

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016672.D
 Acq On : 02 Oct 2021 15:56
 Operator : CG/JU
 Sample : PB139443BS
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139443BS

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: BN016672.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	15	18	20	rBV	7367	10216	2.14%	0.129%
2	3.281	20	22	51	rVB	5601	28239	5.91%	0.358%
3	3.595	51	56	78	rVB	6519	31008	6.49%	0.393%
4	5.263	231	237	256	rVB	14701	56872	11.91%	0.721%
5	6.822	401	406	418	rBV	24241	61776	12.94%	0.783%
6	6.978	418	423	429	rVV	16862	36889	7.73%	0.467%
7	7.080	429	434	440	rVV	37209	76055	15.93%	0.964%
8	7.200	440	447	460	rVB	12367	33214	6.96%	0.421%
9	7.523	478	482	489	rVB	7052	15630	3.27%	0.198%
10	7.642	490	495	514	rVB2	50161	123580	25.88%	1.566%
11	7.956	524	529	538	rVB2	49072	112275	23.51%	1.423%
12	8.168	547	552	563	rVB	3459	9378	1.96%	0.119%
13	8.430	571	577	594	rVB3	21588	50617	10.60%	0.641%
14	8.696	594	598	601	rBV	5111	9547	2.00%	0.121%
15	8.784	601	605	606	rBV	32953	62460	13.08%	0.791%
16	8.822	606	608	616	rVB	27373	51309	10.75%	0.650%
17	9.342	645	649	652	rBV	46511	78139	16.36%	0.990%
18	9.519	660	663	666	rBV	3123	6150	1.29%	0.078%
19	9.596	666	669	681	rVB	8498	15663	3.28%	0.198%
20	9.836	685	688	702	rBV	16408	28722	6.02%	0.364%
21	10.052	702	705	713	rVB	3978	8683	1.82%	0.110%
22	10.407	729	733	735	rBV	108571	198261	41.52%	2.512%
23	10.457	735	737	741	rVV	112368	184474	38.63%	2.337%
24	10.571	743	746	756	rVV	27465	59997	12.57%	0.760%
25	10.749	756	760	763	rVB	33729	58234	12.20%	0.738%
26	11.306	801	804	813	rBV	1891	4854	1.02%	0.062%
27	11.709	853	865	895	rBV	13457	25468	5.33%	0.323%
28	12.003	920	931	939	rBV	58769	96102	20.13%	1.218%
29	12.074	939	947	971	rVV	131820	214179	44.85%	2.714%
30	12.296	987	997	1021	rVV	131848	206665	43.28%	2.619%
31	12.695	1056	1059	1062	rBV	16917	28514	5.97%	0.361%
32	12.759	1062	1064	1071	rVB	11793	24793	5.19%	0.314%
33	12.886	1071	1074	1078	rBV	120018	203821	42.69%	2.583%
34	13.140	1088	1094	1097	rBV	81295	136765	28.64%	1.733%
35	13.736	1138	1141	1143	rBV	11956	17185	3.60%	0.218%
36	13.850	1147	1150	1153	rVB	18995	27636	5.79%	0.350%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	13.939	1155	1157	1158	rBV	5296	8576	1.80%	0.109%
38	13.990	1158	1161	1164	rVB	95476	156871	32.85%	1.988%
39	14.269	1180	1183	1185	rBV	139278	199523	41.79%	2.528%
40	14.332	1185	1188	1191	rVB	172376	251029	52.57%	3.181%
41	14.637	1209	1212	1220	rBV3	16164	43618	9.13%	0.553%
42	14.814	1224	1226	1230	rBV	5333	9209	1.93%	0.117%
43	14.903	1230	1233	1236	rBV	7478	11221	2.35%	0.142%
44	15.106	1246	1249	1252	rBV	8871	11470	2.40%	0.145%
45	15.322	1263	1266	1270	rBV2	234561	361392	75.69%	4.579%
46	15.411	1270	1273	1280	rVV2	2945	8047	1.69%	0.102%
47	15.537	1280	1283	1287	rVV	38000	63956	13.39%	0.810%
48	15.614	1287	1289	1298	rVV2	42068	65422	13.70%	0.829%
49	15.766	1298	1301	1311	rVB2	13499	22528	4.72%	0.285%
50	16.227	1334	1338	1341	rBV2	59711	93608	19.60%	1.186%
51	16.324	1343	1346	1350	rVB	49473	75495	15.81%	0.957%
52	16.506	1358	1361	1372	rVB	20074	34194	7.16%	0.433%
53	16.677	1372	1375	1384	rBV	19631	34733	7.27%	0.440%
54	17.018	1400	1403	1405	rBV	97427	161512	33.82%	2.046%
55	17.066	1405	1407	1410	rVV	159089	225369	47.20%	2.856%
56	17.151	1411	1414	1434	rVB	116793	190548	39.91%	2.414%
57	17.431	1434	1437	1453	rBV	88513	141354	29.60%	1.791%
58	18.015	1482	1485	1505	rVB	5433	7503	1.57%	0.095%
59	19.068	1686	1697	1699	rBV	115413	161531	33.83%	2.047%
60	19.098	1699	1703	1743	rVB	191609	272177	57.00%	3.449%
61	19.460	1766	1776	1813	rBV	186415	261786	54.83%	3.317%
62	19.678	1813	1820	1857	rVB	112770	145341	30.44%	1.842%
63	20.378	1918	1921	1924	rBV	45586	58440	12.24%	0.740%
64	21.174	1993	1996	1998	rBV	50294	63733	13.35%	0.808%
65	21.227	1998	2001	2003	rVV2	200872	409814	85.83%	5.193%
66	21.270	2003	2005	2017	rVB	213358	285627	59.82%	3.619%
67	22.056	2076	2079	2082	rBV	64738	81532	17.08%	1.033%
68	22.810	2217	2230	2236	rBV	126675	209228	43.82%	2.651%
69	22.855	2236	2243	2301	rVB	135872	255712	53.55%	3.240%
70	23.385	2385	2398	2416	rBV	83715	183637	38.46%	2.327%
71	23.484	2417	2427	2486	rVB	95532	209591	43.89%	2.656%
72	24.087	2594	2603	2621	rBV	5467	10298	2.16%	0.130%
73	24.857	2818	2828	2850	rVB2	5152	11438	2.40%	0.145%
74	25.778	3068	3097	3180	rBV4	120343	477493	100.00%	6.050%
75	26.459	3274	3296	3366	rBV	65760	224458	47.01%	2.844%

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Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

