

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016653.D
 Acq On : 02 Oct 2021 03:23
 Operator : CG/JU
 Sample : PB139433BS
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139433BS

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: BN016653.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	6285	9350	1.89%	0.125%
2	3.281	20	22	48	rVB	5212	26305	5.32%	0.350%
3	3.594	51	56	82	rVB	6024	29621	5.99%	0.395%
4	5.254	231	236	254	rBV	13577	52657	10.64%	0.701%
5	6.822	401	406	418	rBV	22458	57484	11.62%	0.766%
6	6.978	418	423	429	rVV	15560	34299	6.93%	0.457%
7	7.080	429	434	440	rVV	34000	69542	14.05%	0.926%
8	7.200	440	447	460	rVB	11694	30600	6.18%	0.408%
9	7.522	478	482	489	rVB	6620	14466	2.92%	0.193%
10	7.642	490	495	514	rVB2	46861	115747	23.39%	1.542%
11	7.956	524	529	538	rVB2	44852	103394	20.90%	1.377%
12	8.168	547	552	557	rBV2	3012	7212	1.46%	0.096%
13	8.430	571	577	594	rVB3	20117	46950	9.49%	0.625%
14	8.696	594	598	601	rBV	4463	8515	1.72%	0.113%
15	8.784	601	605	606	rBV	29772	58065	11.73%	0.773%
16	8.822	606	608	616	rVB	25227	47399	9.58%	0.631%
