

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016676.D
 Acq On : 02 Oct 2021 18:21
 Operator : CG/JU
 Sample : PB139402BS
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139402BS

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: BN016676.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	7680	11004	2.04%	0.126%
2	3.281	20	22	38	rVB	5632	26451	4.90%	0.304%
3	3.595	51	56	77	rVB	6904	32757	6.06%	0.376%
4	5.264	231	237	253	rBV	15868	61557	11.39%	0.707%
5	6.822	401	406	418	rBV	26588	67723	12.54%	0.778%
6	6.979	418	423	429	rVV	19484	42419	7.85%	0.487%
7	7.080	429	434	440	rVV	39156	80992	14.99%	0.931%
8	7.200	440	447	459	rVB	13662	36073	6.68%	0.415%
9	7.523	478	482	489	rVB	7637	16690	3.09%	0.192%
10	7.642	490	495	506	rVB2	54289	132795	24.58%	1.526%
11	7.956	524	529	539	rVB2	52700	119474	22.12%	1.373%
12	8.168	547	552	557	rVV	3454	8293	1.54%	0.095%
13	8.430	571	577	585	rBV3	23494	54908	10.16%	0.631%
14	8.696	594	598	601	rBV	5445	10165	1.88%	0.117%
15	8.784	601	605	606	rBV	36170	69476	12.86%	0.798%
16	8.822	606	608	616	rVB	30568	57201	10.59%	0.657%
17	9.342	645	649	652	rBV	50639	86217	15.96%	0.991%
18	9.520	660	663	666	rBV	3445	6781	1.26%	0.078%
19	9.596	666	669	677	rVB	9509	16973	3.14%	0.195%
20	9.836	685	688	702	rVB	17200	30634	5.67%	0.352%
21	10.052	702	705	713	rVB	4453	9526	1.76%	0.109%
22	10.407	729	733	735	rBV	118735	215986	39.98%	2.482%
23	10.457	735	737	740	rVV	119896	196186	36.32%	2.254%
24	10.571	743	746	756	rVV	31781	69654	12.89%	0.800%
25	10.749	756	760	763	rVB	35937	61866	11.45%	0.711%
26	11.709	852	865	903	rBV	14714	28618	5.30%	0.329%
27	12.003	921	931	939	rBV	62901	102893	19.05%	1.182%
28	12.074	939	947	971	rVV	138574	229380	42.46%	2.636%
29	12.296	987	997	1021	rVV	141469	220647	40.84%	2.536%
30	12.696	1056	1059	1062	rBV	18850	31553	5.84%	0.363%
31	12.772	1062	1065	1071	rVB	13136	27569	5.10%	0.317%
32	12.886	1071	1074	1078	rBV	129363	218204	40.39%	2.507%
33	13.140	1090	1094	1097	rBV	85023	142827	26.44%	1.641%
34	13.736	1138	1141	1143	rBV	13290	18820	3.48%	0.216%
35	13.850	1147	1150	1153	rVB	21250	30938	5.73%	0.356%
36	13.939	1155	1157	1158	rBV	5960	9542	1.77%	0.110%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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37	13.990	1158	1161	1164	rVB	102418	171862	31.81%	1.975%
38	14.269	1180	1183	1185	rBV	153568	219203	40.58%	2.519%
39	14.332	1185	1188	1191	rVB	184264	269612	49.91%	3.098%
40	14.637	1209	1212	1220	rBV3	18263	48095	8.90%	0.553%
41	14.814	1224	1226	1230	rVV	5977	10336	1.91%	0.119%
42	14.903	1230	1233	1246	rVB	8449	14396	2.66%	0.165%
43	15.106	1246	1249	1252	rBV	9752	12613	2.33%	0.145%
44	15.322	1263	1266	1269	rBV2	258644	391736	72.51%	4.502%
45	15.411	1271	1273	1280	rVV2	3047	7543	1.40%	0.087%
46	15.538	1280	1283	1287	rVV	42683	70673	13.08%	0.812%
47	15.614	1287	1289	1298	rVV2	47039	72953	13.50%	0.838%
48	15.766	1298	1301	1311	rVB2	14591	24746	4.58%	0.284%
49	16.227	1334	1338	1341	rBV2	64454	102083	18.90%	1.173%
50	16.324	1343	1346	1349	rVV	52338	80431	14.89%	0.924%
51	16.506	1358	1361	1372	rBV	22746	38036	7.04%	0.437%
52	16.677	1372	1375	1384	rBV	20493	37432	6.93%	0.430%
53	17.018	1400	1403	1405	rBV	113614	180754	33.46%	2.077%
54	17.066	1405	1407	1410	rVV	164355	243228	45.02%	2.795%
55	17.151	1411	1414	1434	rVB	128580	208067	38.51%	2.391%
56	17.431	1434	1437	1453	rBV	95985	155998	28.88%	1.793%
57	18.016	1482	1485	1504	rVB6	6267	8284	1.53%	0.095%
58	19.063	1685	1696	1699	rBV	130259	186580	34.54%	2.144%
59	19.093	1699	1702	1747	rVB	216350	289947	53.67%	3.332%
60	19.460	1767	1776	1813	rBV	209726	292641	54.17%	3.363%
61	19.679	1813	1820	1848	rBV	119263	159837	29.59%	1.837%
62	20.378	1918	1921	1924	rBV	56892	66815	12.37%	0.768%
63	21.164	1992	1995	1997	rBV	55571	71218	13.18%	0.818%
64	21.217	1997	2000	2003	rVV2	233662	476680	88.24%	5.478%
65	21.270	2003	2005	2017	rVB	227351	306236	56.69%	3.519%
66	22.056	2076	2079	2082	rBV	77303	99861	18.49%	1.148%
67	22.807	2216	2229	2235	rBV	141436	236517	43.78%	2.718%
68	22.848	2235	2241	2289	rVB	151814	282553	52.30%	3.247%
69	23.385	2384	2398	2415	rBV	95423	214504	39.71%	2.465%
70	23.485	2416	2427	2475	rVB	113053	236462	43.77%	2.717%
71	24.087	2593	2603	2622	rBV	7990	15729	2.91%	0.181%
72	24.854	2816	2827	2850	rBV	8076	18824	3.48%	0.216%
73	25.774	3069	3096	3197	rBV3	134261	540224	100.00%	6.208%
74	26.456	3272	3295	3368	rBV	72780	249772	46.23%	2.870%
75	26.822	3388	3402	3434	rVB	2065	6959	1.29%	0.080%

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Integrator: RTE
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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