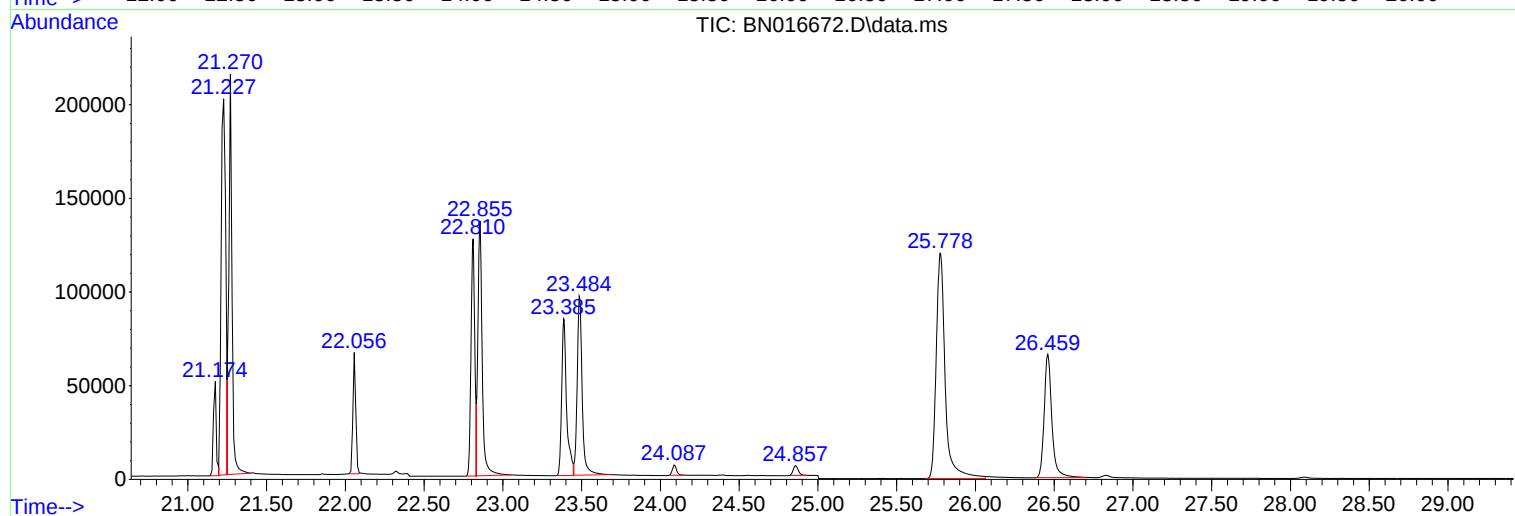
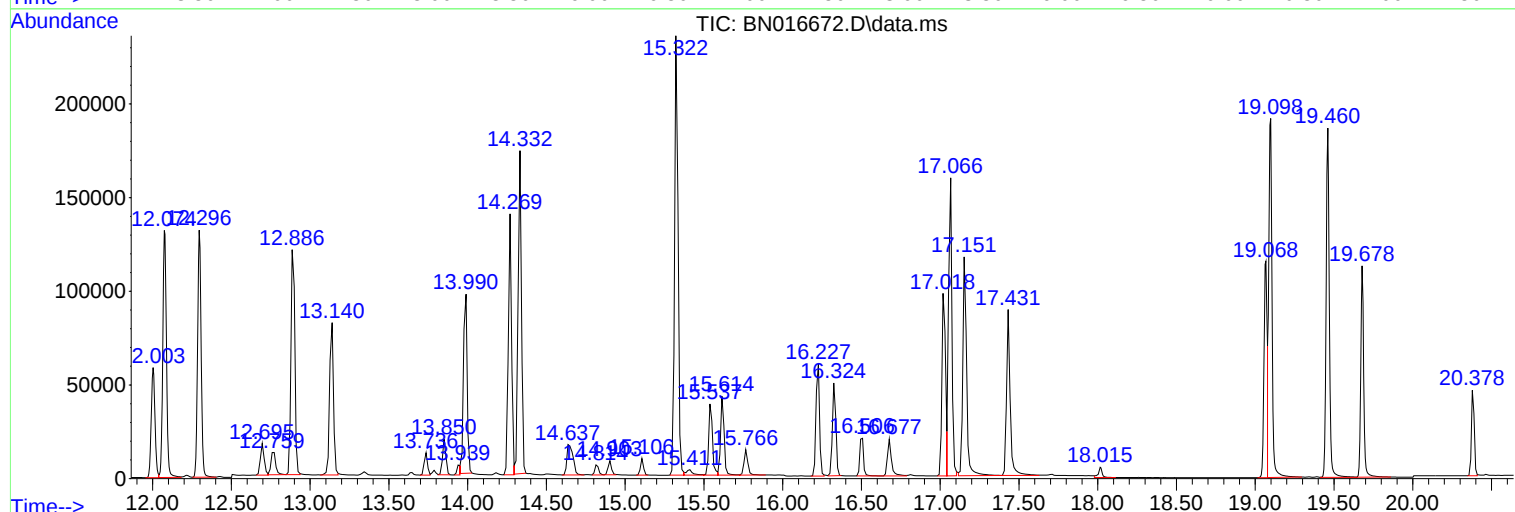
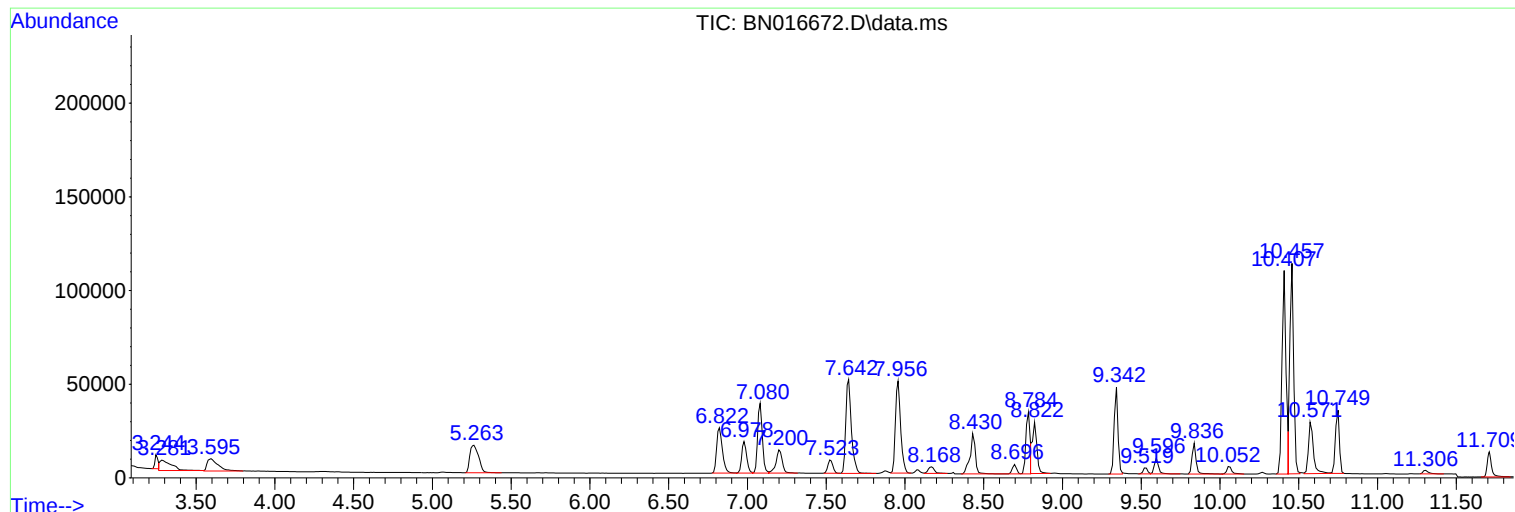
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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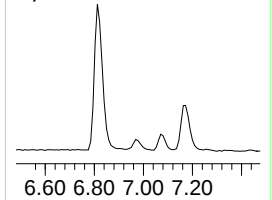
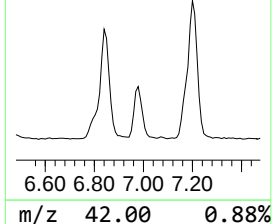
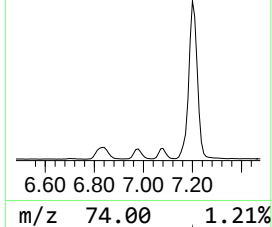
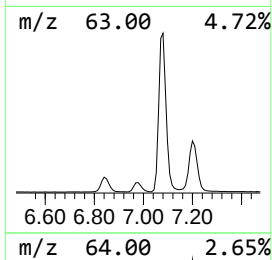
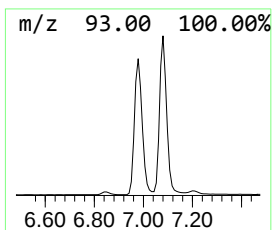
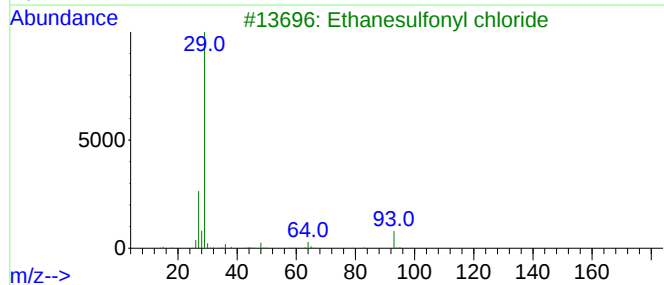
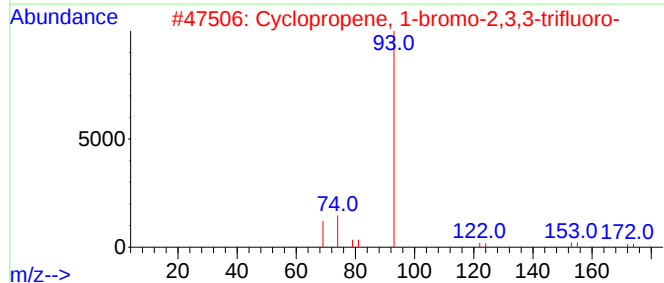
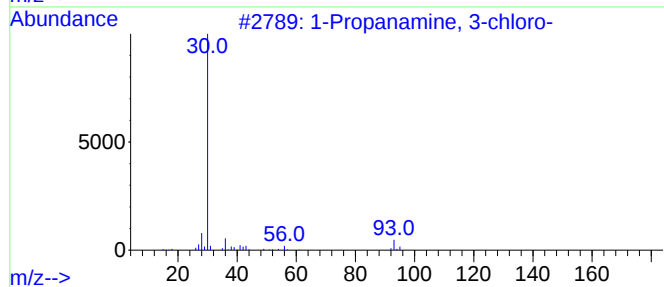
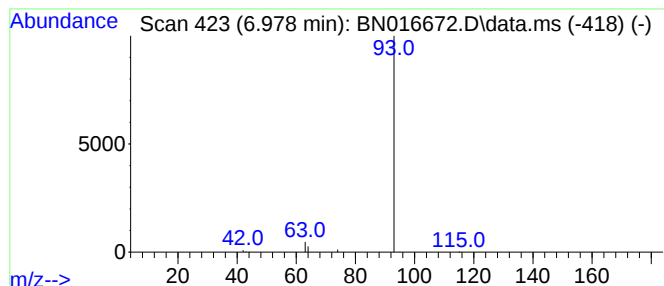
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
6.978	0.12 ng	36889	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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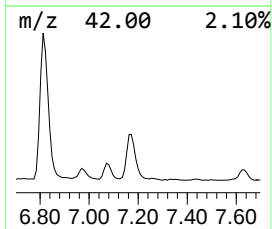
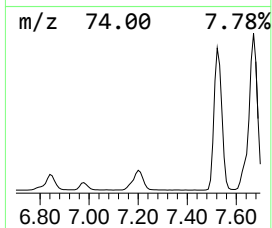
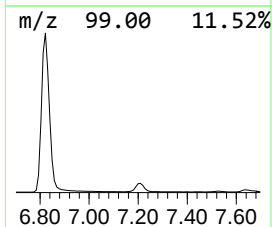
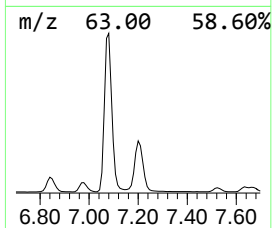
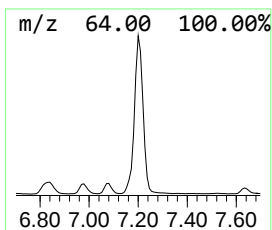
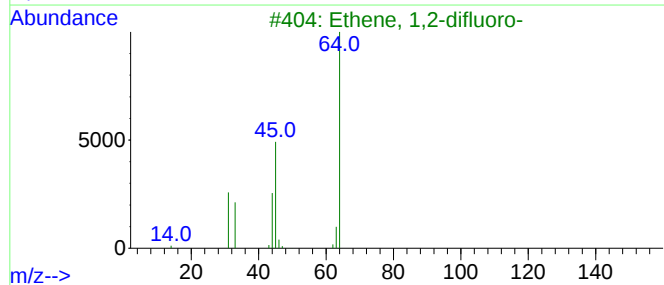
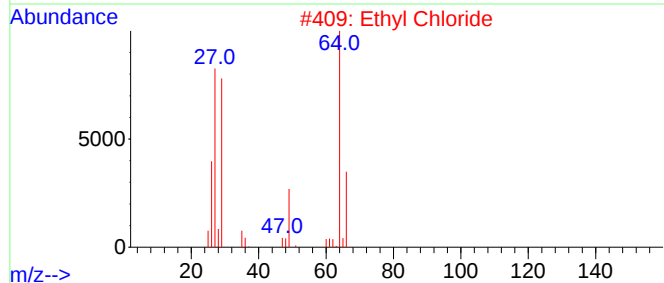
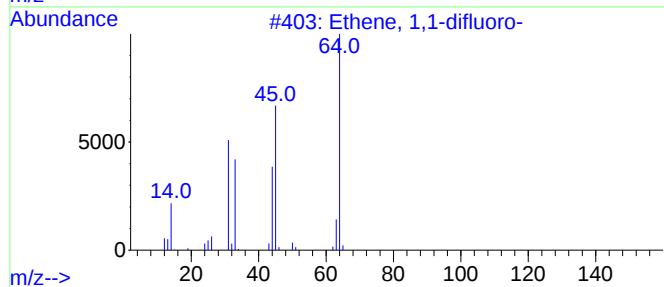
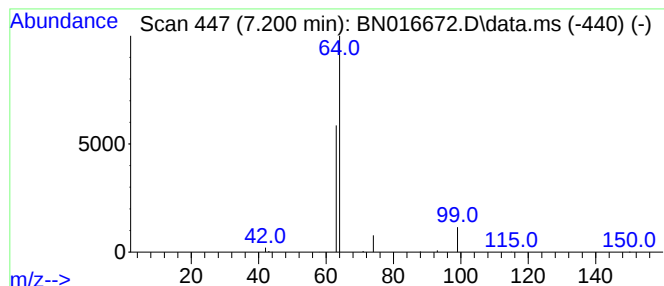
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	33214	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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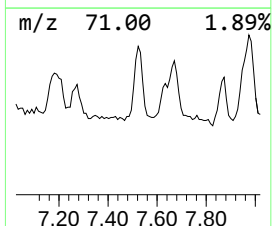
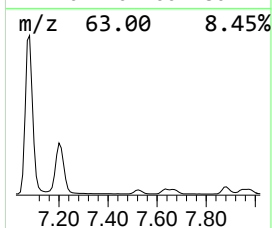
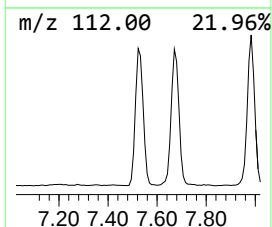
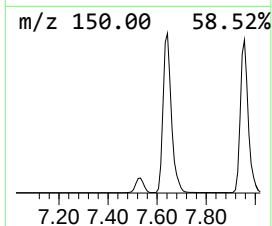
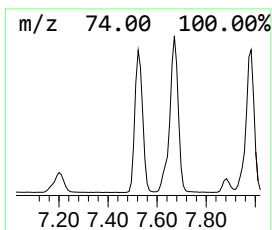
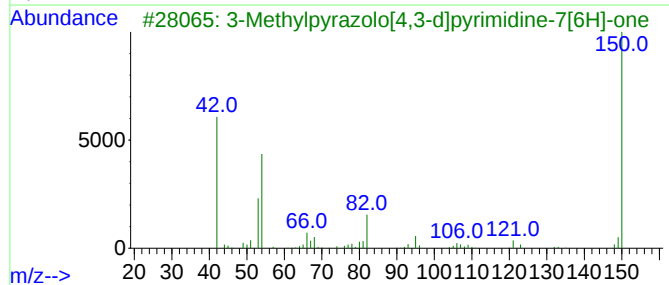
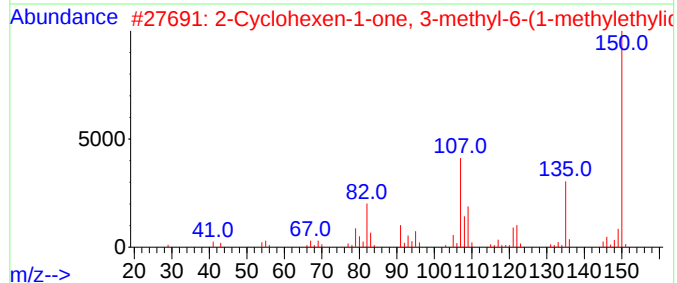
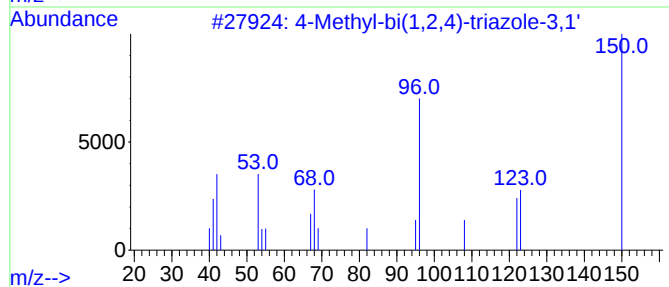
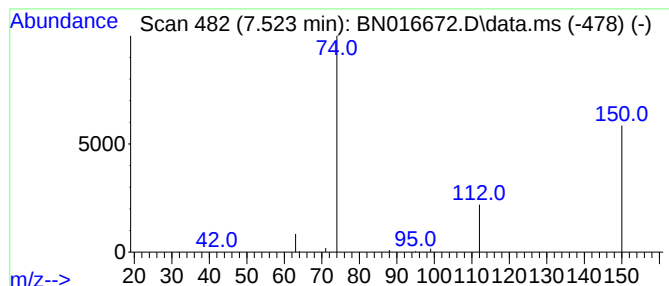
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Methyl-bi(1,2,4)-triazole... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	15630	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-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
4		N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2
5		Propanoic acid	74	C3H6O2	000079-09-4	2