17	9.342	645	649	652	rBV	42356	71940	14.54%	0.958%
18	9.519	660	663	666	rBV	2970	5822	1.18%	0.078%
19	9.595	666	669	679	rVB	8145	14688	2.97%	0.196%
20	9.836	685	688	702	rVV	14665	26338	5.32%	0.351%
21	10.052	702	705	719	rVB	3830	8632	1.74%	0.115%
22	10.407	729	733	735	rBV	102870	188018	38.00%	2.505%
23	10.457	735	737	741	rVV	101773	168999	34.15%	2.251%
24	10.571	743	746	756	rVV	25785	56814	11.48%	0.757%
25	10.749	756	760	763	rVB	30597	53511	10.81%	0.713%
26	11.709	853	865	888	rBV	12876	23613	4.77%	0.315%
27	12.003	921	931	939	rBV	54806	89085	18.00%	1.187%
28	12.074	939	947	971	rVV	121137	199118	40.24%	2.652%
29	12.296	987	997	1020	rVV	122956	192089	38.82%	2.559%
30	12.695	1056	1059	1062	rBV	15951	27083	5.47%	0.361%
31	12.759	1062	1064	1071	rVB	11385	23752	4.80%	0.316%
32	12.886	1071	1074	1078	rBV	113190	189225	38.24%	2.521%
33	13.139	1090	1094	1097	rBV	73445	124429	25.15%	1.657%
34	13.736	1138	1141	1143	rBV	11034	15765	3.19%	0.210%
35	13.850	1147	1150	1153	rVB	17719	25693	5.19%	0.342%
36	13.939	1155	1157	1158	rBV	4977	7962	1.61%	0.106%