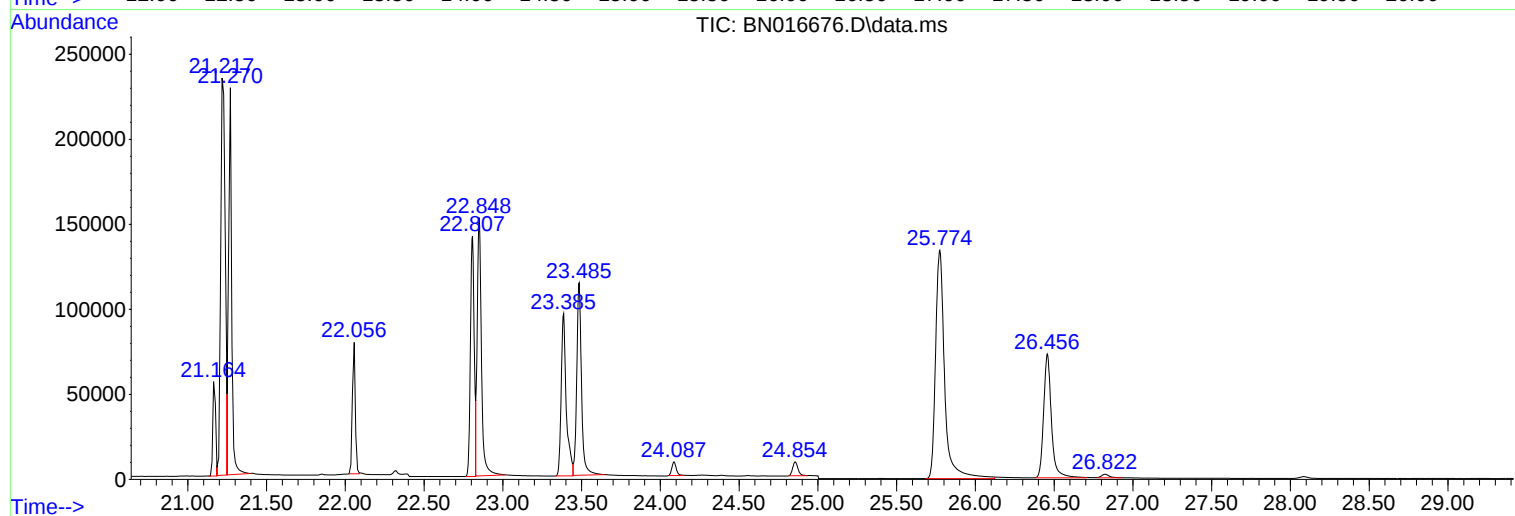
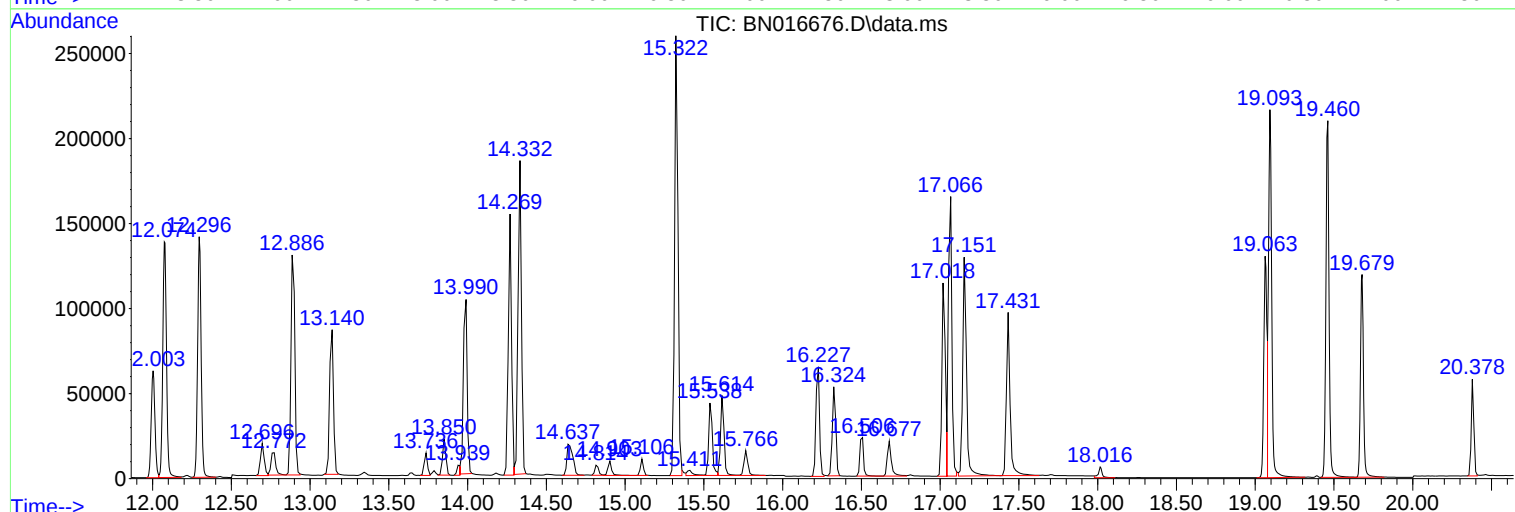
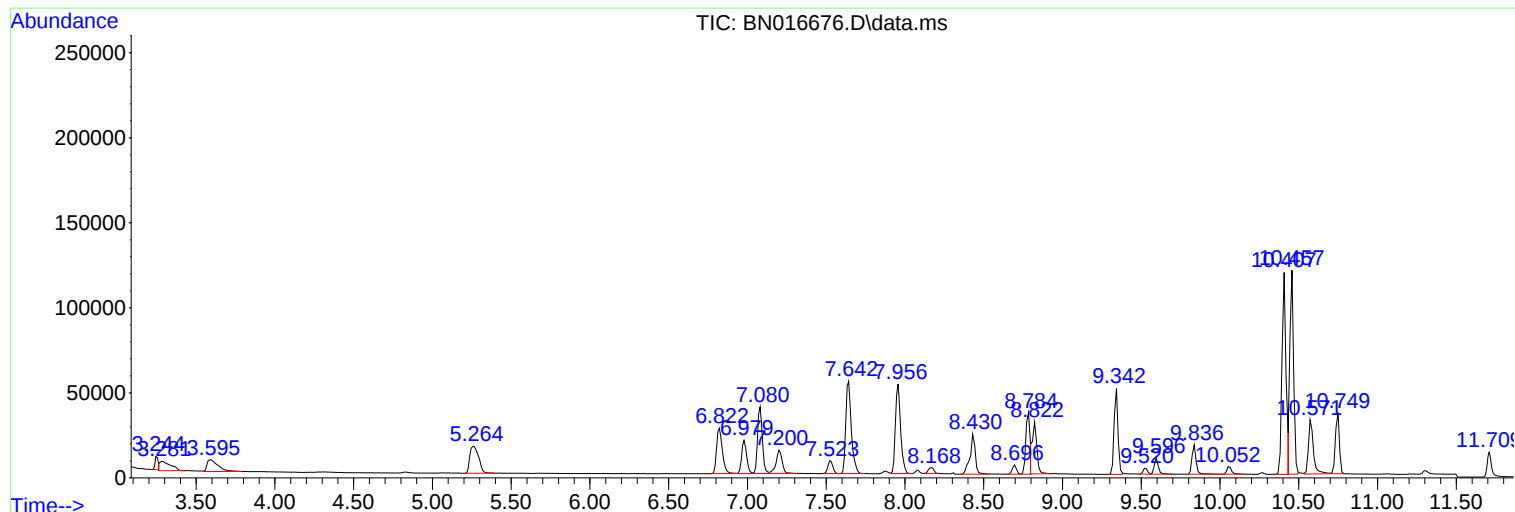
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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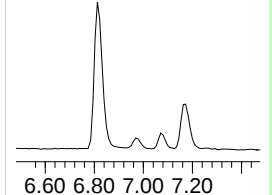
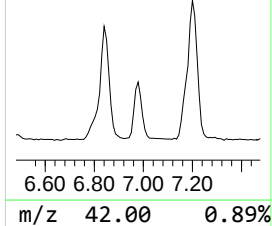
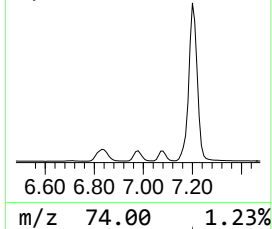
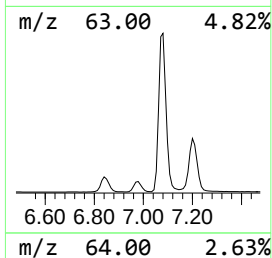
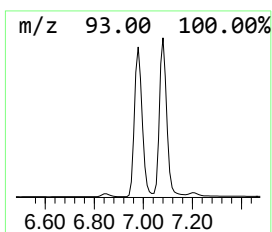
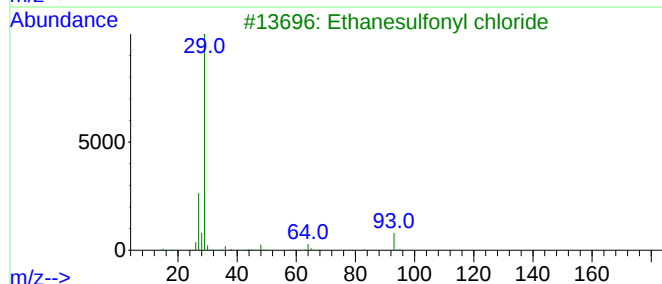
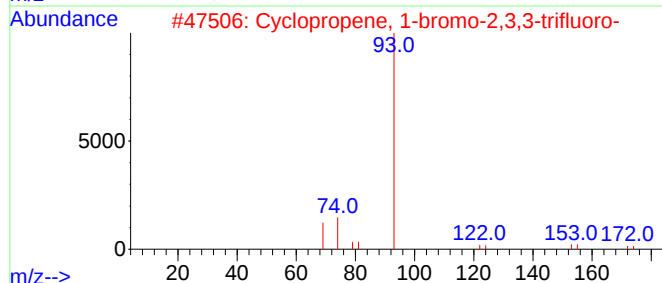
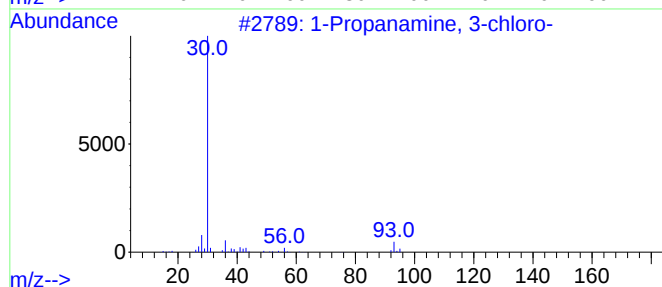
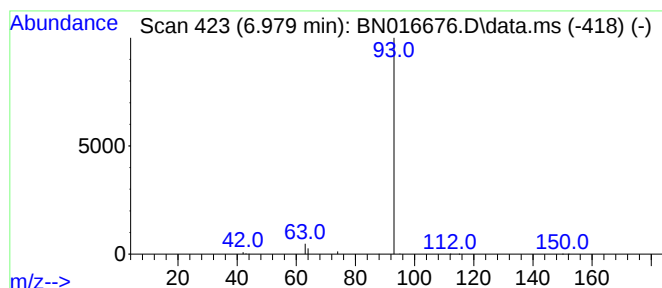
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.13 ng	42419	1,4-Dichlorobenzene-d4	7.642

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



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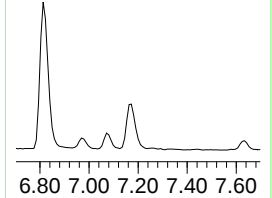
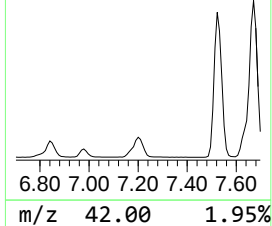
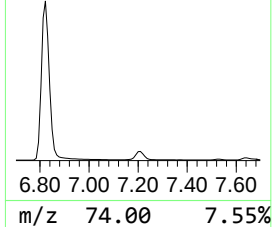
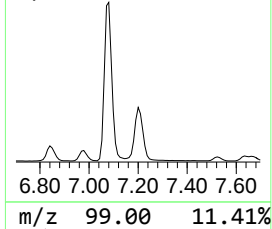
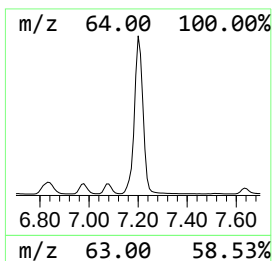
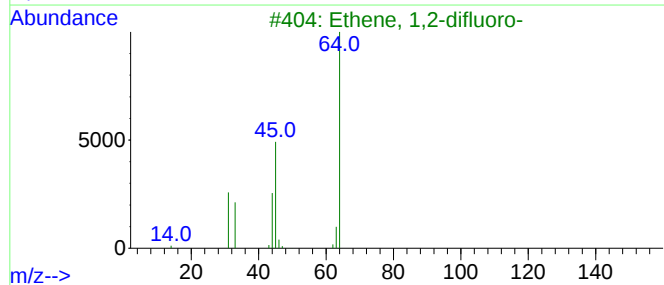
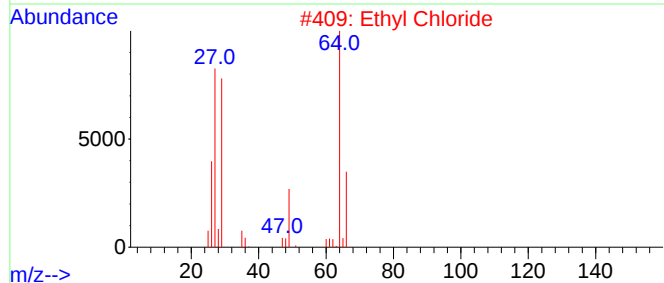
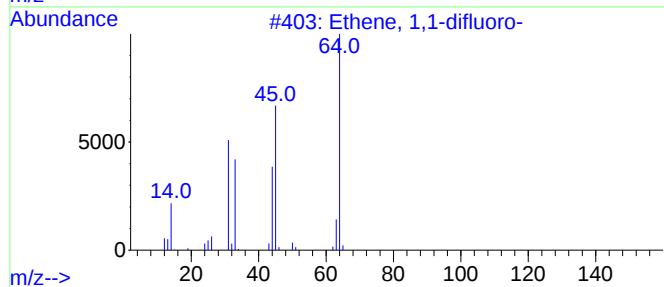
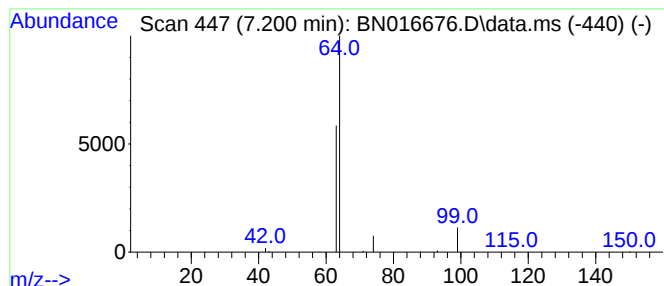
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	36073	1,4-Dichlorobenzene-d4	7.642

