 2-...	13.139	0.3	ng	131746	3	14.268	199501	0.4
Benzene, 2-meth...	13.850	0.1	ng	33366	3	14.268	199501	0.4
Benzene, 1-meth...	14.636	0.1	ng	49108	3	14.268	199501	0.4
Succinic acid, ...	15.537	0.1	ng	67867	3	14.268	199501	0.4
Benzenecarbothi...	15.613	0.1	ng	74013	3	14.268	199501	0.4
5-Fluoro-2-meth...	17.431	0.4	ng	156049	4	17.017	166010	0.4
Benzyl butyl ph...	20.378	0.1	ng	107054	5	21.238	466385	0.4
.beta.-Alanine,...	22.055	0.2	ng	182133	5	21.238	466385	0.4