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37	13.990	1158	1161	1164	rVB	85039	145489	29.40%	1.938%
38	14.269	1180	1183	1185	rBV	134011	188650	38.12%	2.513%
39	14.332	1185	1188	1191	rVB	158752	233087	47.10%	3.105%
40	14.637	1209	1212	1220	rBV3	15331	40299	8.14%	0.537%
41	14.814	1224	1226	1230	rBV	5019	8693	1.76%	0.116%
42	14.903	1230	1233	1236	rBV	7081	10588	2.14%	0.141%
43	15.106	1246	1249	1252	rBV	8049	10567	2.14%	0.141%
44	15.322	1263	1266	1270	rBV2	223909	335994	67.90%	4.476%
45	15.537	1280	1283	1287	rBV	36290	58343	11.79%	0.777%
46	15.614	1287	1289	1292	rVB2	38941	56217	11.36%	0.749%
47	15.766	1298	1301	1311	rVB2	12922	21538	4.35%	0.287%
48	16.226	1334	1338	1341	rBV2	54035	87382	17.66%	1.164%
49	16.324	1343	1346	1349	rVV	46335	69536	14.05%	0.926%
50	16.494	1358	1360	1372	rVB	18728	31563	6.38%	0.420%
51	16.677	1372	1375	1384	rBV	18305	32742	6.62%	0.436%
52	17.017	1400	1403	1405	rBV	96969	156717	31.67%	2.088%
53	17.066	1405	1407	1410	rVV	138524	208058	42.05%	2.771%
54	17.151	1411	1414	1434	rVV	110050	177472	35.87%	2.364%
55	17.431	1434	1437	1453	rVV	78520	129969	26.27%	1.731%
56	18.015	1482	1485	1507	rVB7	5090	6796	1.37%	0.091%