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



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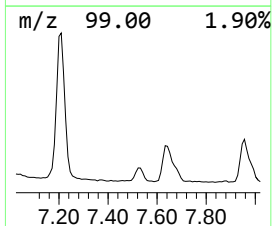
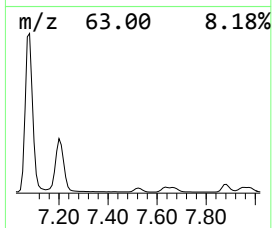
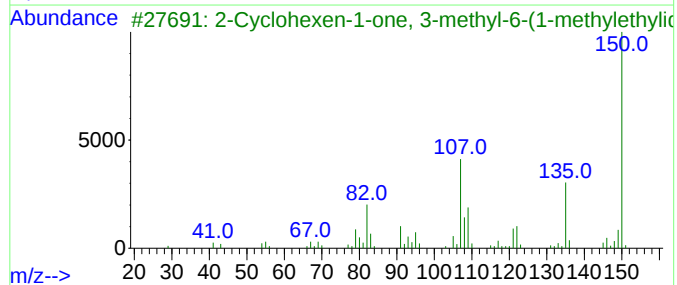
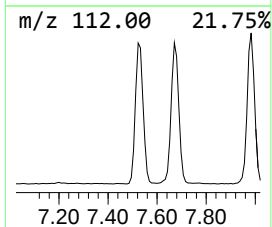
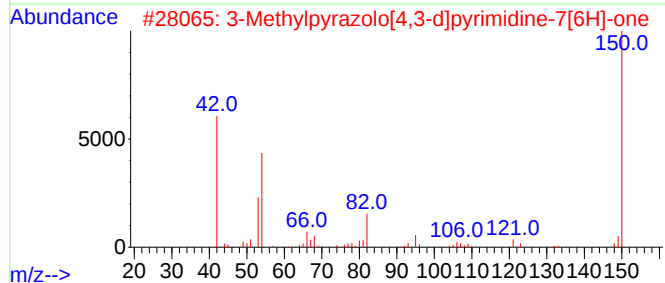
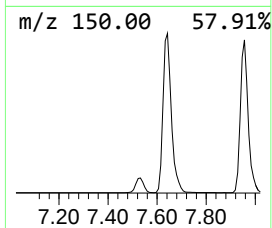
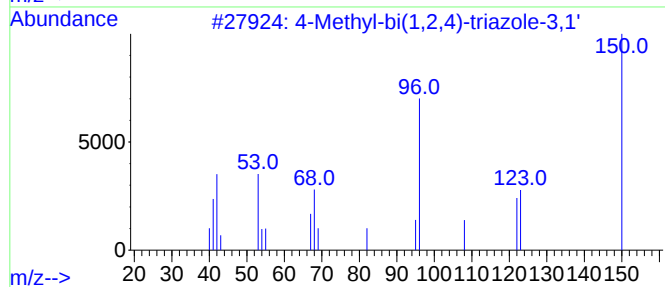
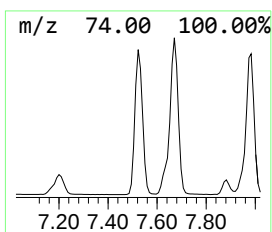
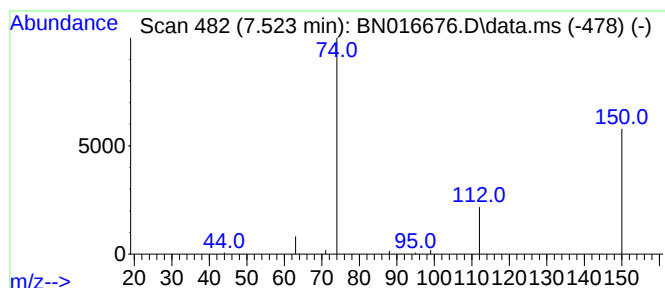
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	16690	1,4-Dichlorobenzene-d4	7.642

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



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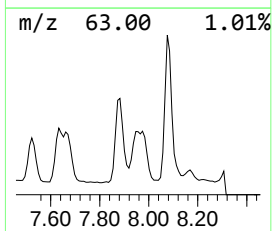
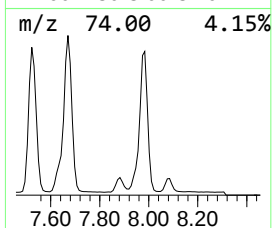
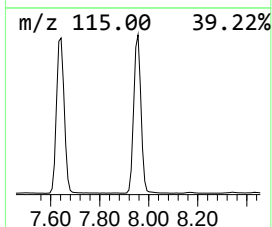
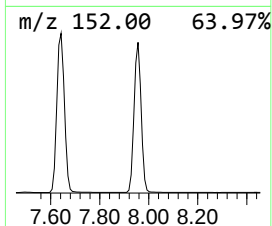
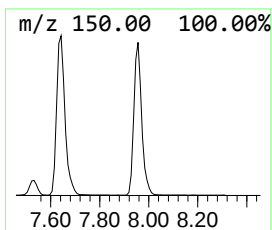
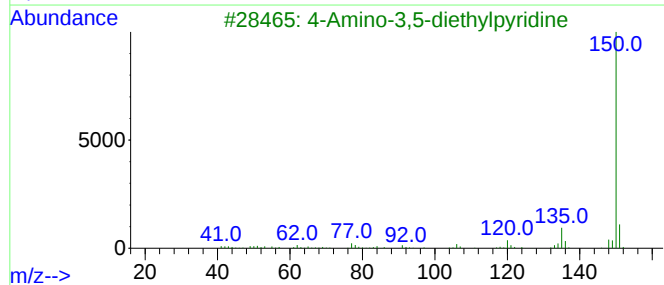
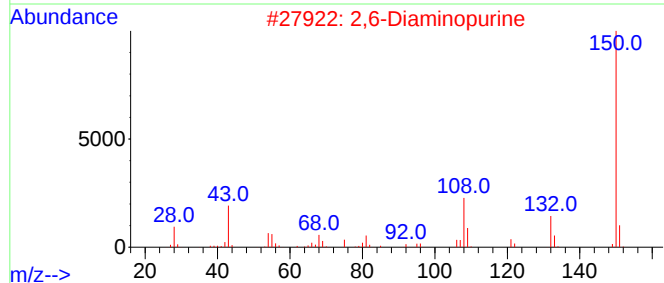
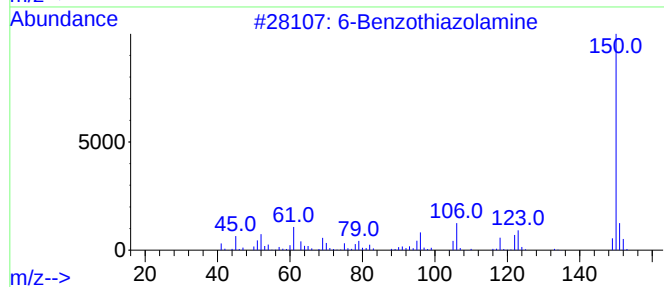
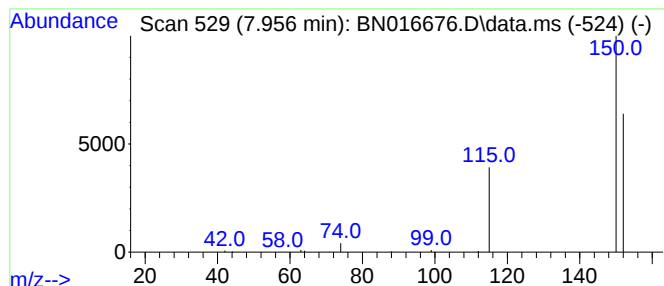
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	119474	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 : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