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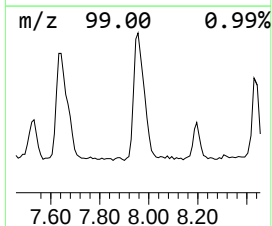
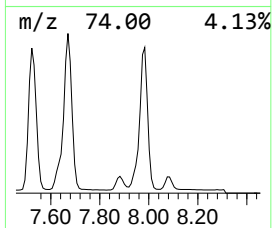
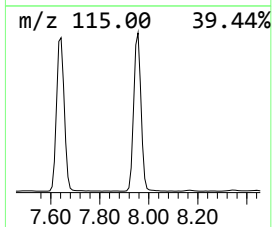
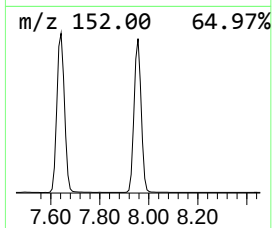
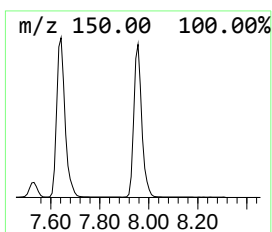
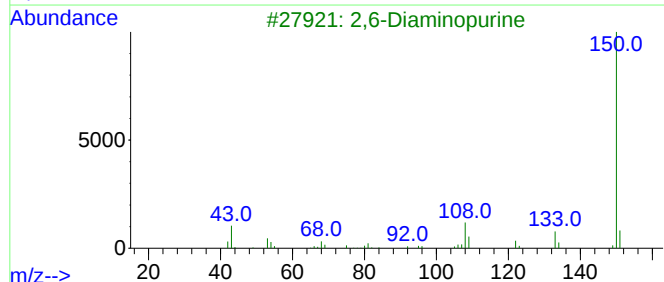
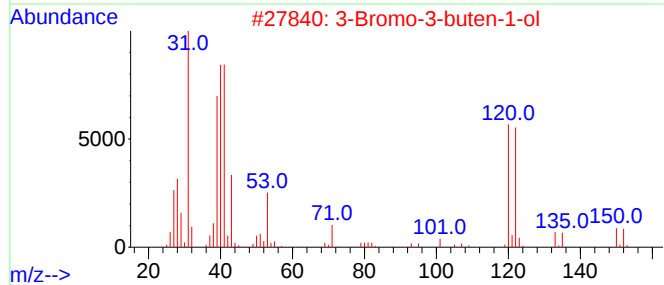
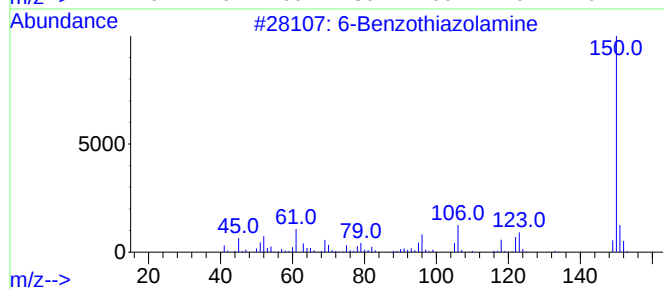
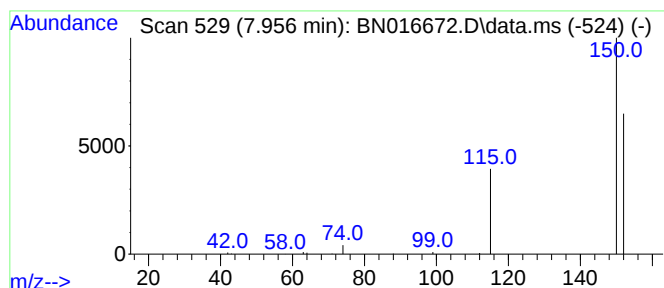
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	112275	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Benzothiazolamine	150	C7H6N2S	000533-30-2	4
2			3-Bromo-3-buten-1-ol	150	C4H7BrO	076334-36-6	3
3			2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
4			9-Methylpoxanthine	150	C6H6N4O	000875-31-0	2
5			5,6,7,8-Tetrahydro-6-oxopteridine	150	C6H6N4O	051036-16-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