57	19.063	1685	1696	1699	rBV	113437	158807	32.09%	2.115%
58	19.093	1699	1702	1747	rVB	184482	248622	50.24%	3.312%
59	19.460	1766	1776	1812	rBV	178465	251109	50.75%	3.345%
60	19.673	1813	1819	1867	rVB	104694	138544	28.00%	1.845%
61	20.378	1918	1921	1924	rBV	51425	59203	11.96%	0.789%
62	21.164	1992	1995	1997	rBV	51411	59067	11.94%	0.787%
63	21.217	1997	2000	2003	rVV2	204127	410773	83.01%	5.472%
64	21.270	2003	2005	2016	rVB	173735	254713	51.48%	3.393%
65	22.056	2075	2079	2082	rBV	57534	80040	16.18%	1.066%
66	22.803	2216	2228	2234	rBV	124540	204583	41.34%	2.725%
67	22.848	2234	2241	2286	rVB	137442	248846	50.29%	3.315%
68	23.382	2384	2397	2415	rBV	83259	188756	38.15%	2.514%
69	23.481	2415	2426	2474	rVB	97234	205893	41.61%	2.743%
70	24.083	2592	2602	2621	rBV	8556	16722	3.38%	0.223%
71	24.850	2815	2826	2855	rBV	8471	19764	3.99%	0.263%
72	25.771	3068	3095	3171	rBV3	126276	494825	100.00%	6.591%
73	26.449	3271	3293	3344	rBV	68310	226234	45.72%	3.014%
74	26.818	3386	3401	3429	rVB2	2102	6783	1.37%	0.090%

Sum of corrected areas: 7507166

Instrument :

BNA_N