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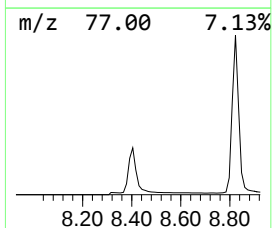
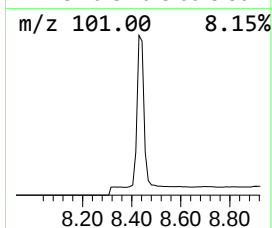
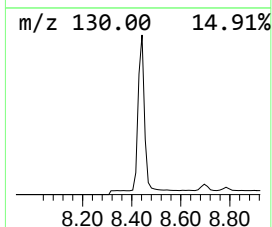
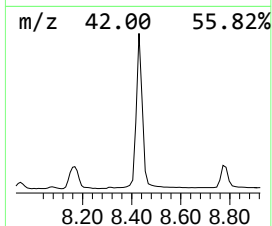
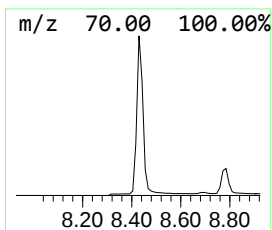
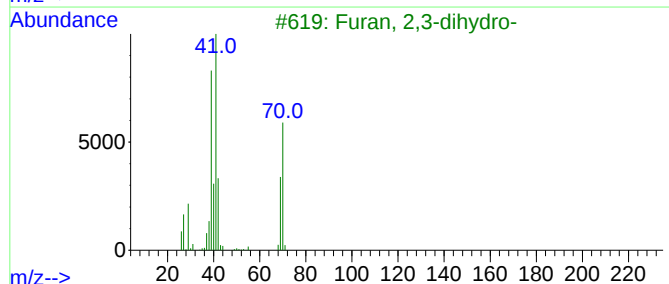
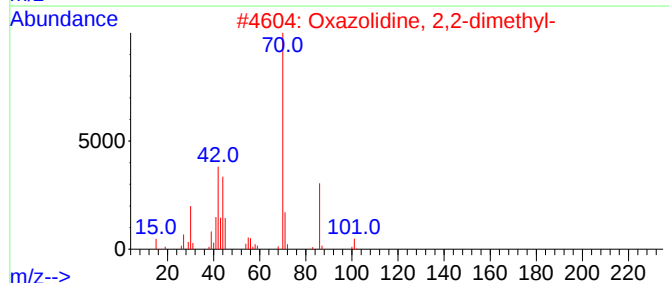
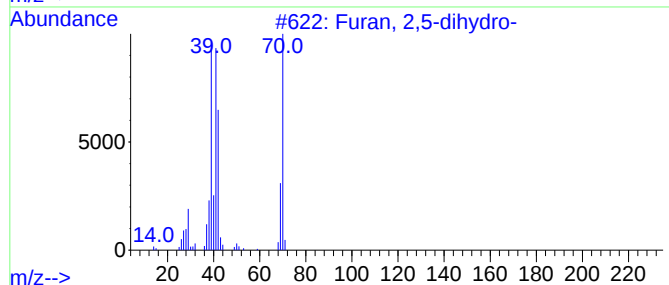
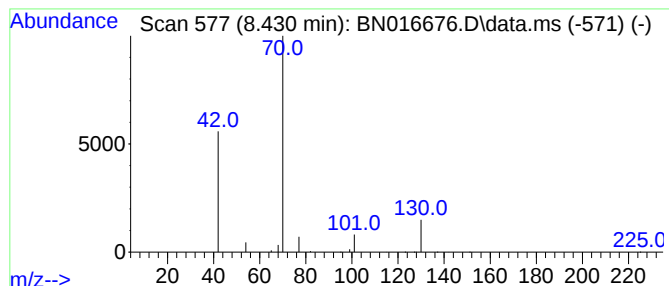
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.17 ng	54908	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 : BN016676.D
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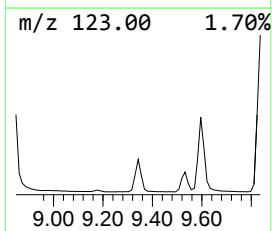
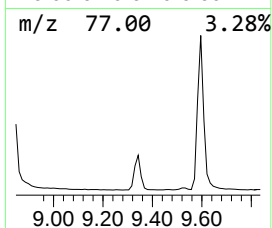
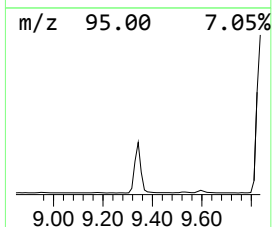
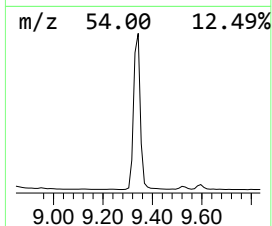
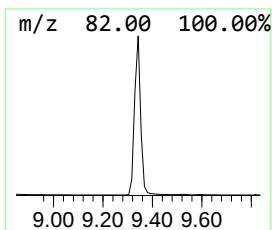
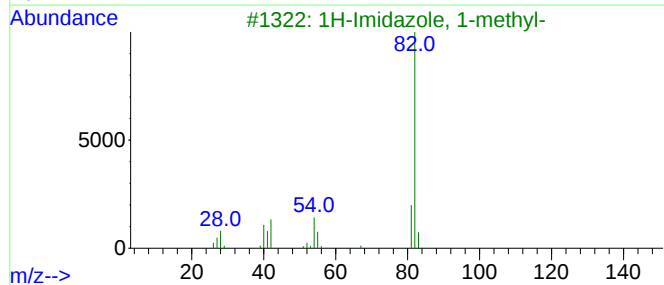
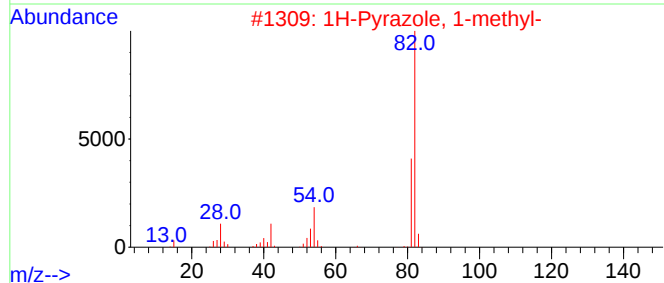
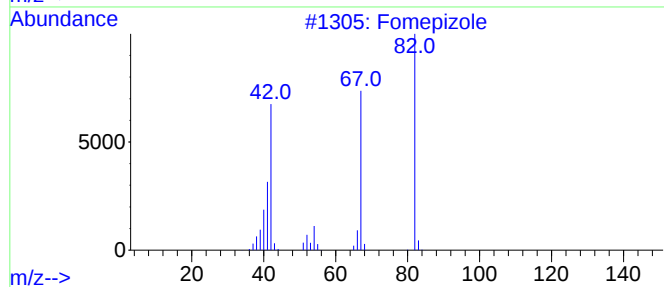
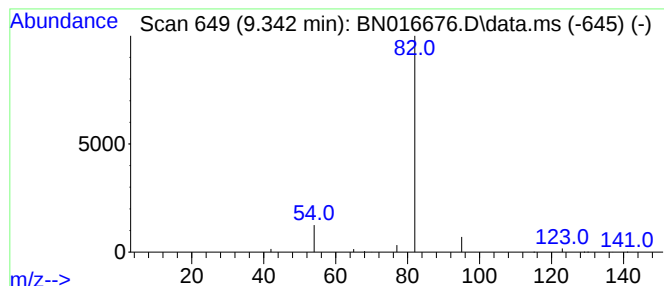
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	86217	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016676.D
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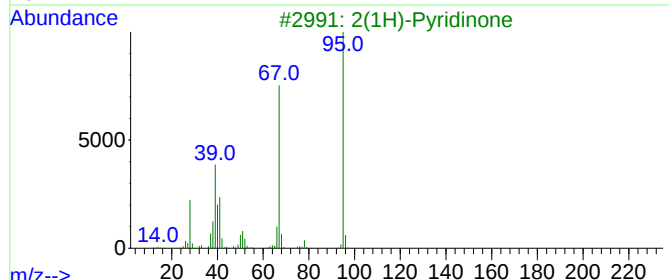
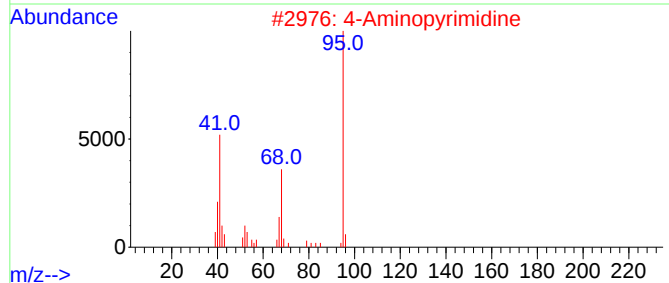
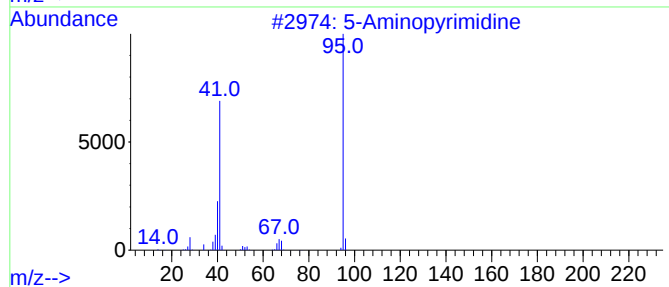
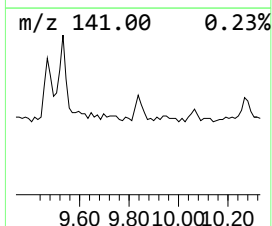
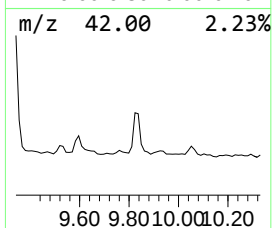
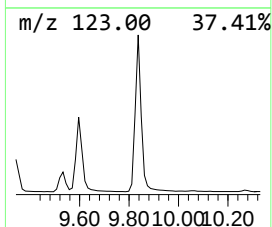
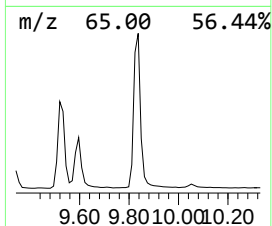
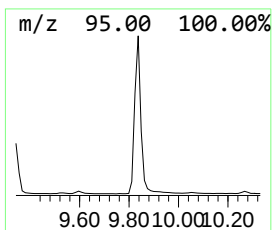
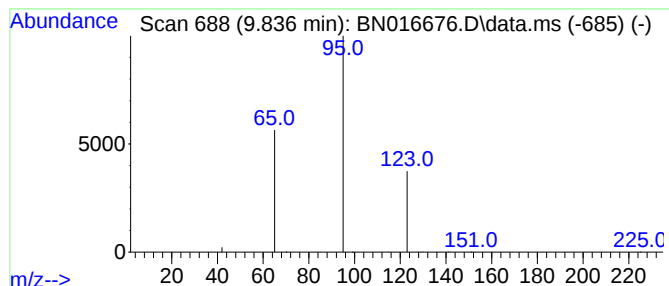
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Aminopyrimidine Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	30634	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\
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Acq On : 02 Oct 2021 18:21
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Misc :
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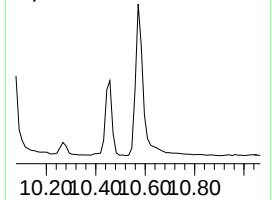
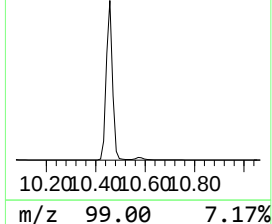
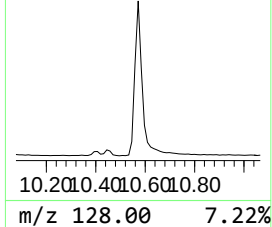
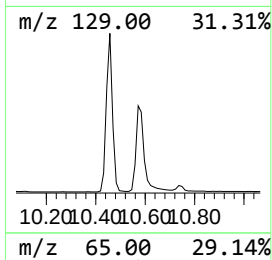
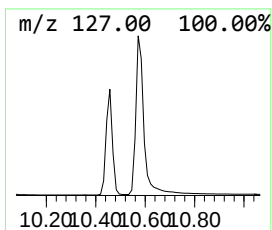
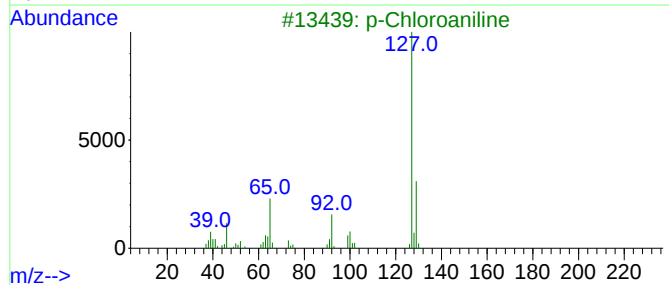
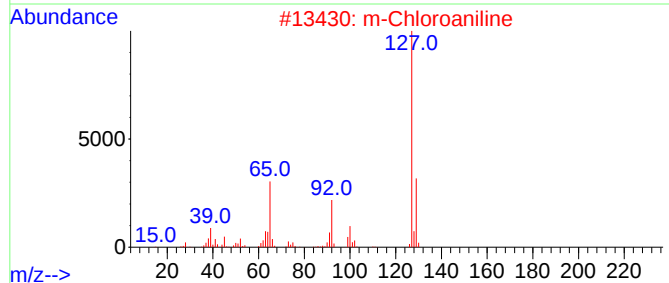
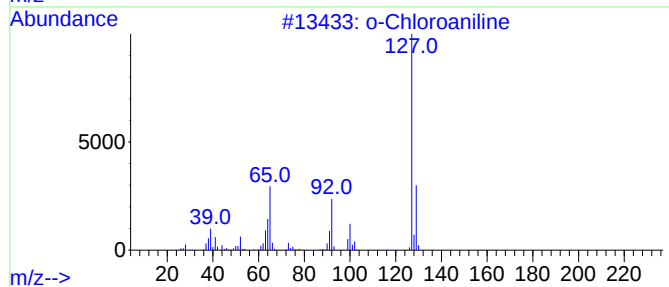
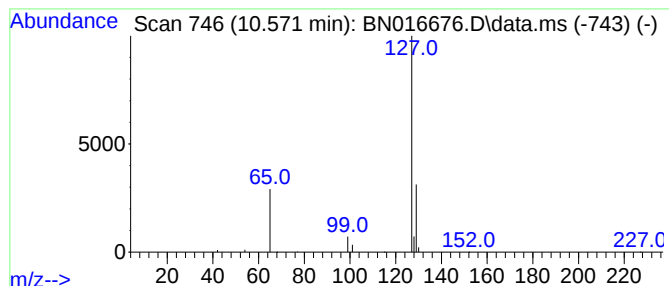
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.13 ng	69654	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Chloroaniline	127	C6H6ClN	000095-51-2	90
2			m-Chloroaniline	127	C6H6ClN	000108-42-9	90
3			p-Chloroaniline	127	C6H6ClN	000106-47-8	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 : BN016676.D
Acq On : 02 Oct 2021 18:21
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Misc :
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ClientSampleId :
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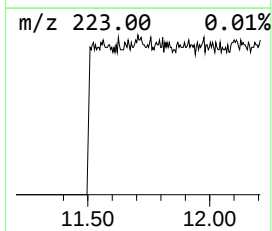
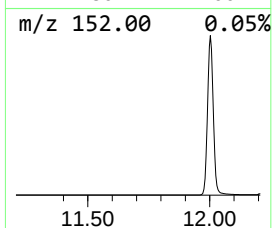
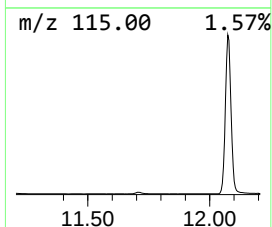
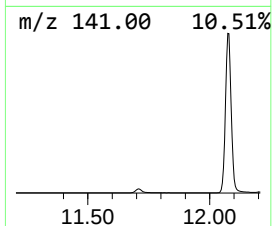
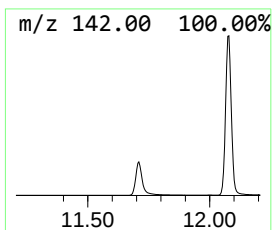
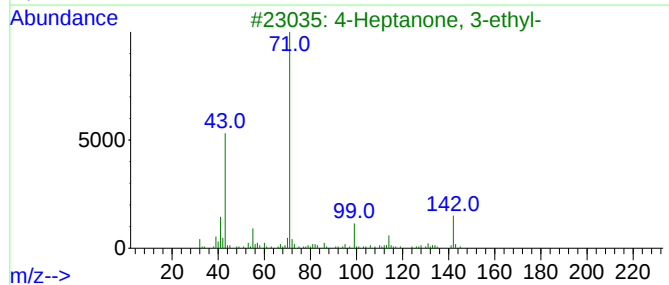
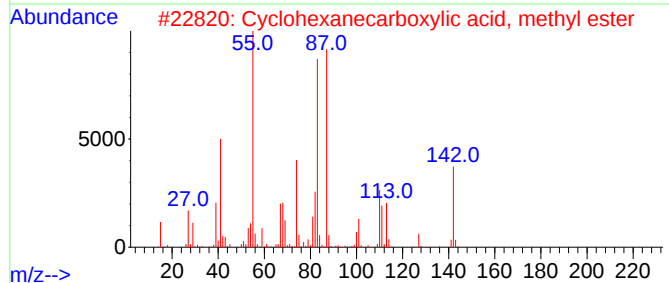
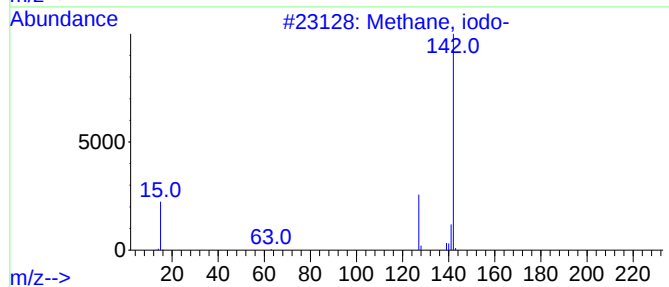
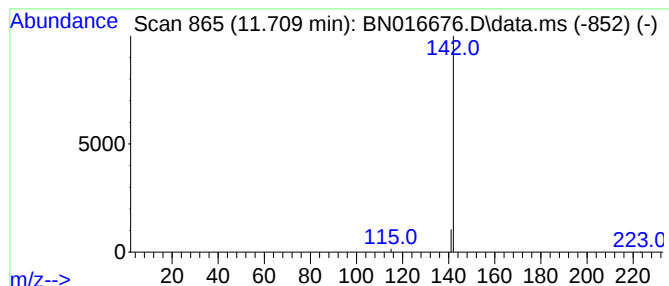
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	28618	Naphthalene-d8	10.407