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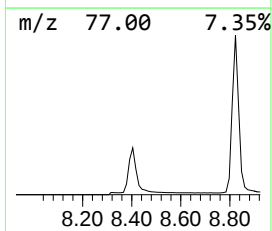
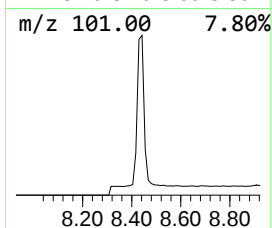
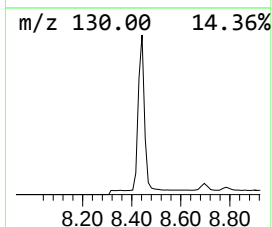
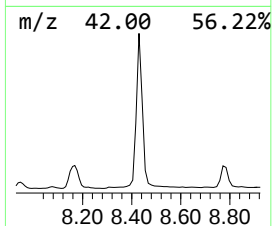
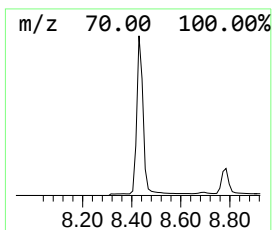
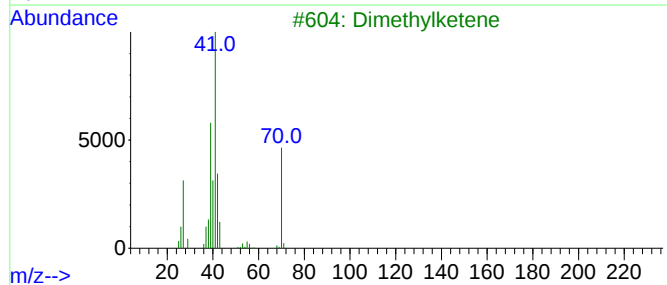
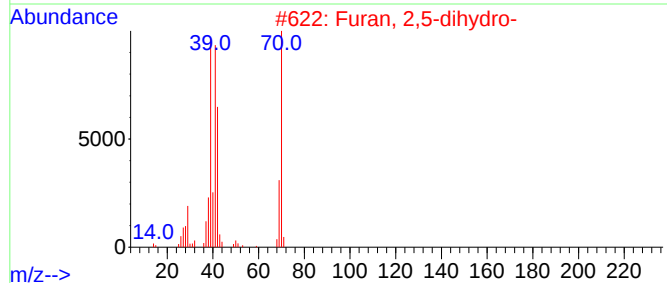
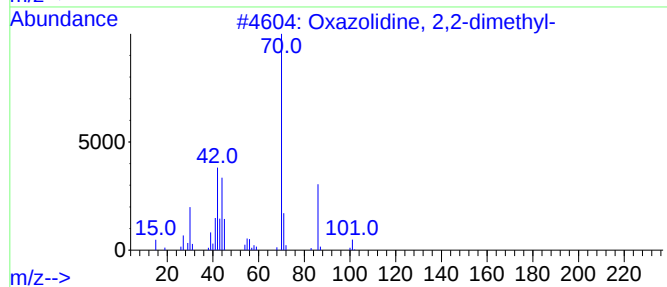
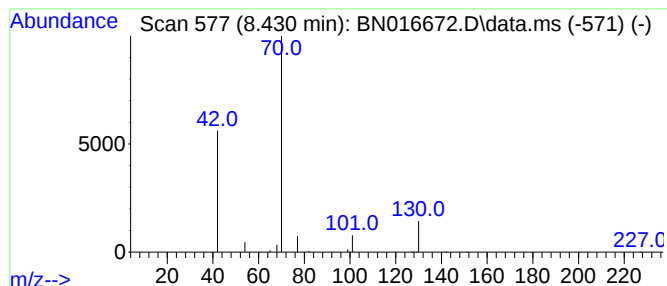
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.16 ng	50617	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			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
3			Dimethylketene	70	C4H6O	000598-26-5	5
4			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
5			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
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Sample : PB139443BS
Misc :
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ClientSampleId :
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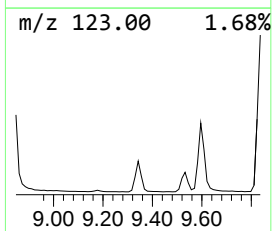
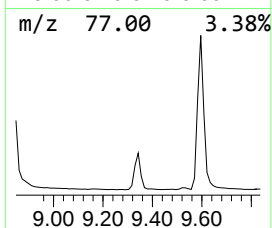
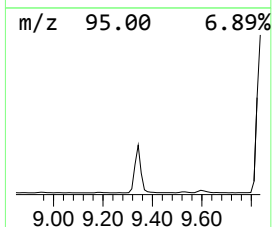
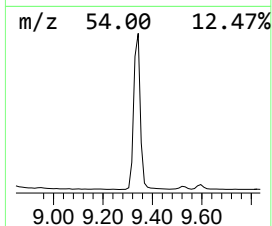
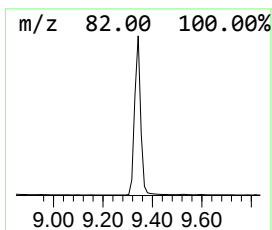
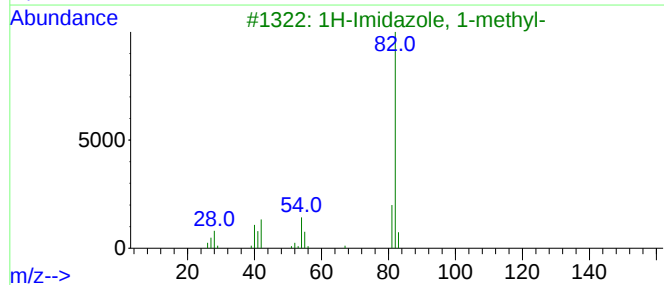
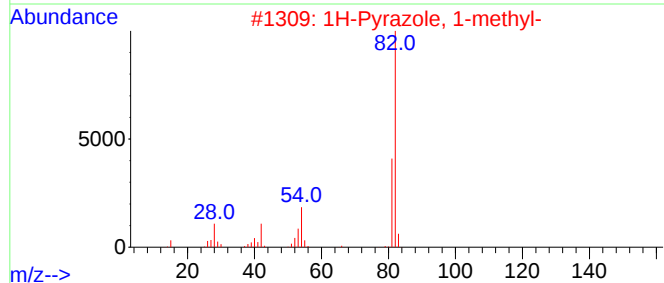
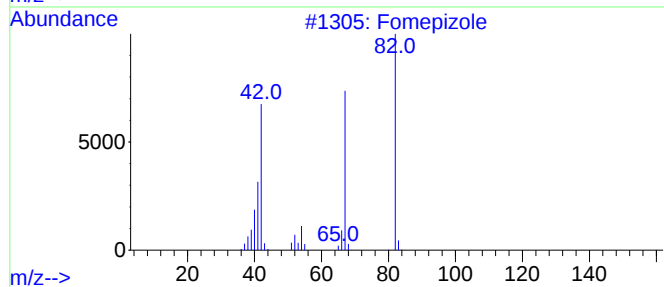
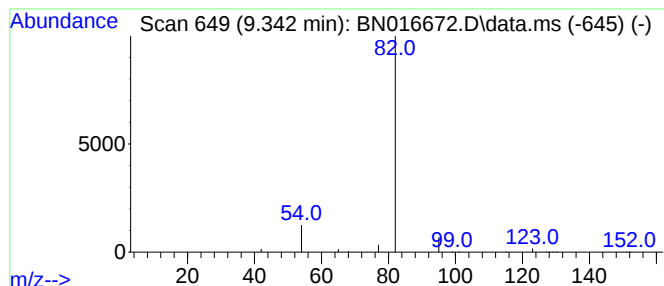
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	78139	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 : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
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Instrument :
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ClientSampleId :
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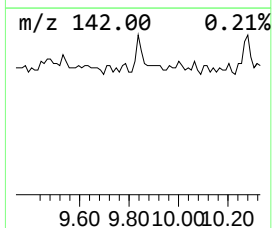
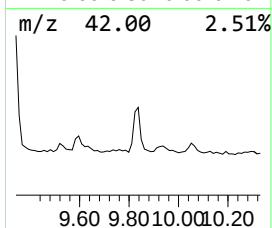
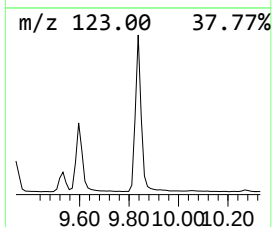
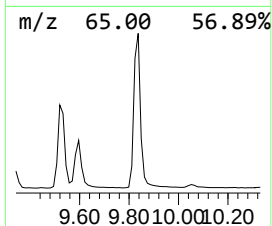
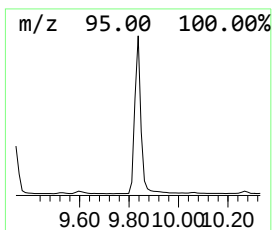
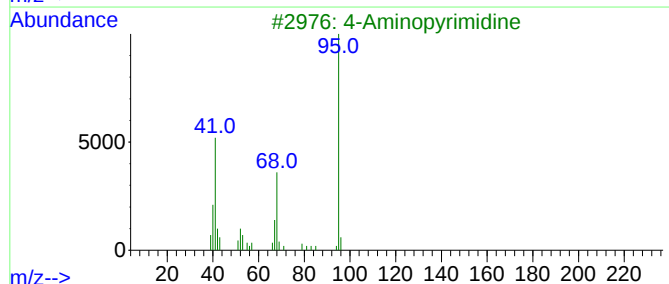
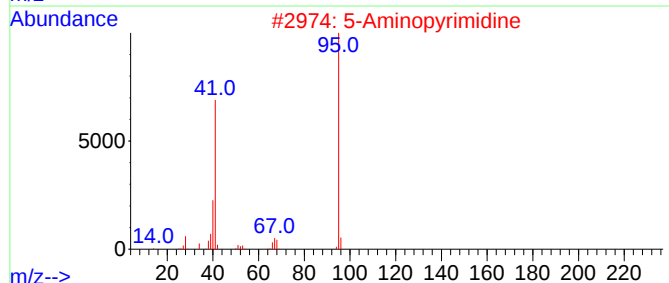
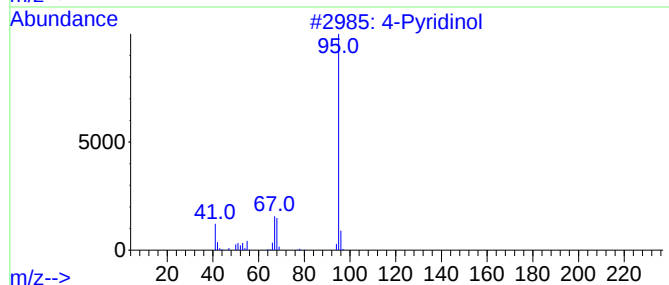
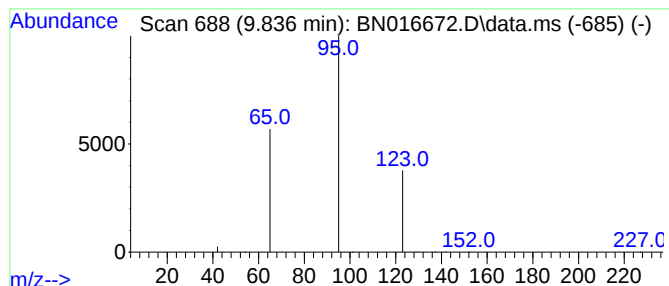
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4-Pyridinol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	28722	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridinol	95	C5H5NO	000626-64-2	4
2			5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
3			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4			2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
5			2-Pyrimidinamine	95	C4H5N3	000109-12-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
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Sample : PB139443BS
Misc :
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Instrument :
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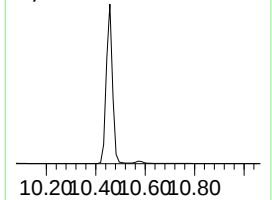
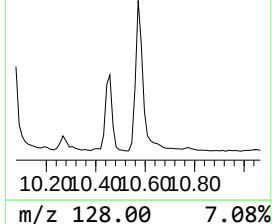
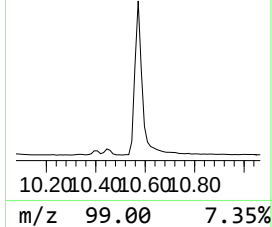
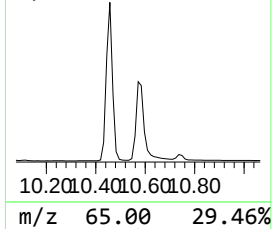
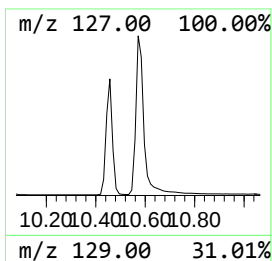
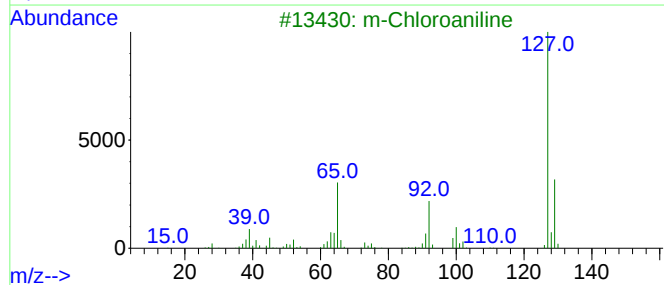
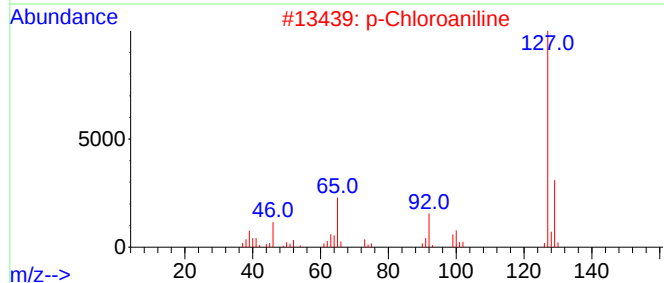
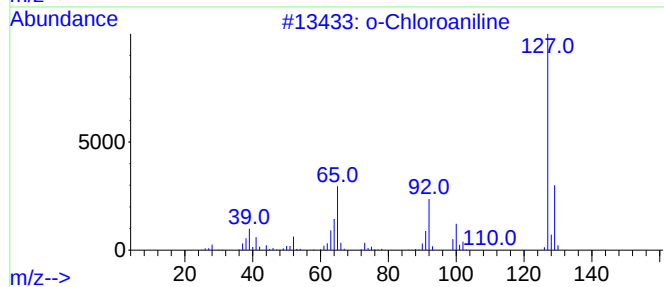
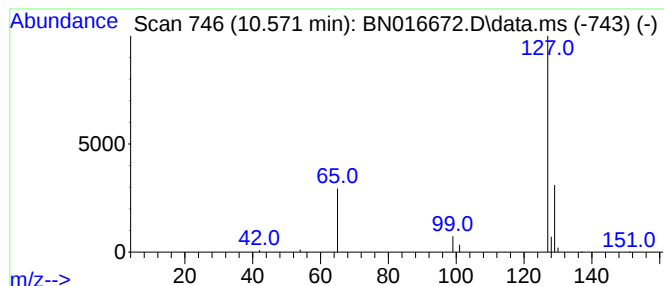
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 o-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	59997	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
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Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