ClientSampleId :

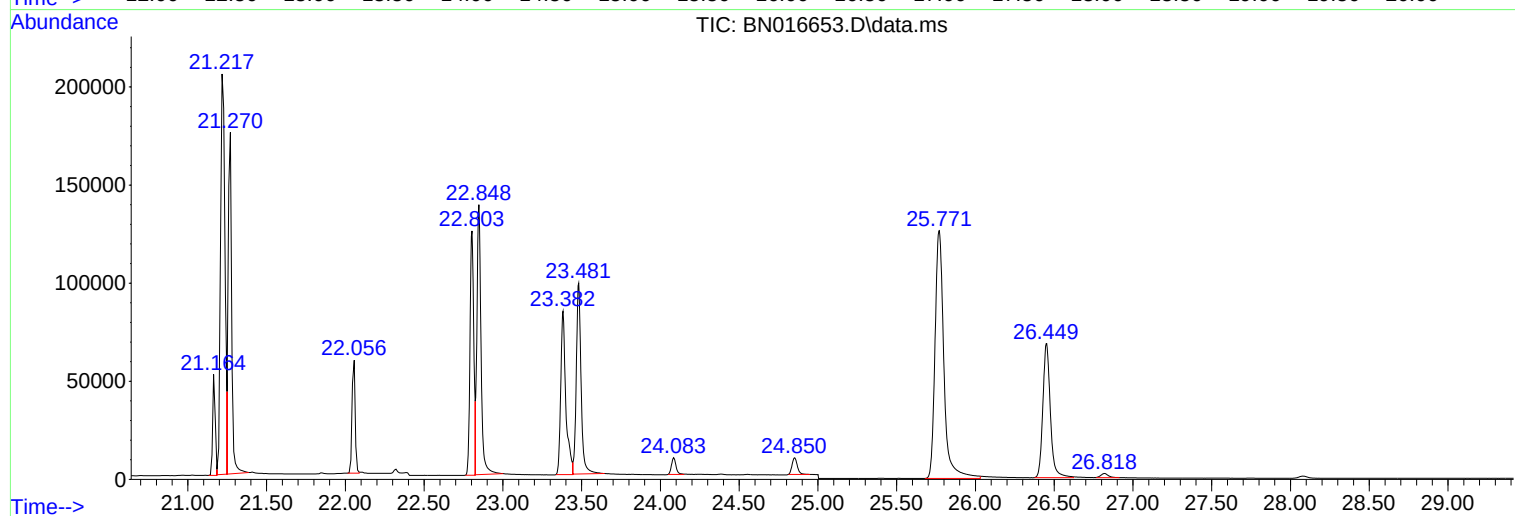
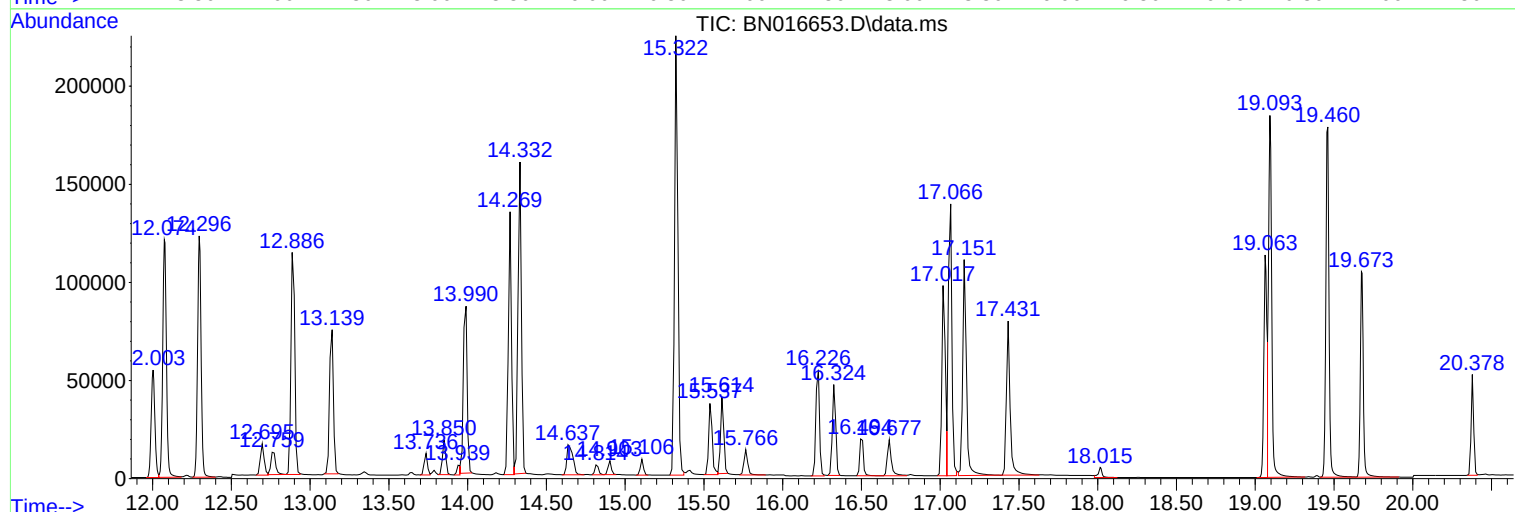
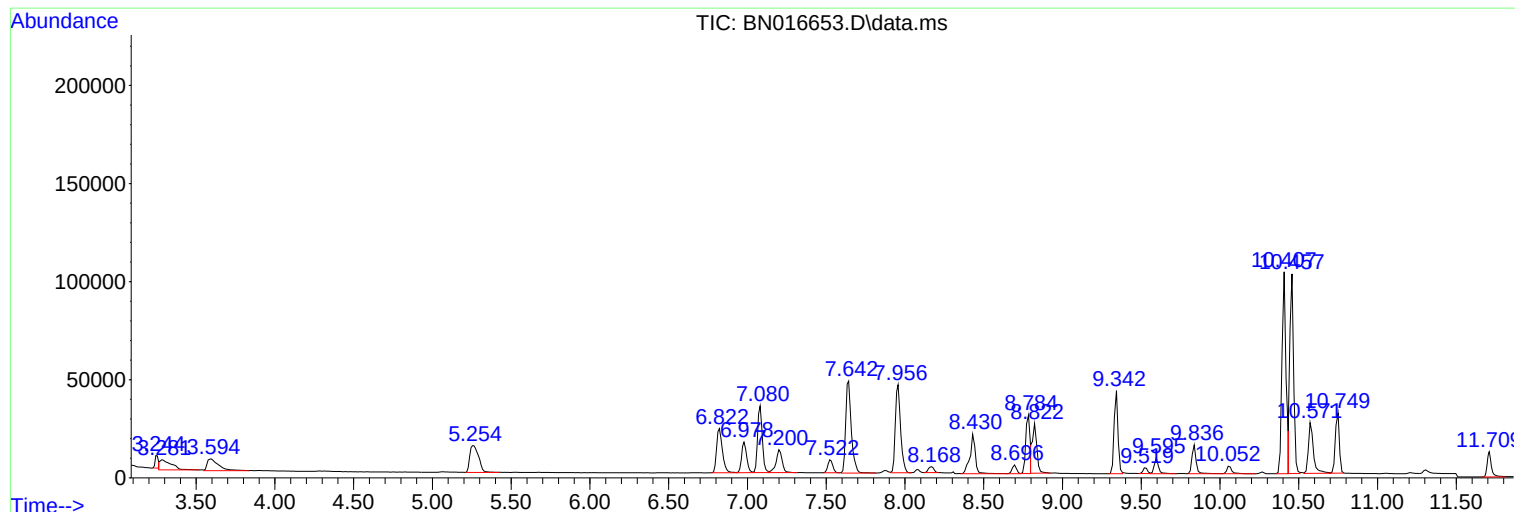
PB139433BS

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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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Acq On : 02 Oct 2021 03:23
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Sample : PB139433BS
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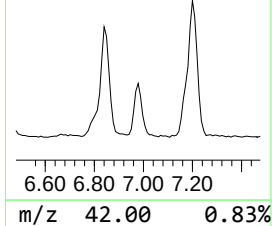
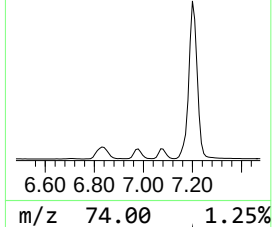
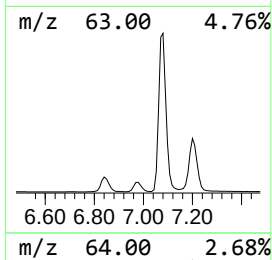
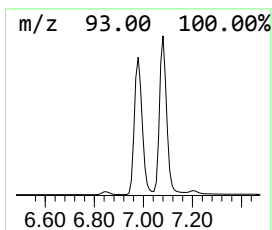
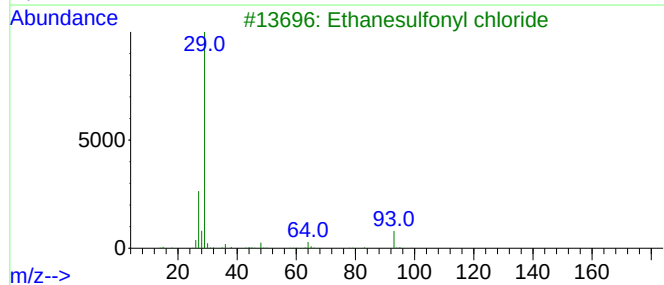
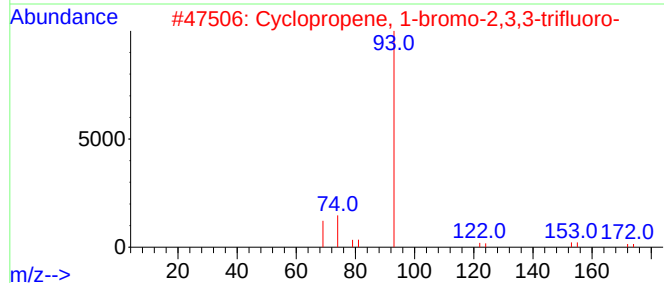
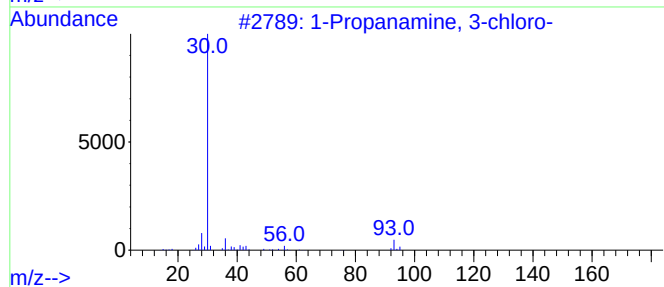
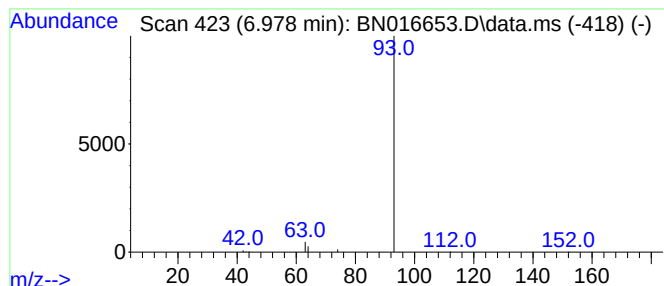
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.12 ng	34299	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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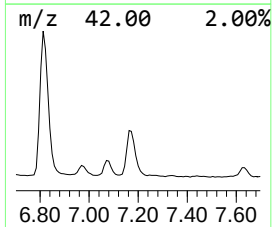
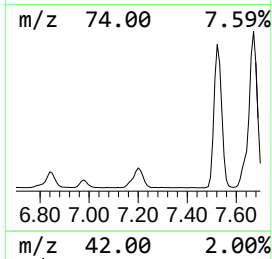
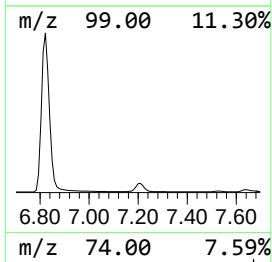