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



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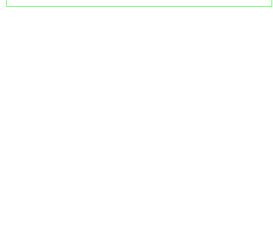
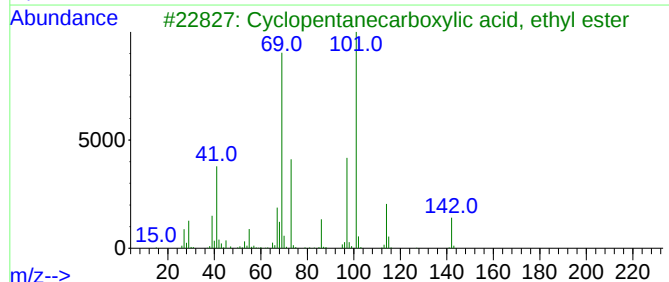
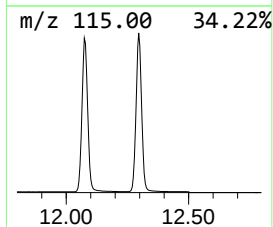
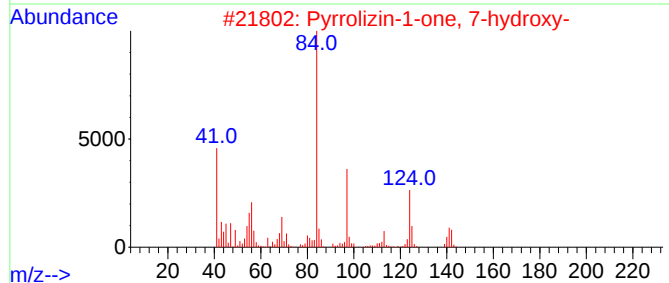
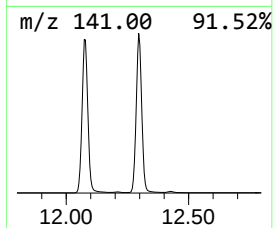
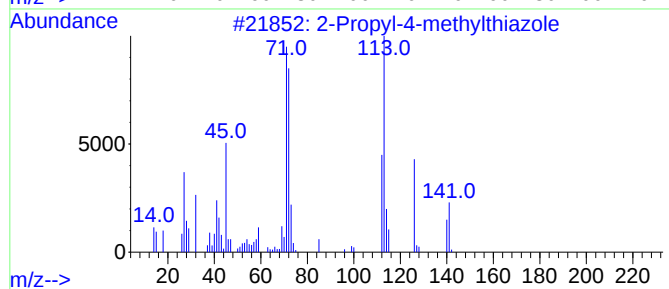
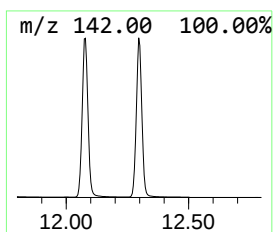
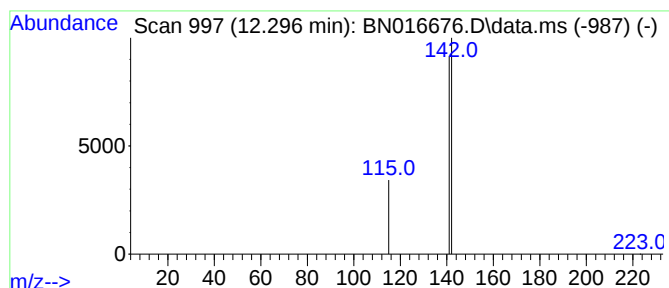
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.41 ng	220647	Naphthalene-d8	10.407	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



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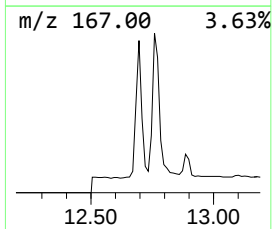
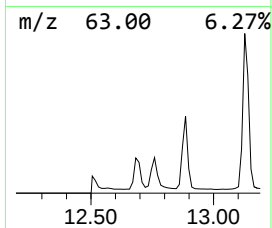
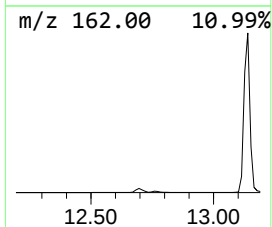
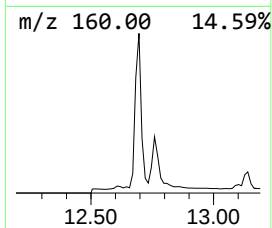
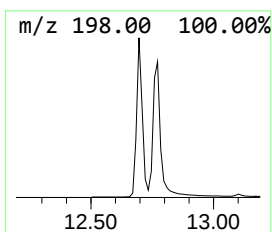
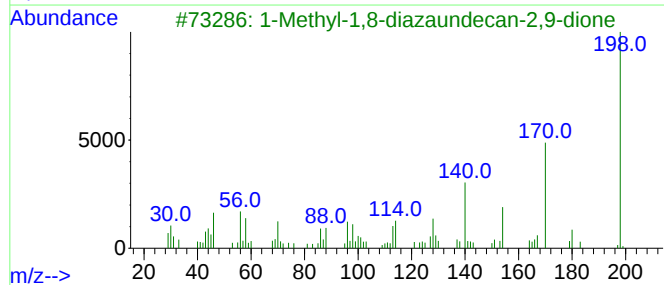
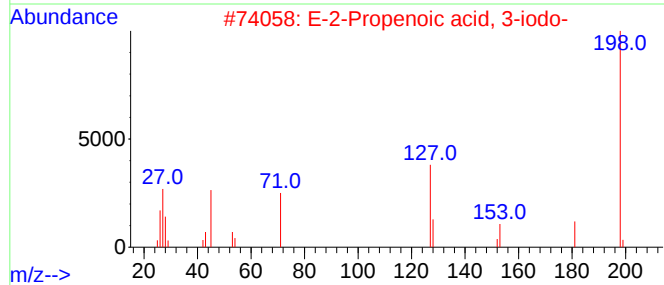
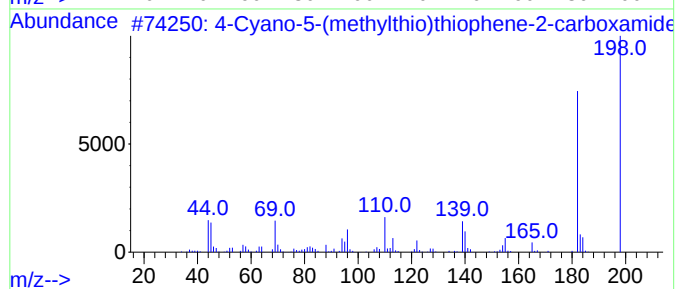
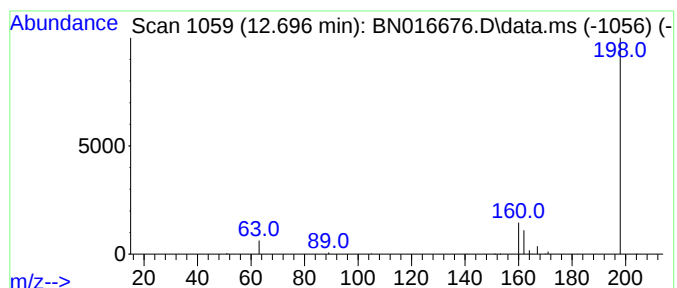
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	31553	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 : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

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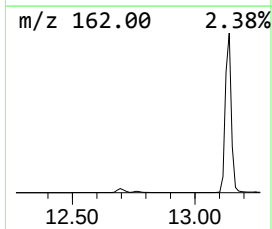
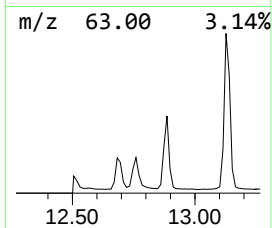
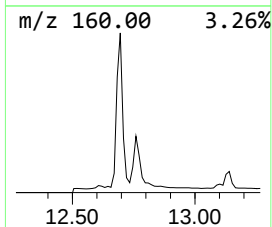
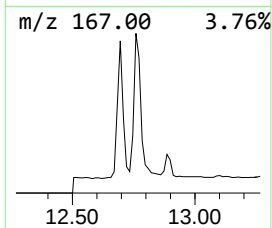
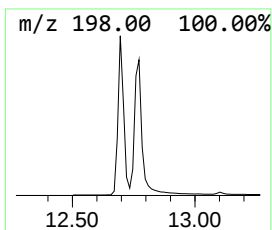
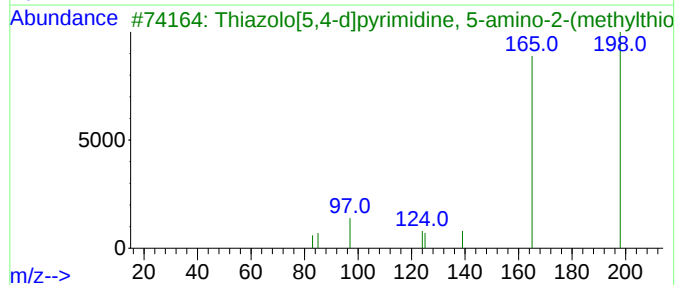
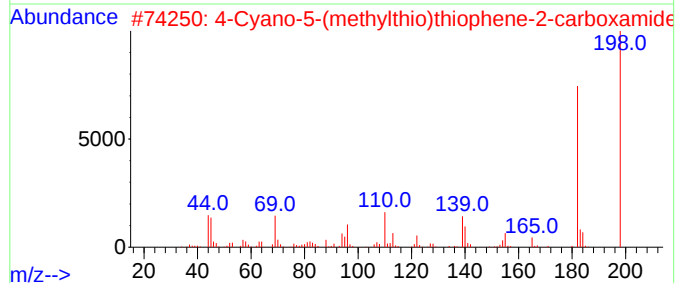
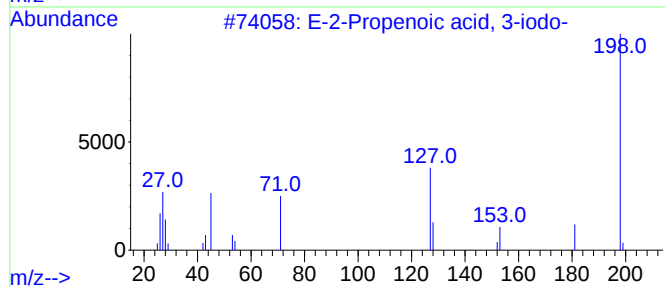
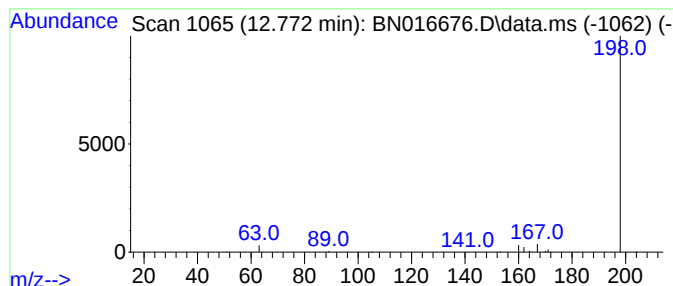
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.05 ng	27569	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