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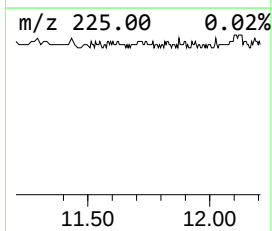
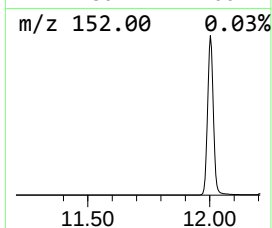
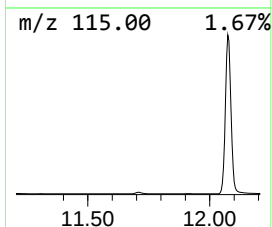
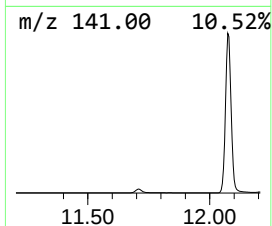
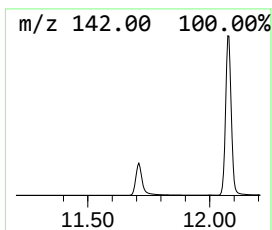
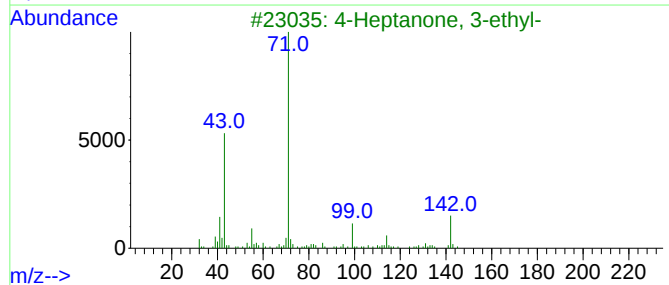
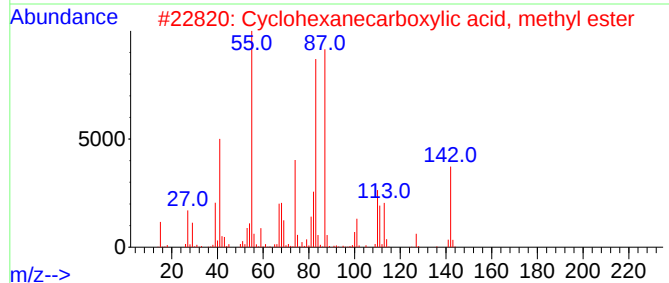
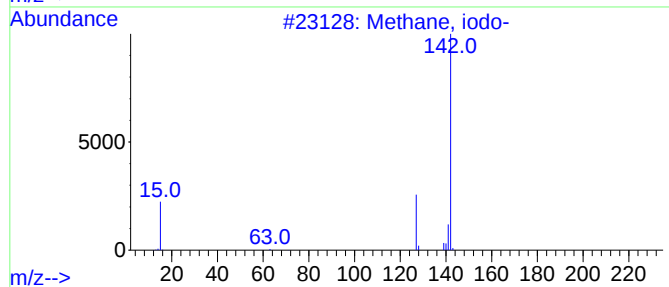
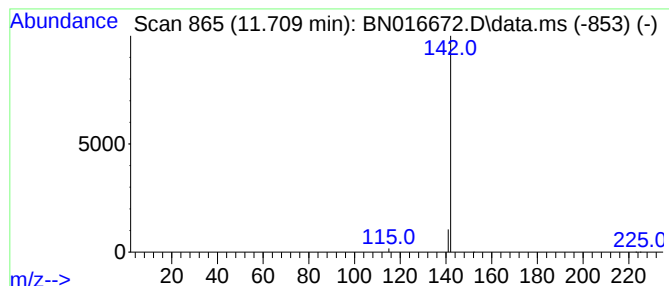
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	25468	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



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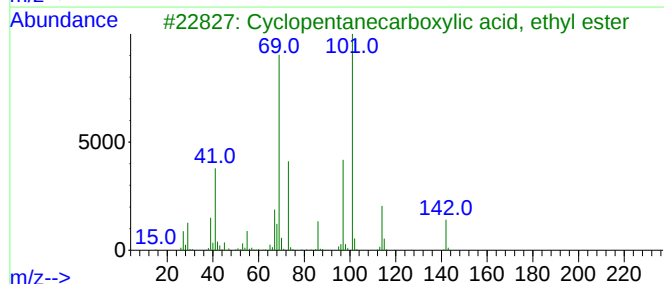
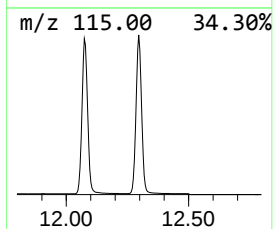
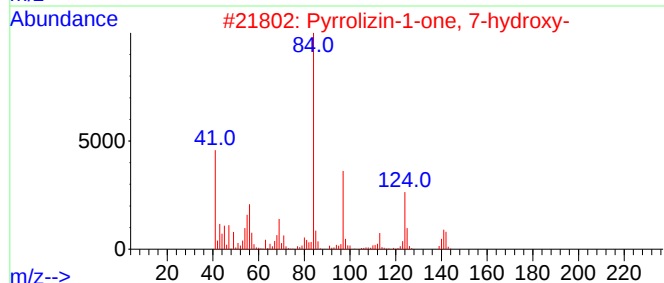
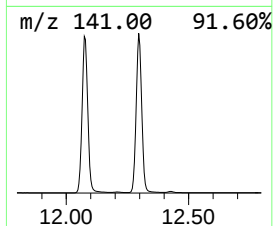
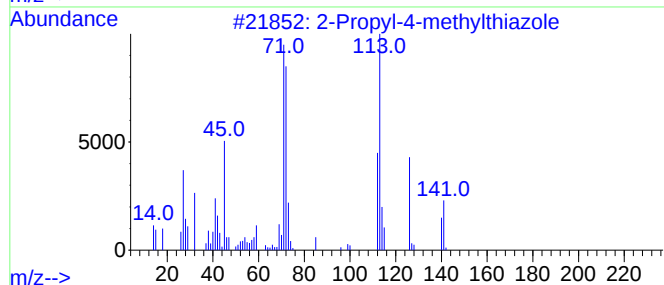
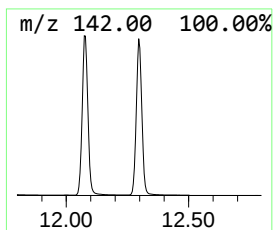
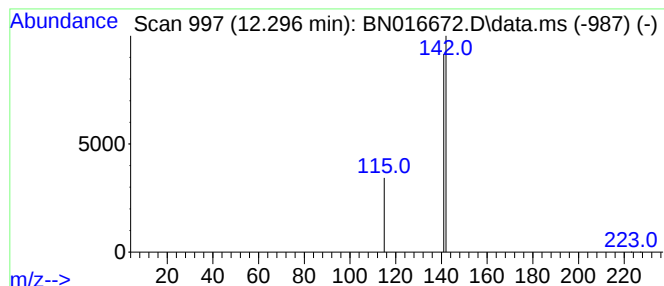
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.42 ng	206665	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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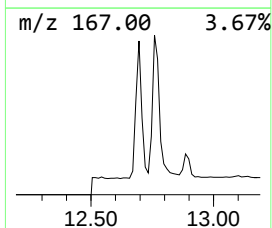
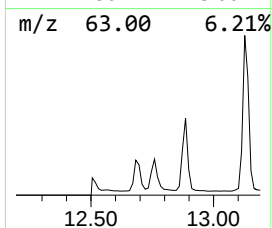
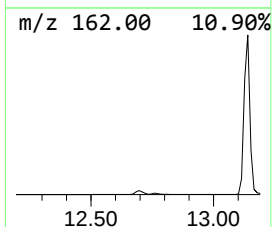
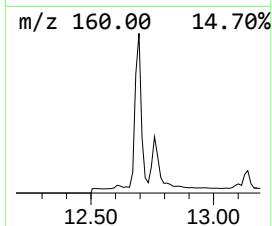
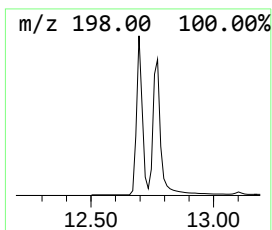
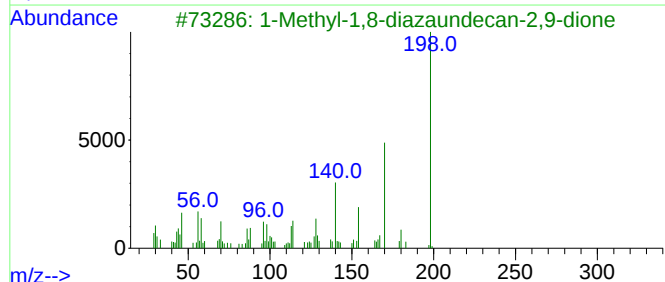
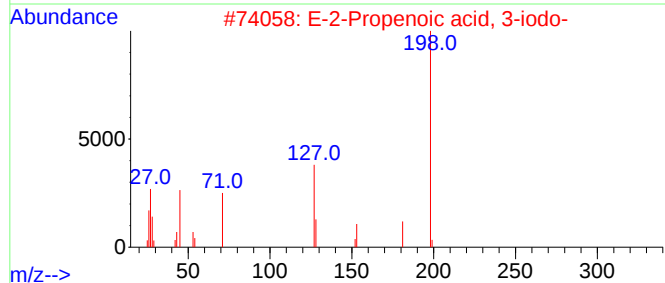
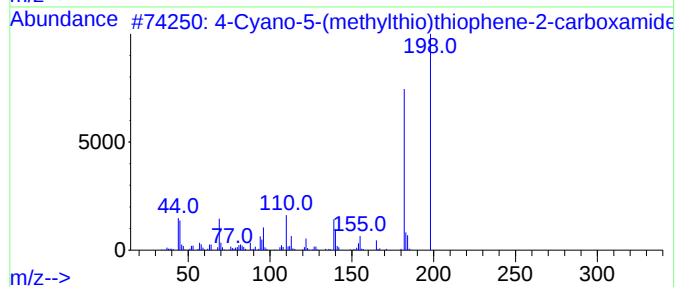
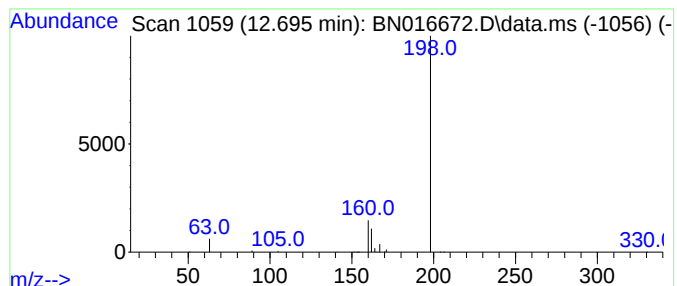
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	28514	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 : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BS