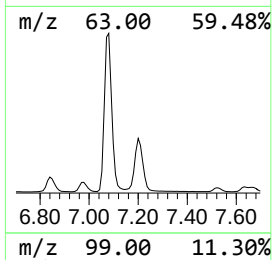
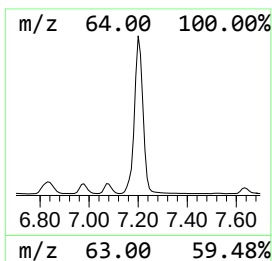
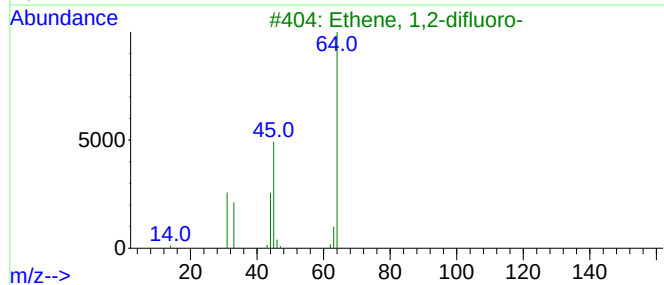
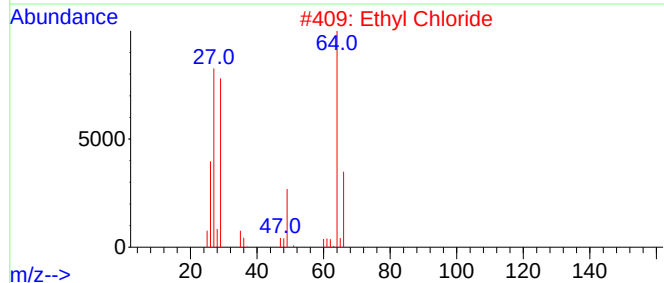
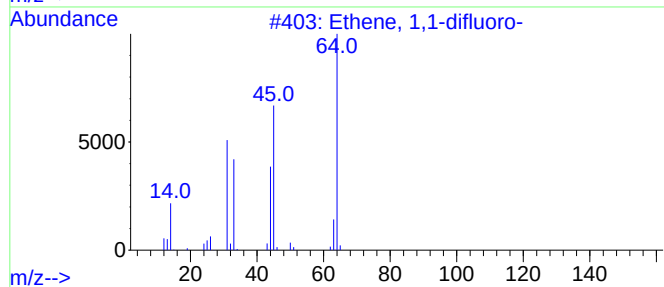
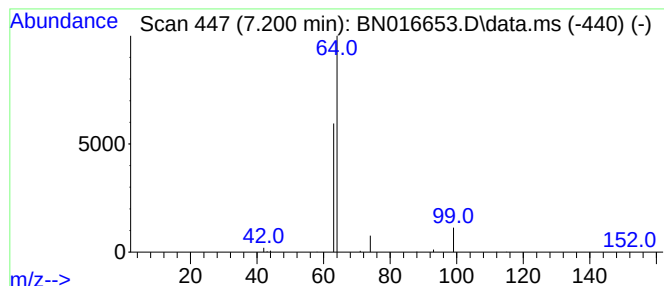
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	30600	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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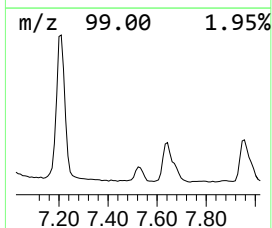
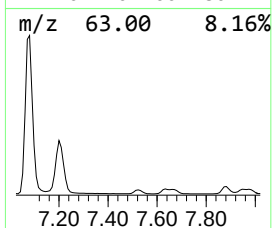
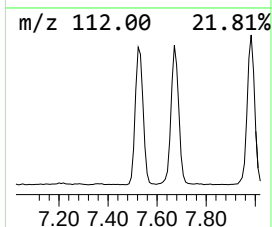
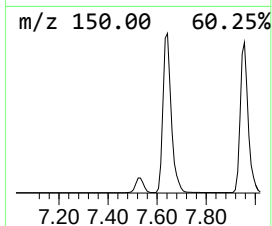
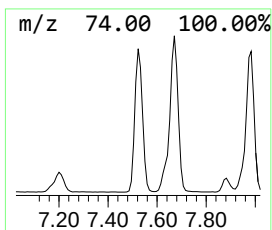
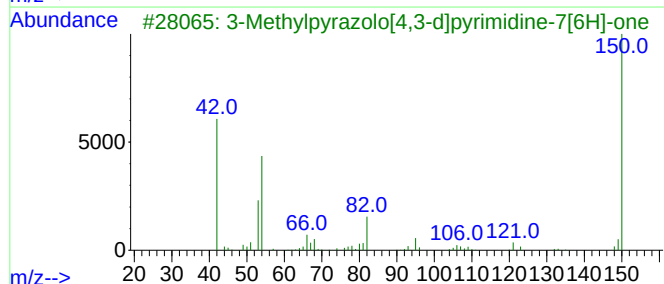
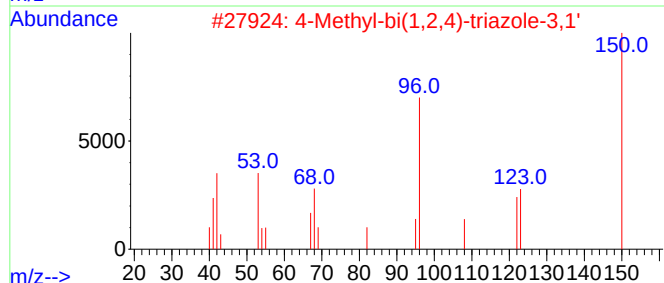
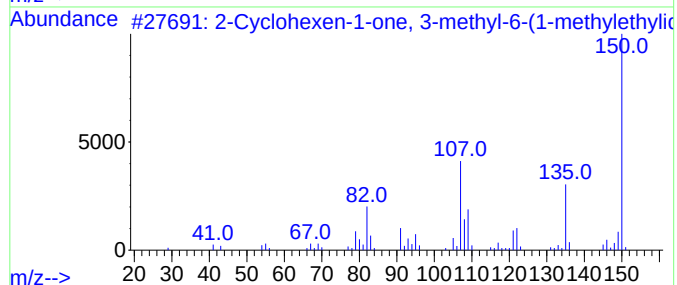
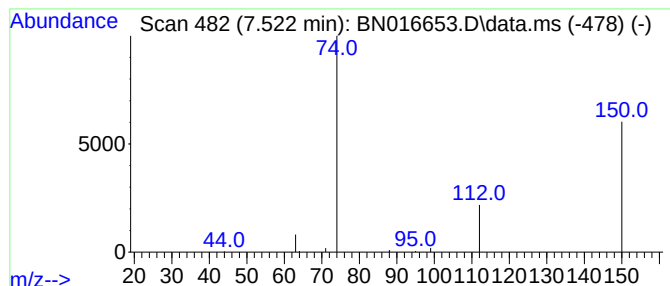
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Cyclohexen-1-one, 3-methy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	14466	1,4-Dichlorobenzene-d4	7.642

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



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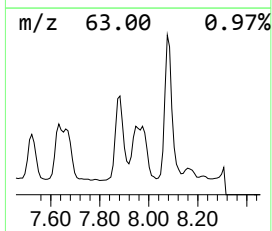