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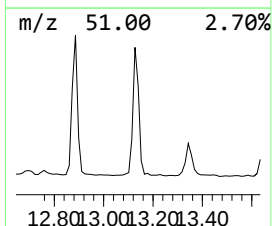
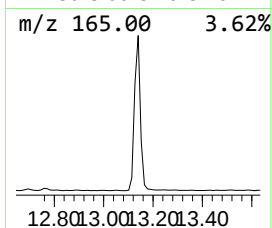
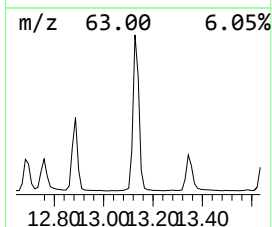
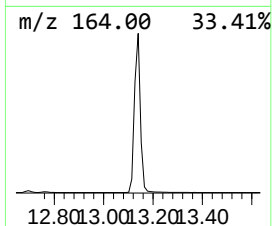
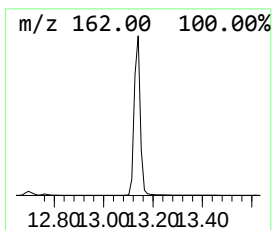
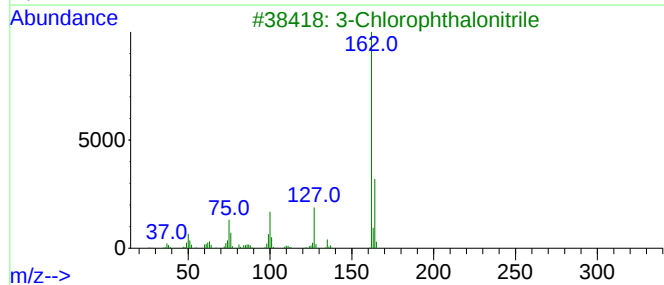
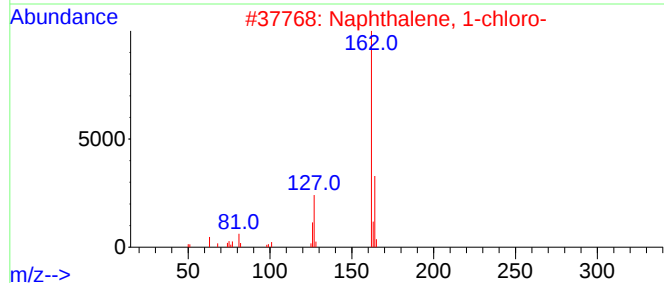
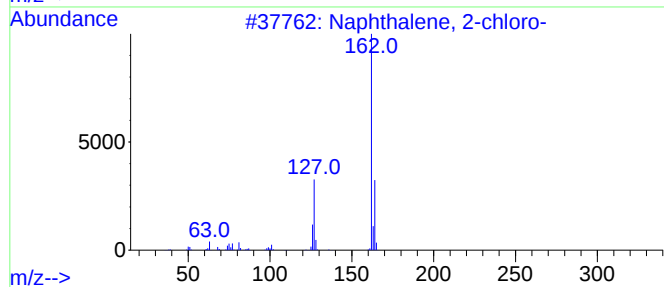
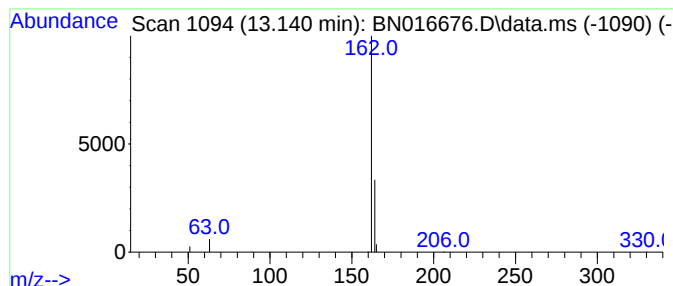
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.26 ng	142827	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	74
2			Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
3			3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
4			2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
5			2-Amino-4-chloro-1,3-thiazole-5-...	162	C4H3ClN2OS	076874-79-8	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016676.D
Acq On : 02 Oct 2021 18:21
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Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

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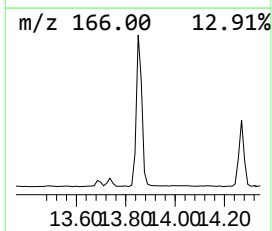
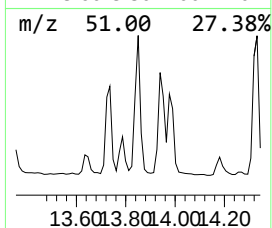
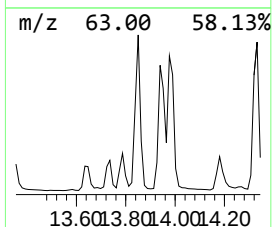
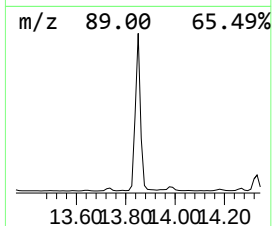
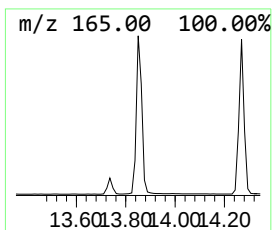
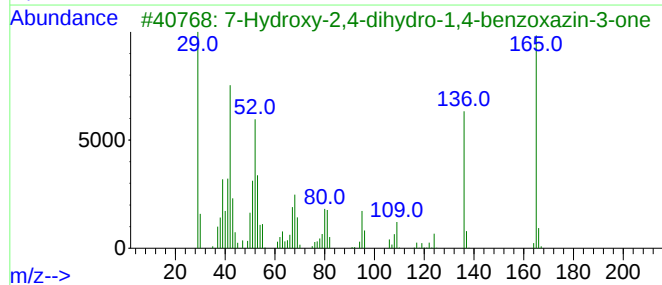
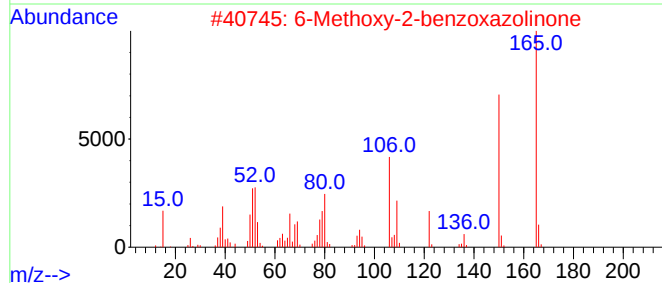
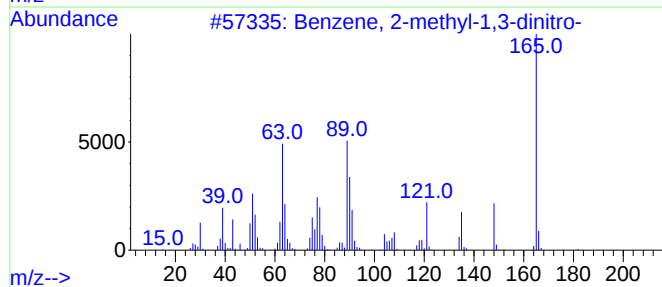
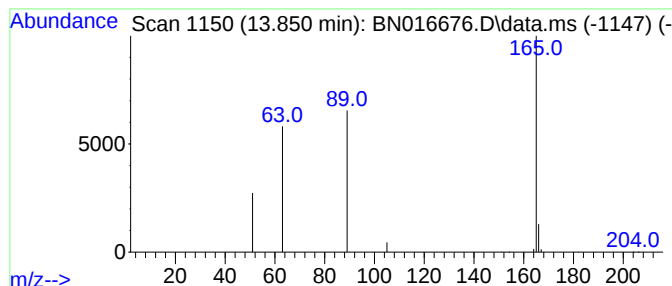
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.06 ng	30938	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	83
2			6-Methoxy-2-benzoxazolinone	165	C8H7NO3	000532-91-2	9
3			7-Hydroxy-2,4-dihydro-1,4-benzox...	165	C8H7NO3	067193-97-9	9
4			Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9
5			Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

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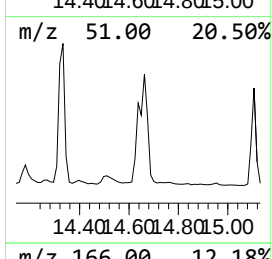
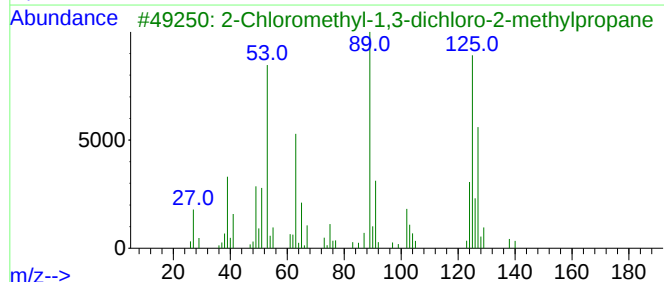
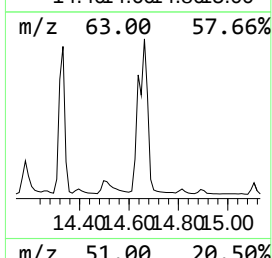
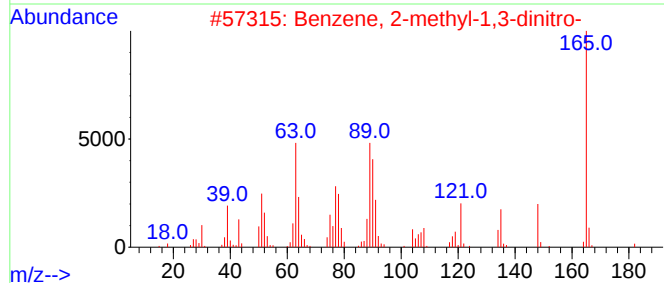
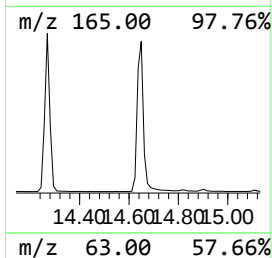
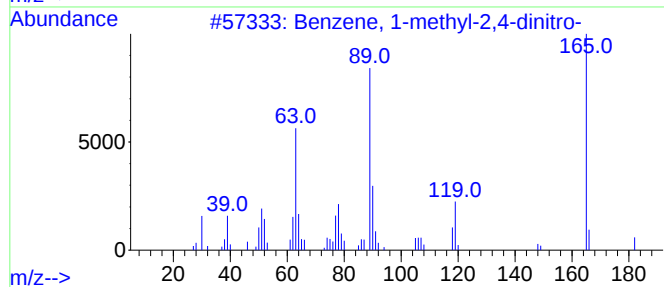
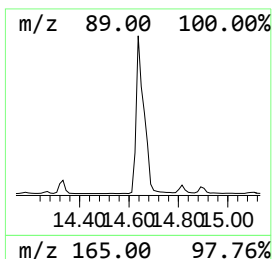
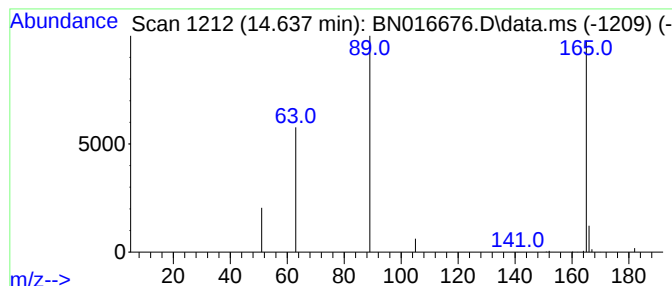
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	48095	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\
Data File : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB139402BS