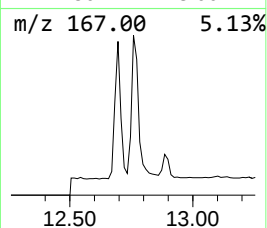
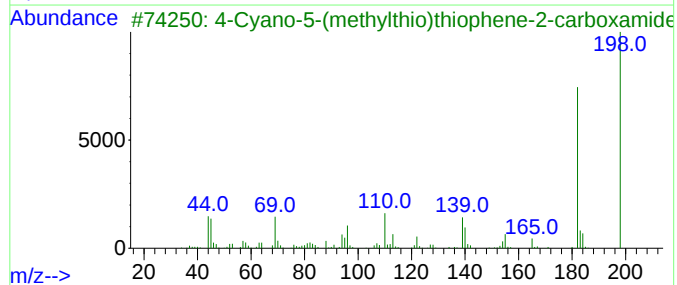
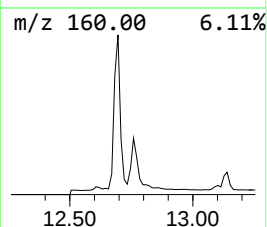
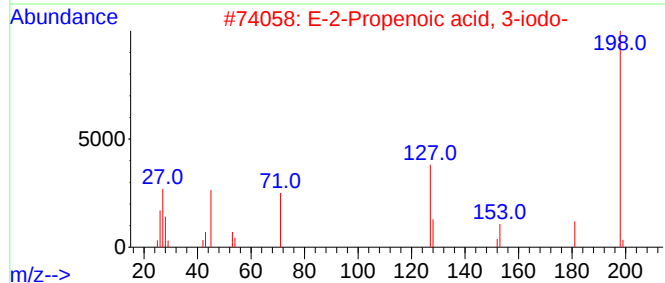
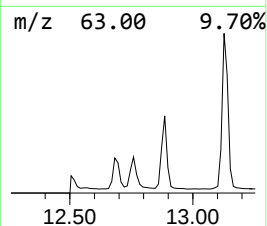
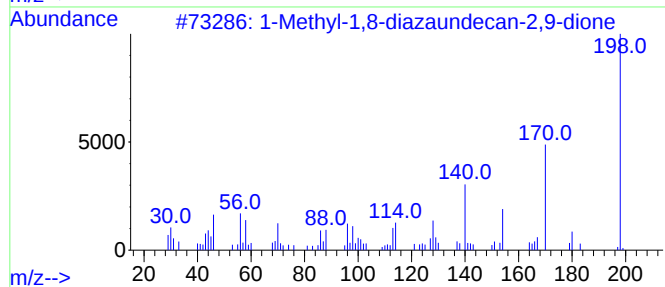
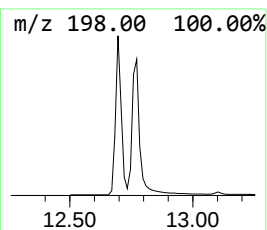
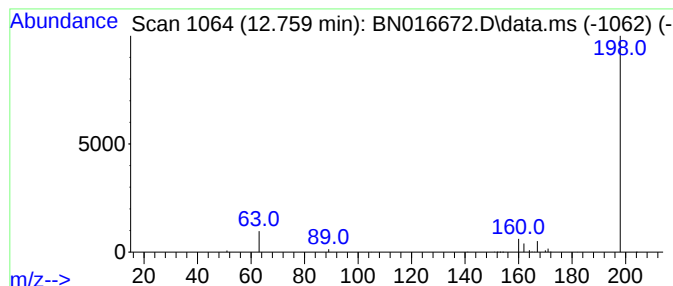
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Methyl-1,8-diazaundecan-2... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	24793	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

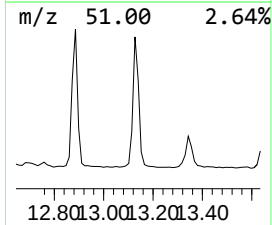
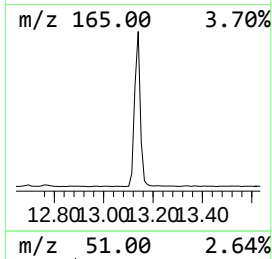
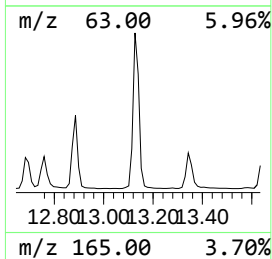
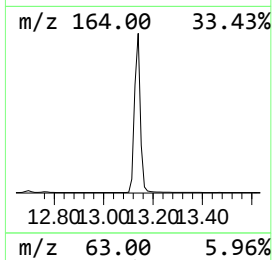
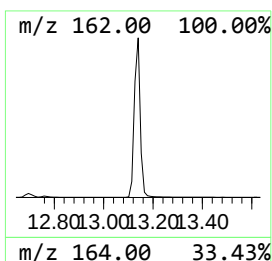
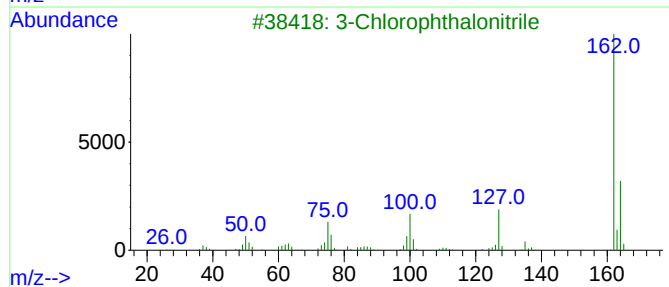
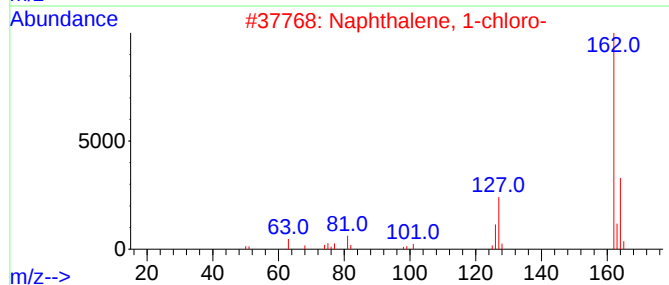
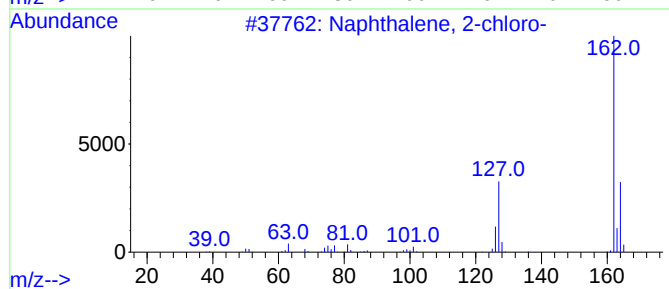
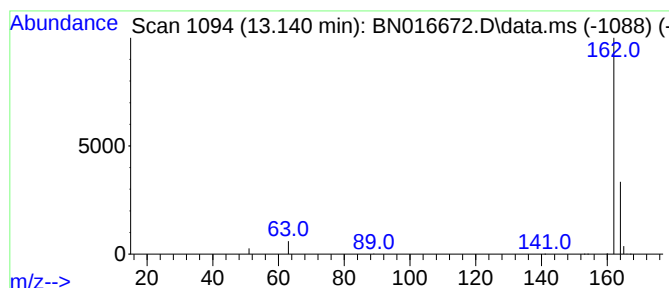
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ClientSampleId :
PB139443BS

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

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.140	0.27 ng	136765	Acenaphthene-d10	14.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	64
2	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	64
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 : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

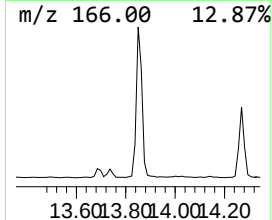
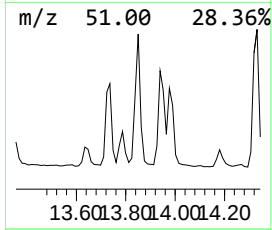
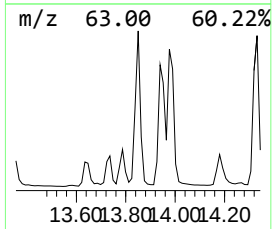
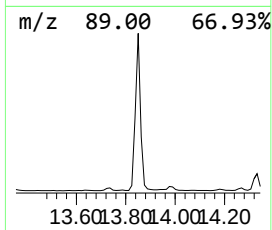
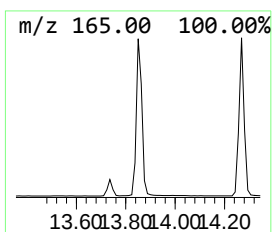
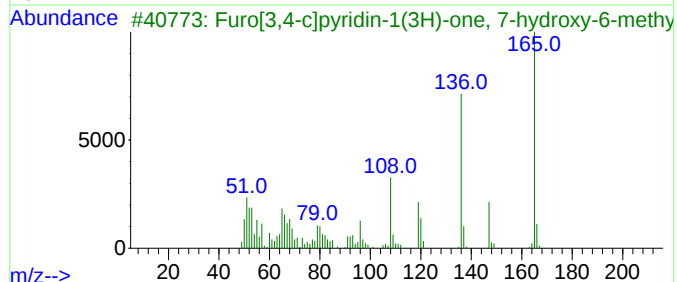
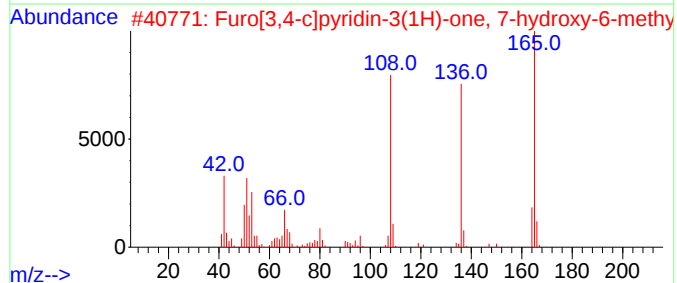
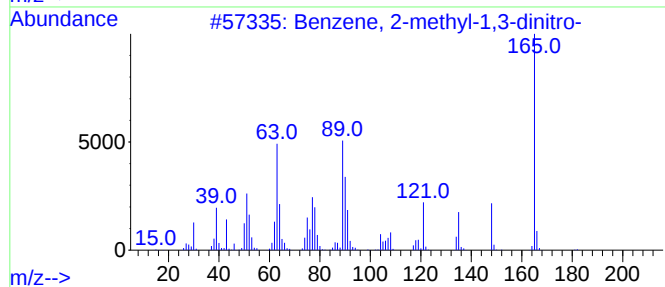
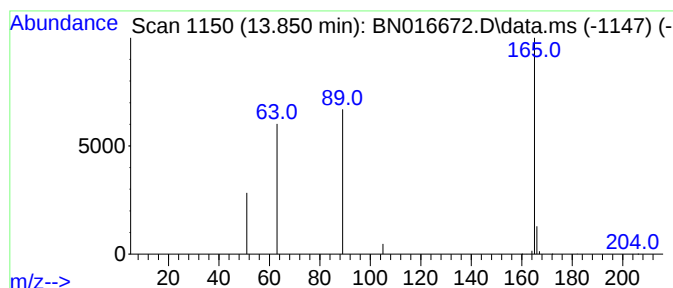
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.850	0.06 ng	27636	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	83
2	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
3	Furo[3,4-c]pyridin-1(3H)-one, 7-...		165	C8H7NO3	004753-19-9	9
4	6-Oxa-3-azabicyclo[3.2.1]octa-1,...		165	C8H7NO3	055255-96-4	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