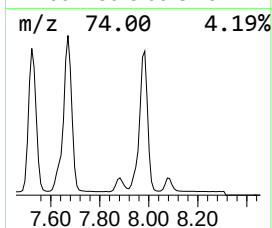
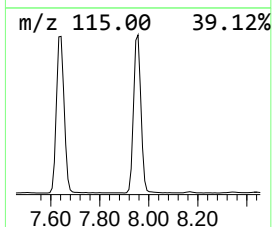
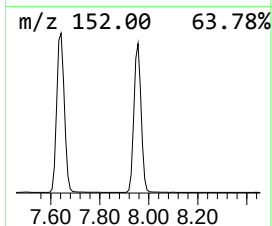
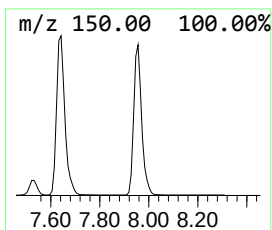
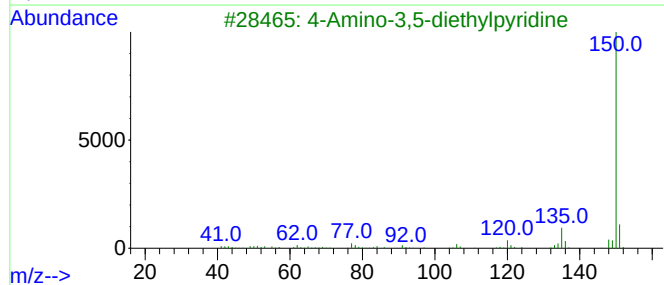
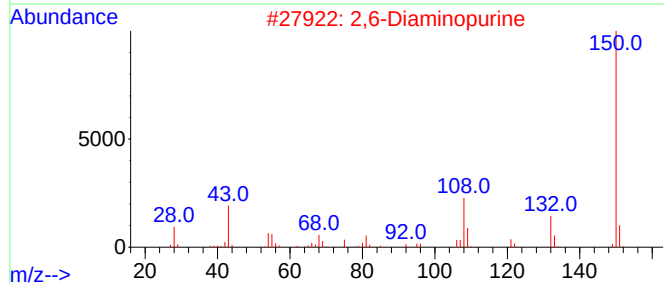
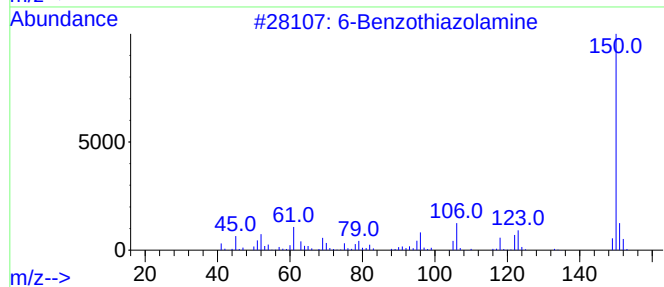
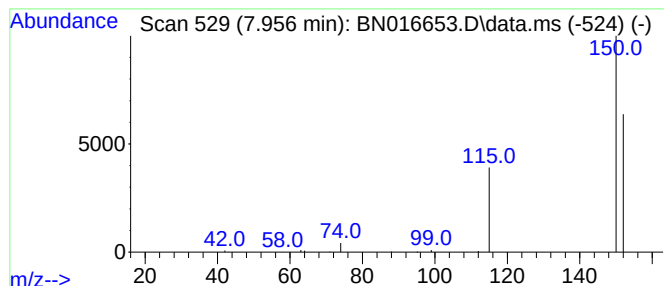
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	103394	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
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Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

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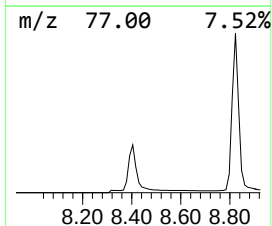
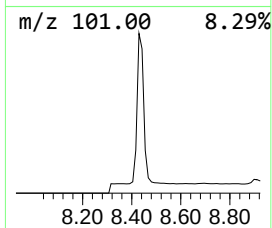
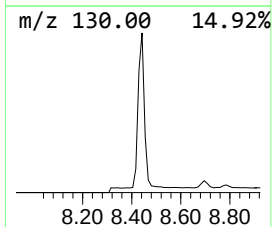
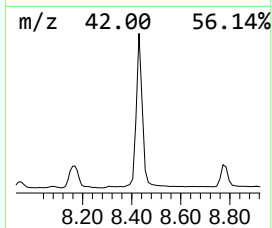
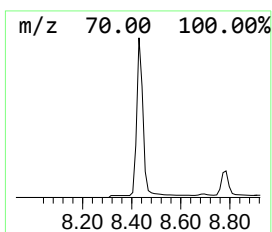
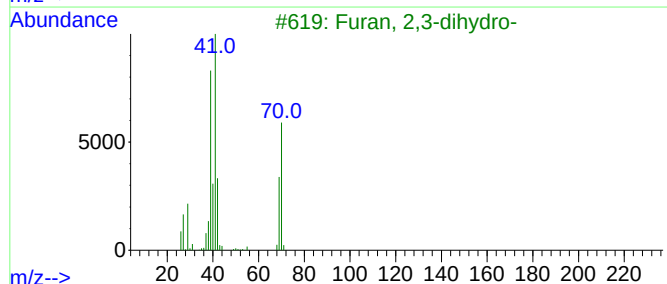
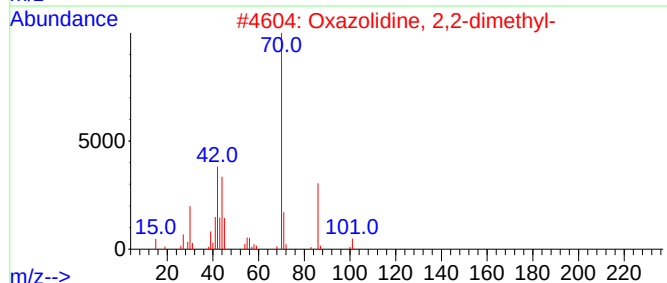
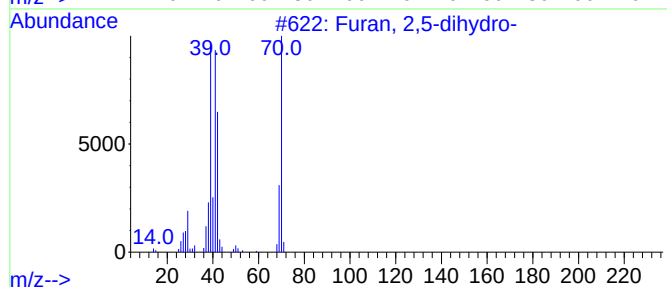
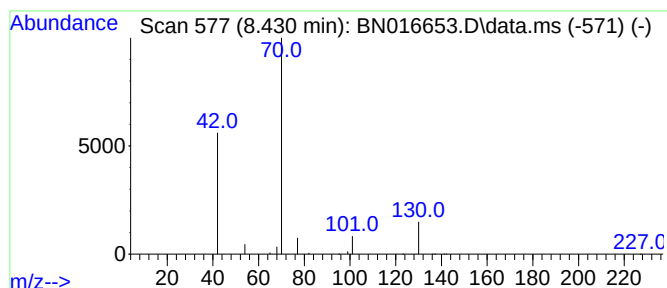
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.16 ng	46950	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