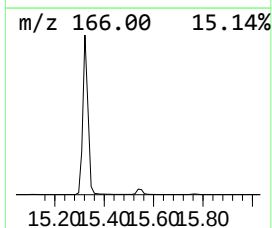
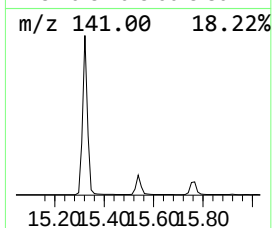
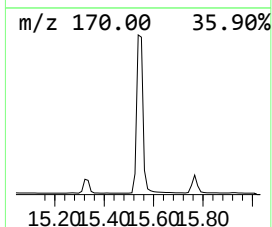
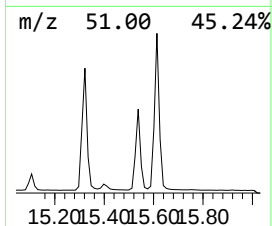
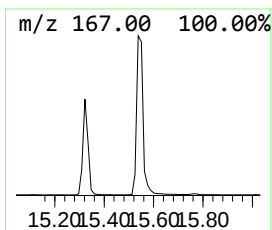
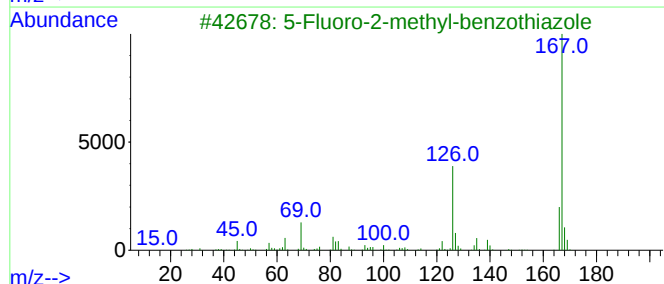
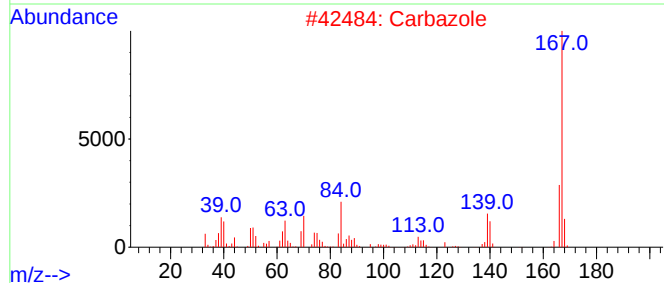
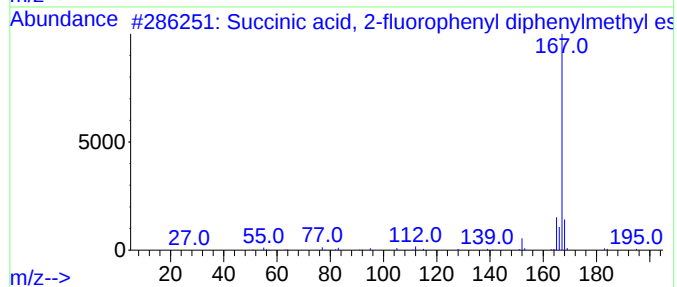
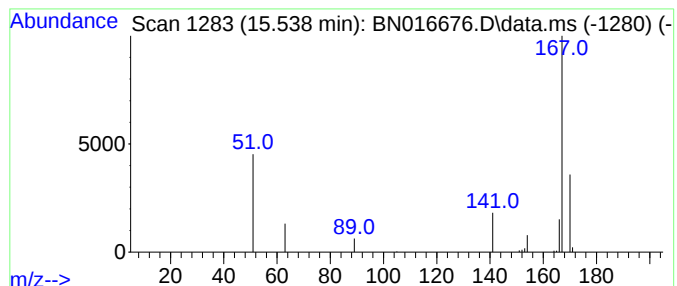
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	70673	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19F04	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5			3,5-Pyridinedicarboxylic acid	167	C7H5NO4	000499-81-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 44 Sample Multiplier: 1

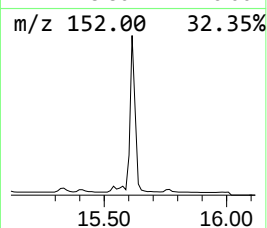
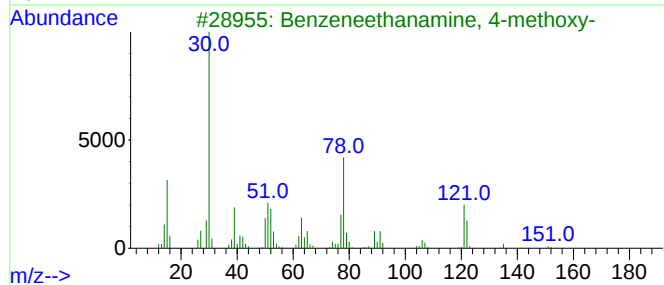
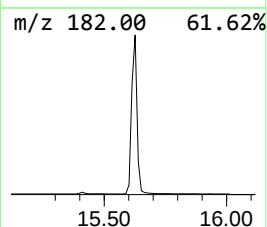
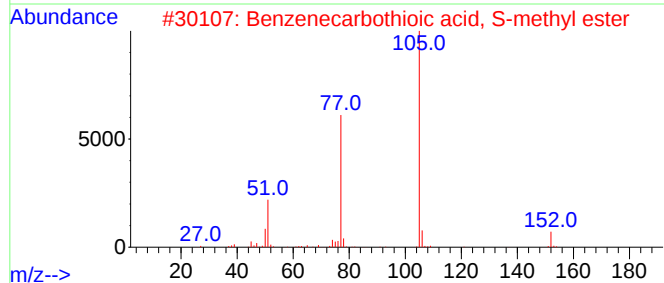
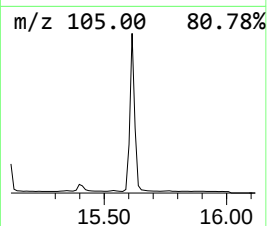
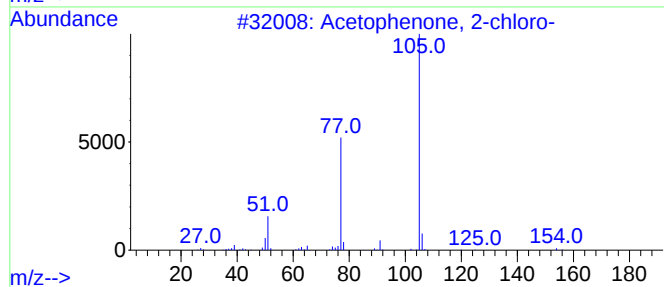
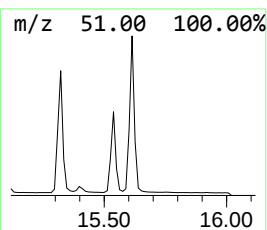
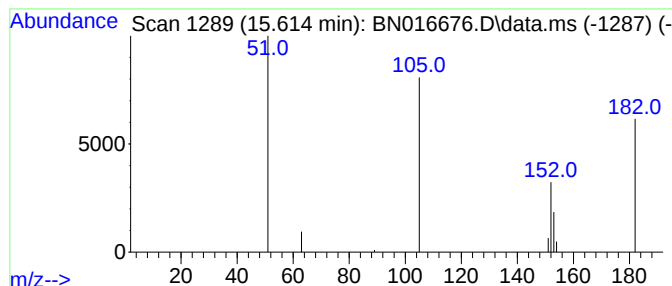
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.614	0.13 ng	72953	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	Propionlonitrile		51	C3HN	001070-71-9	3
5	Propanal, 2-(benzoyloxy)-, (R)-		178	C10H10O3	078871-04-2	2



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Data File : BN016676.D
Acq On : 02 Oct 2021 18:21
Operator : CG/JU
Sample : PB139402BS
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139402BS

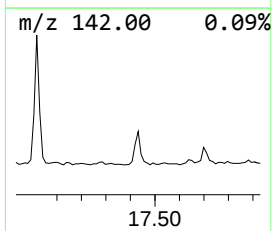
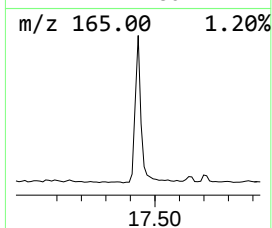
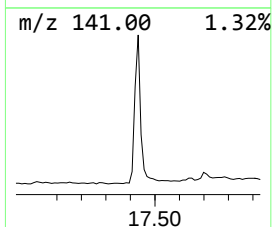
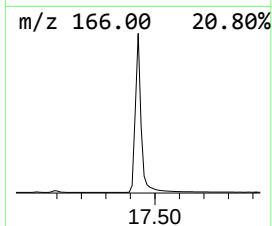
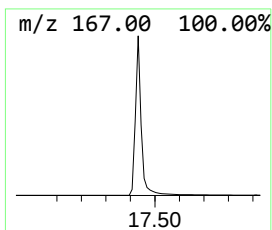
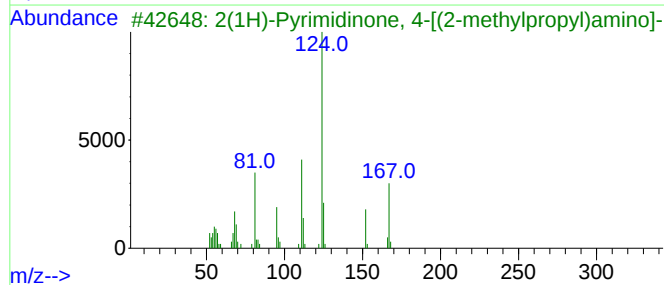
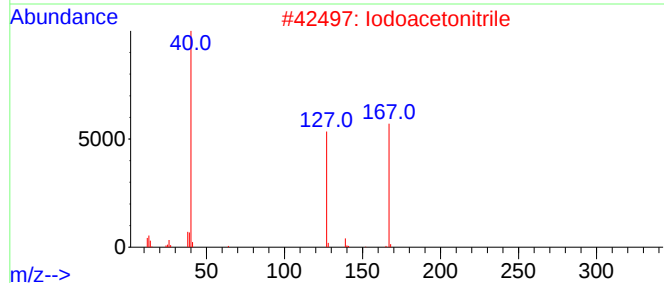
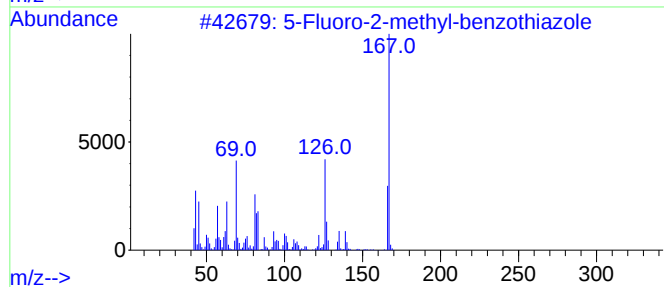
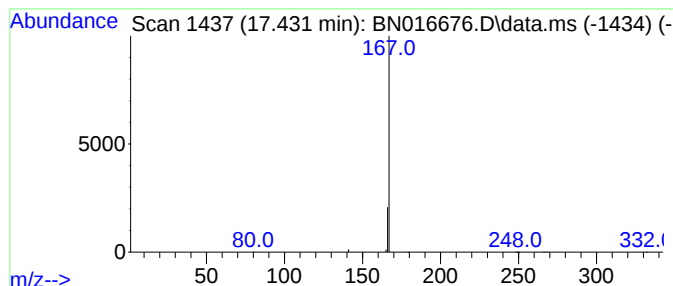
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.35 ng	155998	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		2(1H)-Pyrimidinone, 4-[(2-methyl...	167	C8H13N3O	119608-70-7	4
4		1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
5		1-Cyclopropanecarbonylpiperidin...	167	C9H13NO2	063463-43-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016676.D
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Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139402BS