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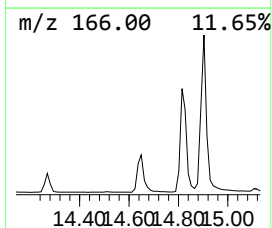
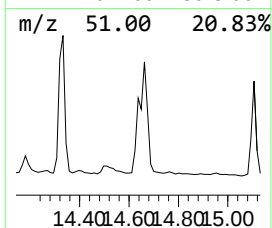
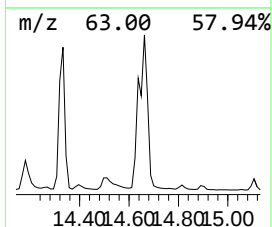
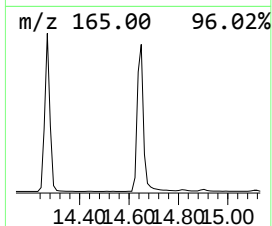
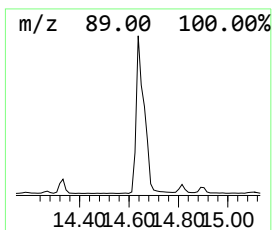
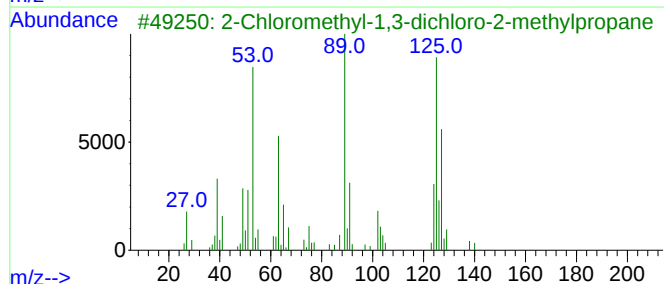
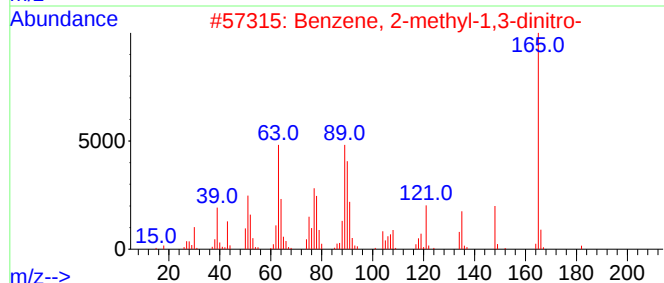
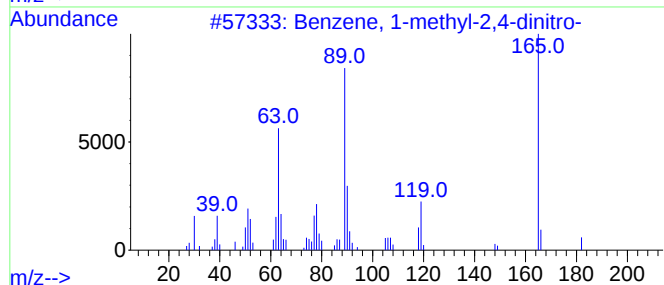
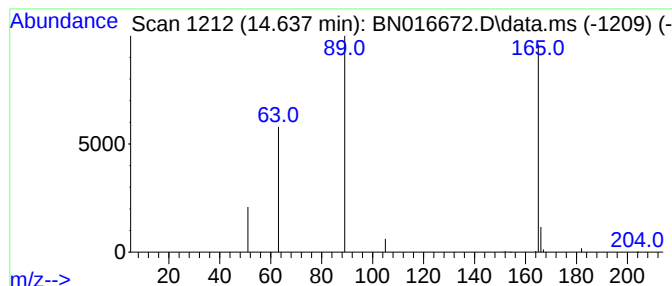
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	43618	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			5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	9
5			6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BS

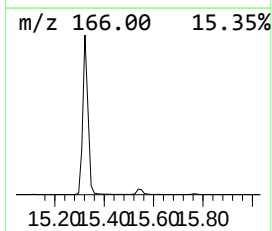
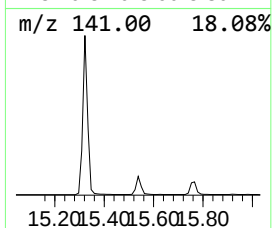
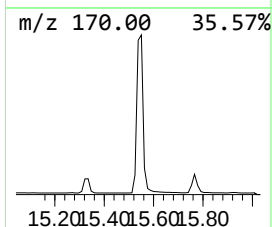
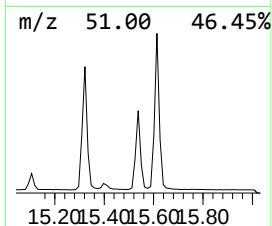
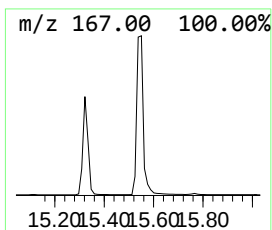
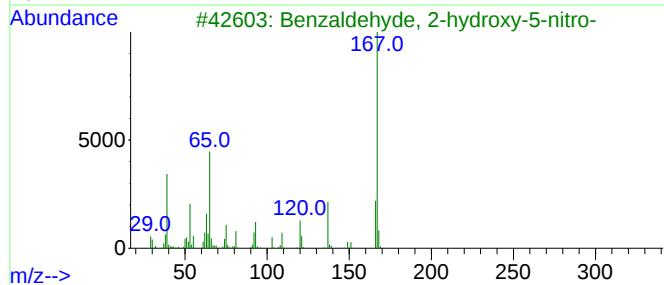
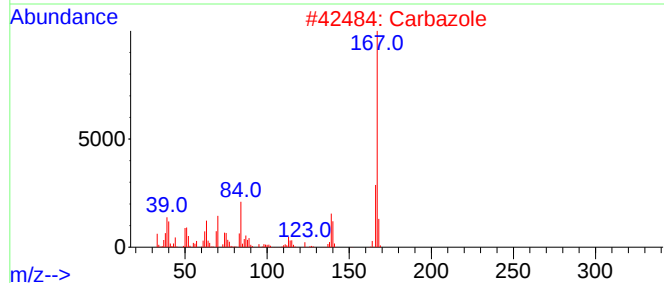
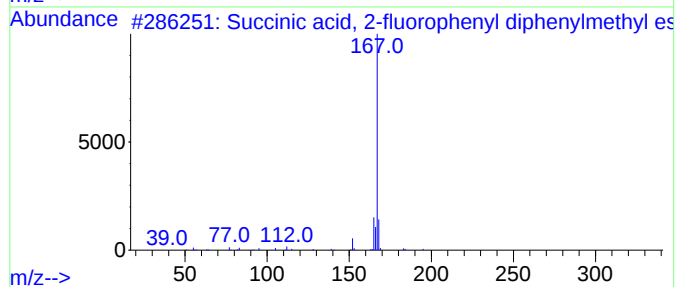
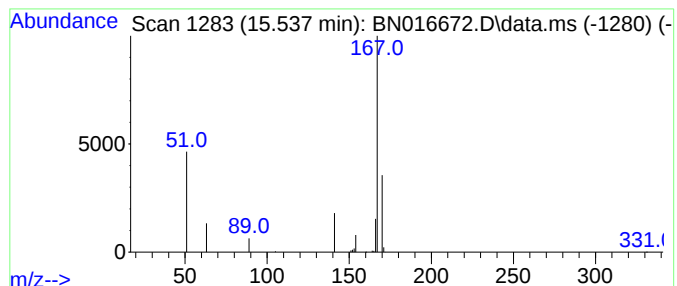
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	63956	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19F04	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5N04	000097-51-8	5
4			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5			Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9N0S	023003-43-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
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Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

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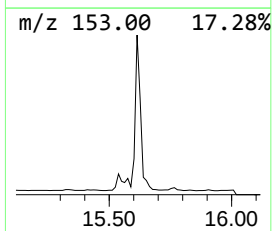
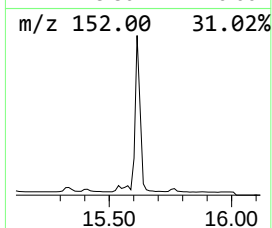
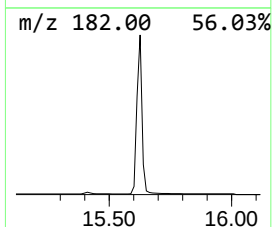
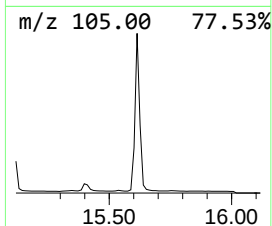
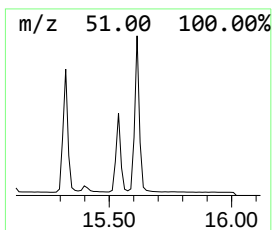
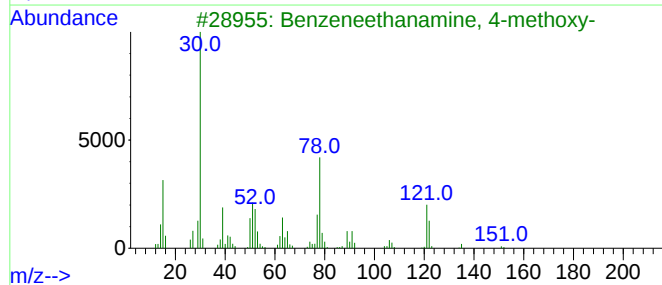
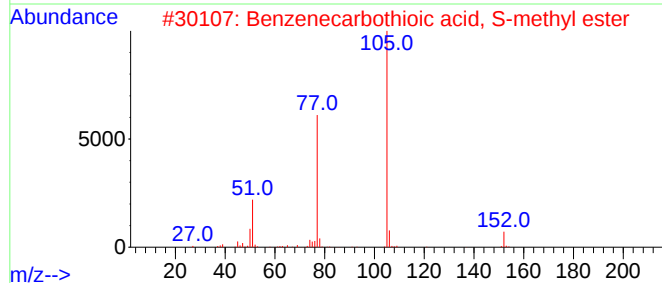
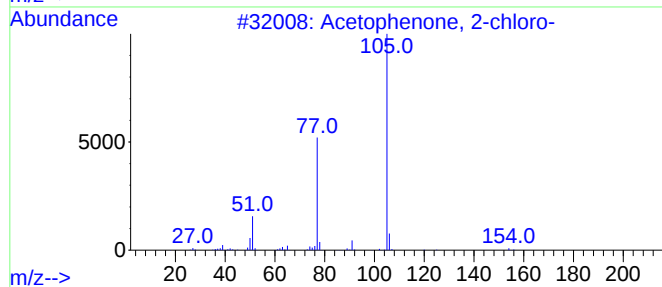
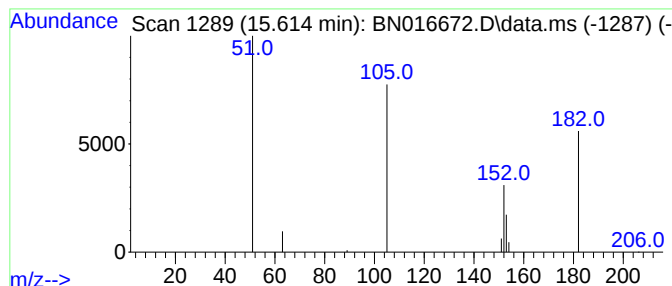
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	65422	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BS