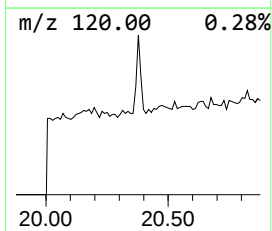
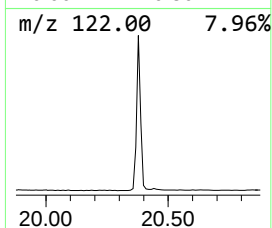
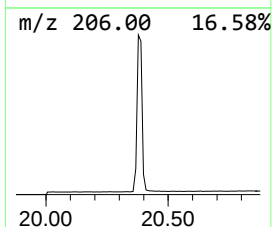
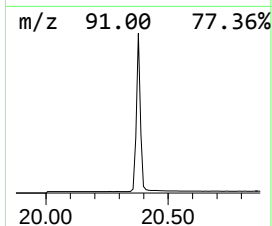
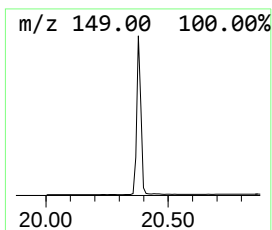
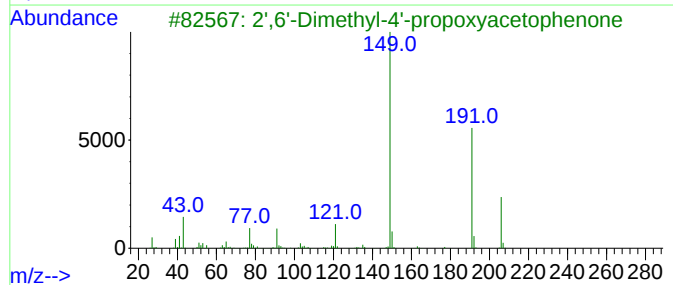
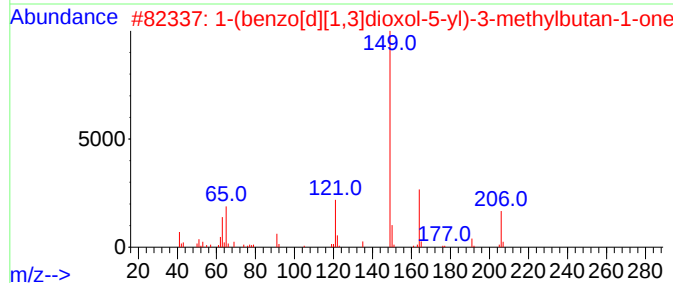
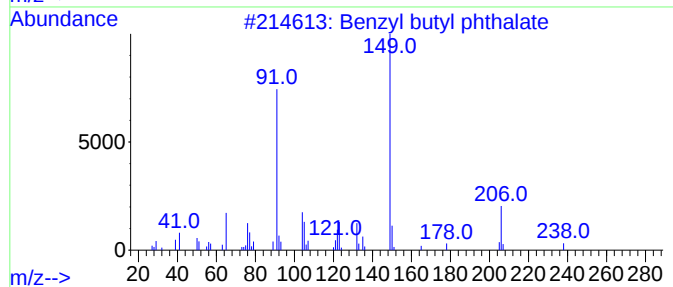
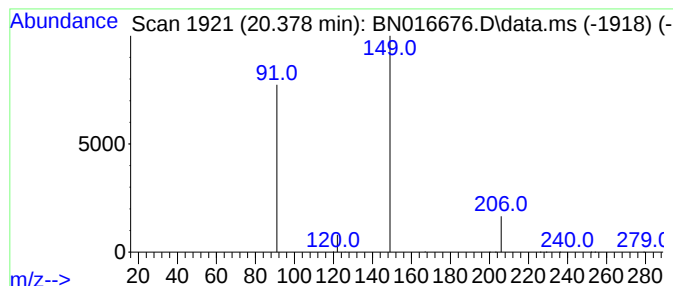
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	66815	Chrysene-d12	21.227

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 44 Sample Multiplier: 1

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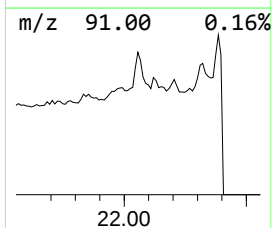
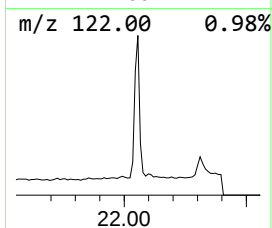
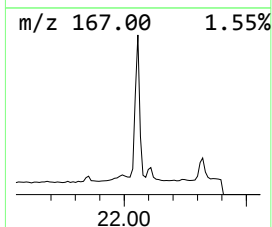
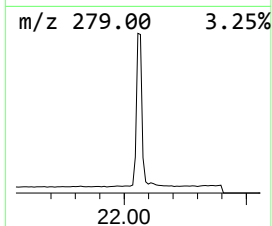
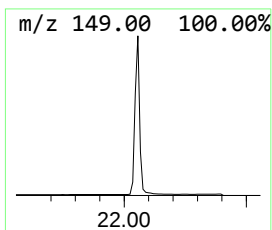
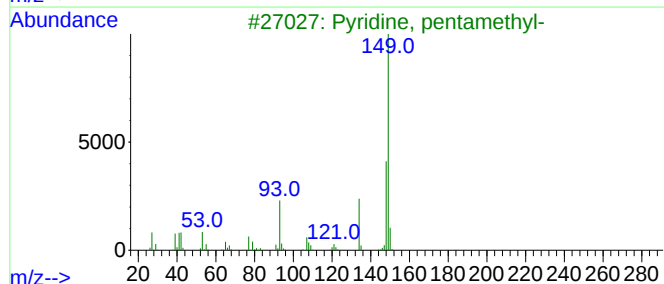
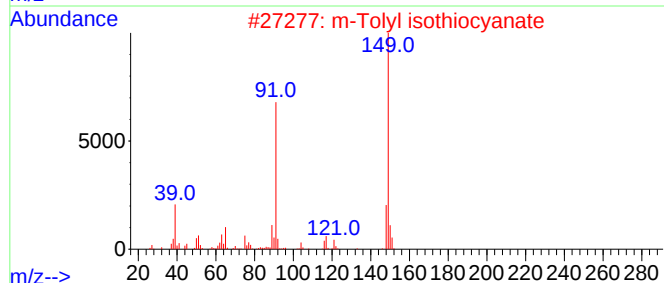
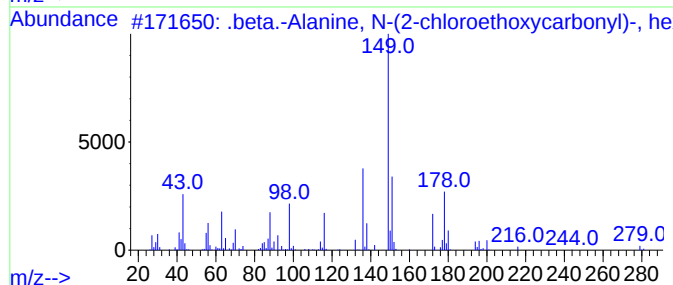
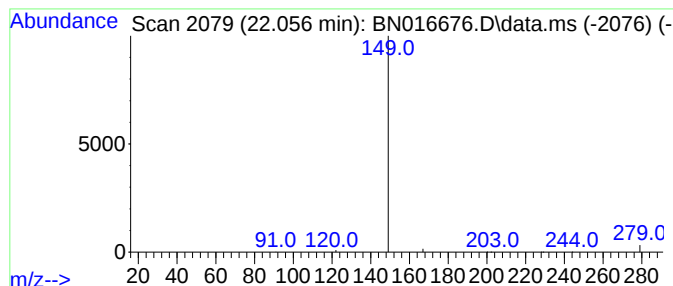
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	99861	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	m-Tolyl		isothiocyanate	149	C8H7NS	000621-30-7	4
3	Pyridine, pentamethyl-			149	C10H15N	003748-83-2	4
4	Phthalic acid, 7-bromoheptyl oct...			454	C23H35BrO4	1000415-52-2	4
5	Benzene, 1-isothiocyanato-4-methyl-			149	C8H7NS	000622-59-3	4



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 Sample : PB139402BS
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
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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, ...	6.979	0.1	ng	42419	1	7.642	132795	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	36073	1	7.642	132795	0.4
4-Methyl-bi(1,2...	7.523	0.1	ng	16690	1	7.642	132795	0.4
6-Benzothiazola...	7.956	0.4	ng	119474	1	7.642	132795	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	54908	1	7.642	132795	0.4
Fomepizole	9.342	0.2	ng	86217	2	10.407	215986	0.4
5-Aminopyrimidine	9.836	0.1	ng	30634	2	10.407	215986	0.4
o-Chloroaniline	10.572	0.1	ng	69654	2	10.407	215986	0.4
Methane, iodo-	11.709	0.1	ng	28618	2	10.407	215986	0.4
2-Propyl-4-meth...	12.296	0.4	ng	220647	2	10.407	215986	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	31553	3	14.269	219203	0.4
E-2-Propenoic a...	12.772	0.1	ng	27569	3	14.269	219203	0.4
Naphthalene, 2-...	13.140	0.3	ng	142827	3	14.269	219203	0.4
Benzene, 2-meth...	13.850	0.1	ng	30938	3	14.269	219203	0.4
Benzene, 1-meth...	14.637	0.1	ng	48095	3	14.269	219203	0.4
Succinic acid, ...	15.538	0.1	ng	70673	3	14.269	219203	0.4
Acetophenone, 2...	15.614	0.1	ng	72953	3	14.269	219203	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	155998	4	17.018	180754	0.4
Benzyl butyl ph...	20.378	0.1	ng	66815	5	21.227	476680	0.4
.beta.-Alanine,...	22.056	0.1	ng	99861	5	21.227	476680	0.4