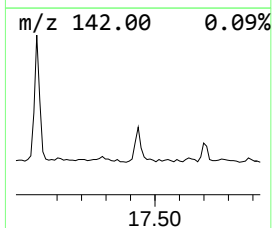
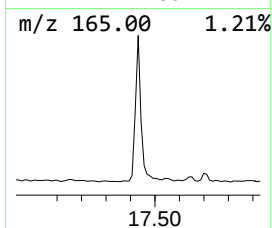
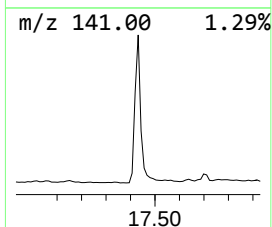
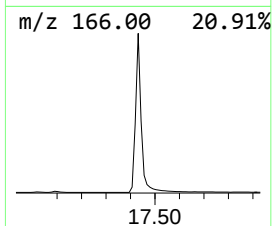
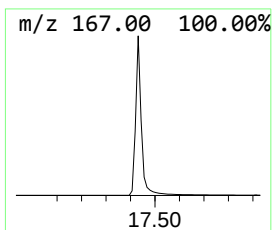
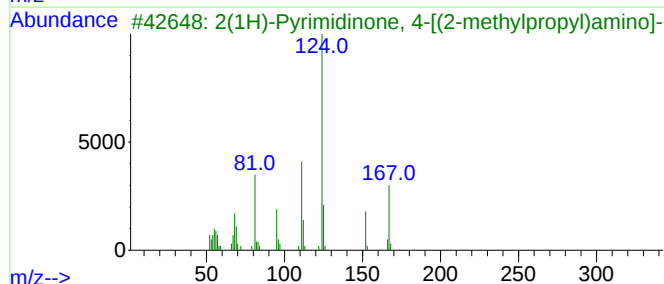
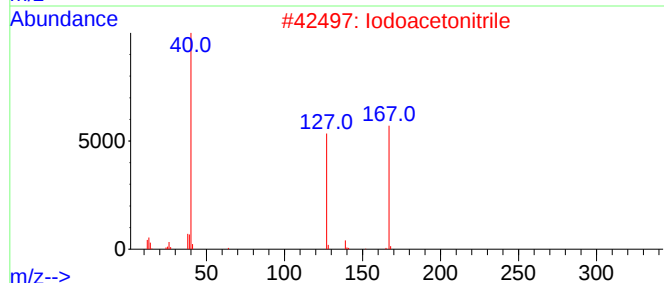
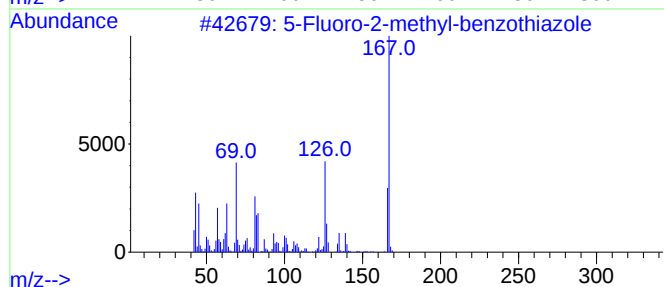
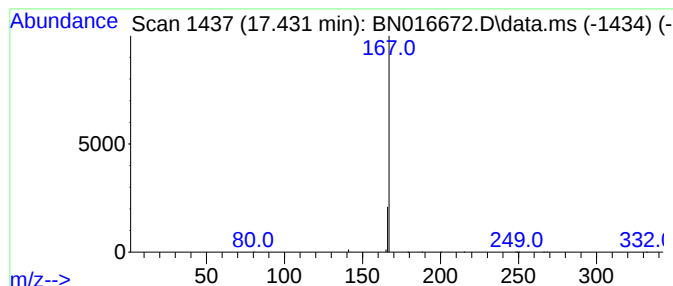
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	141354	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	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 : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BS

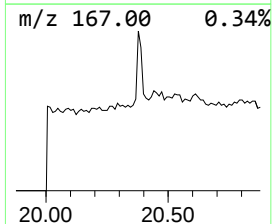
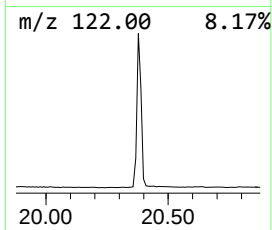
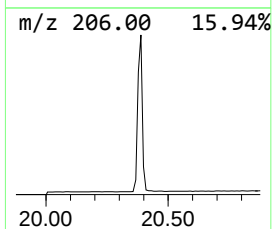
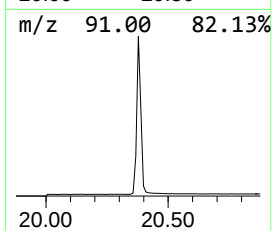
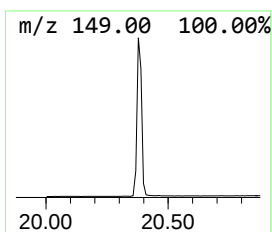
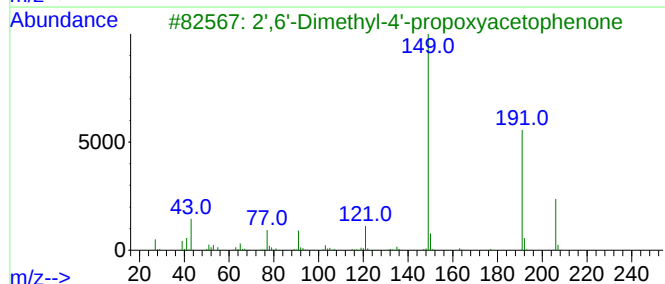
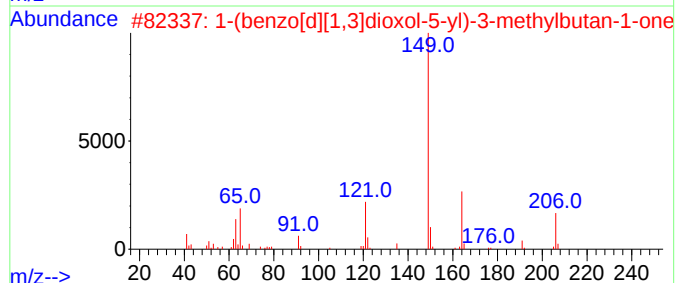
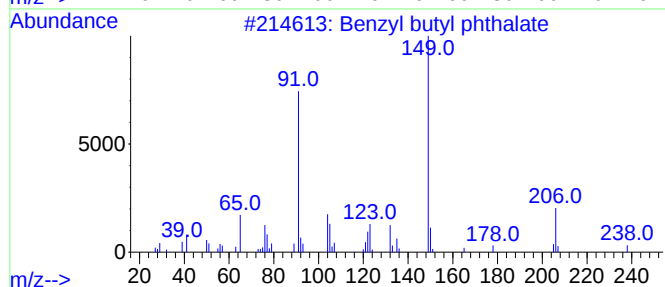
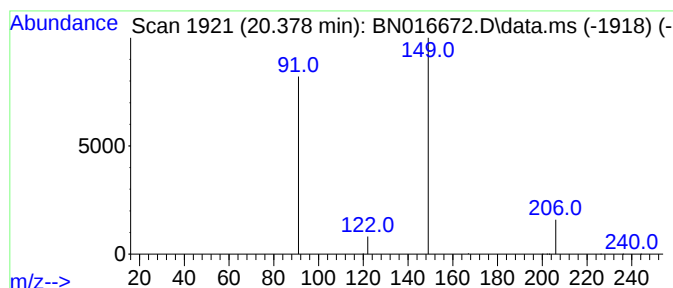
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	58440	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			1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
5			2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
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Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

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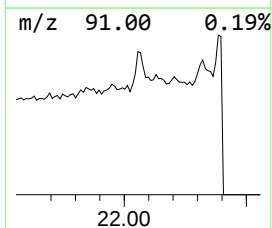
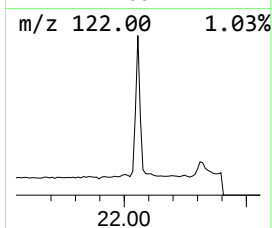
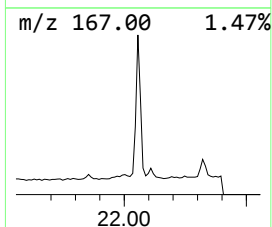
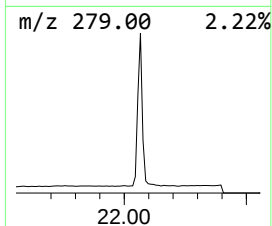
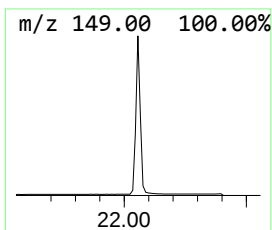
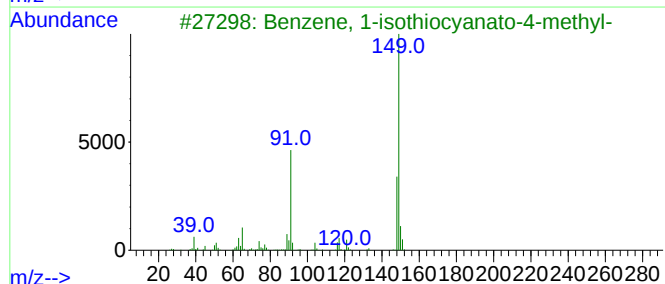
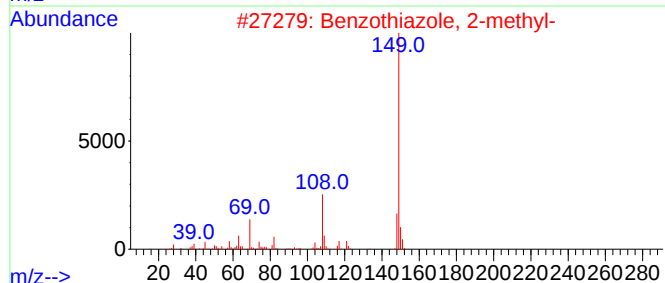
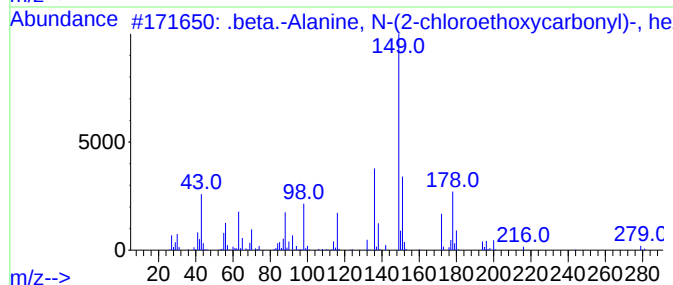
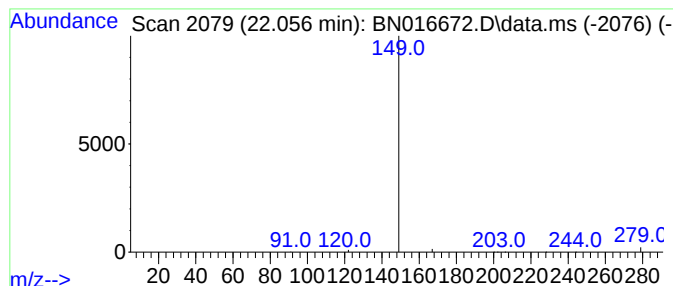
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	81532	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		Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3		Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4		Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016672.D
Acq On : 02 Oct 2021 15:56
Operator : CG/JU
Sample : PB139443BS
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BS

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	36889	1	7.642	123580	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	33214	1	7.642	123580	0.4
4-Methyl-bi(1,2...	7.523	0.1	ng	15630	1	7.642	123580	0.4
6-Benzothiazola...	7.956	0.4	ng	112275	1	7.642	123580	0.4
Oxazolidine, 2,...	8.430	0.2	ng	50617	1	7.642	123580	0.4
Fomepizole	9.342	0.2	ng	78139	2	10.407	198261	0.4
4-Pyridinol	9.836	0.1	ng	28722	2	10.407	198261	0.4
o-Chloroaniline	10.571	0.1	ng	59997	2	10.407	198261	0.4
Methane, iodo-	11.709	0.1	ng	25468	2	10.407	198261	0.4
2-Propyl-4-meth...	12.296	0.4	ng	206665	2	10.407	198261	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	28514	3	14.269	199523	0.4
1-Methyl-1,8-di...	12.759	0.0	ng	24793	3	14.269	199523	0.4
Naphthalene, 2-...	13.140	0.3	ng	136765	3	14.269	199523	0.4
Benzene, 2-meth...	13.850	0.1	ng	27636	3	14.269	199523	0.4
Benzene, 1-meth...	14.637	0.1	ng	43618	3	14.269	199523	0.4
Succinic acid, ...	15.538	0.1	ng	63956	3	14.269	199523	0.4
Acetophenone, 2...	15.614	0.1	ng	65422	3	14.269	199523	0.4
5-Fluoro-2-meth...	17.431	0.4	ng	141354	4	17.017	161512	0.4
Benzyl butyl ph...	20.378	0.1	ng	58440	5	21.238	409814	0.4
.beta.-Alanine,...	22.056	0.1	ng	81532	5	21.238	409814	0.4