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Data File : BN016653.D
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ClientSampleId :
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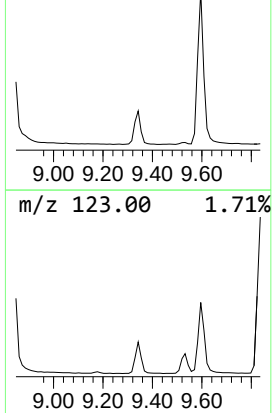
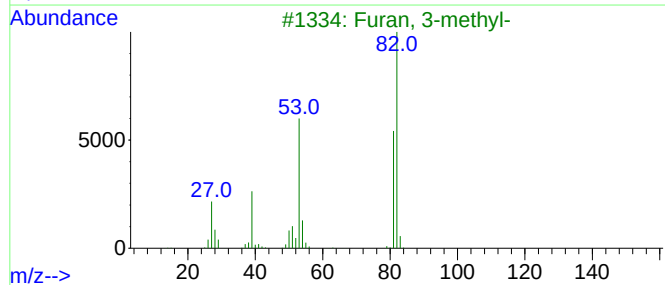
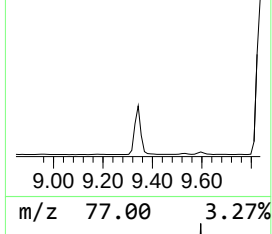
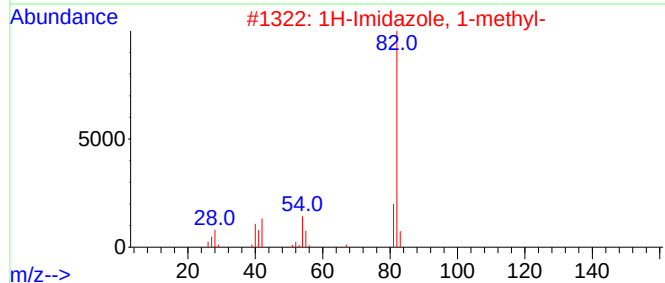
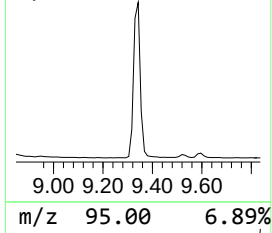
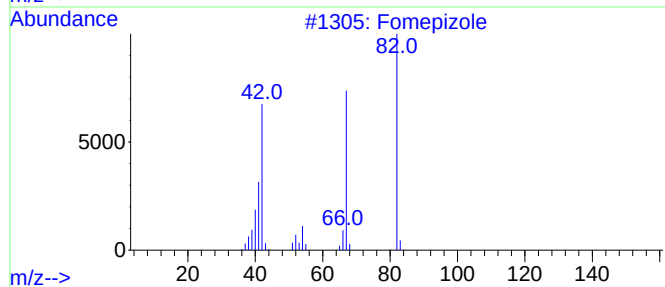
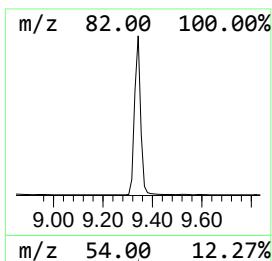
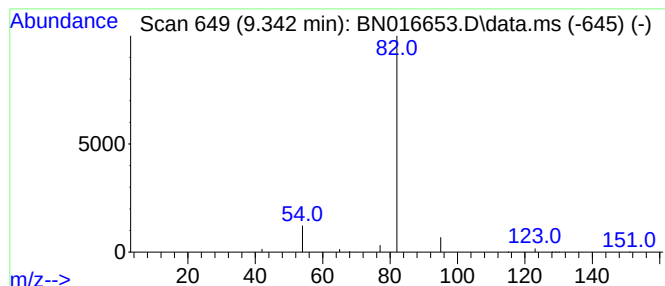
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.15 ng	71940	Naphthalene-d8	10.407

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fomepizole	82	C4H6N2	007554-65-6	5
2		1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
3		Furan, 3-methyl-	82	C5H6O	000930-27-8	4
4		Furan, 2-methyl-	82	C5H6O	000534-22-5	4
5		3-Aminocrotononitrile	82	C4H6N2	001118-61-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
Acq On : 02 Oct 2021 03:23
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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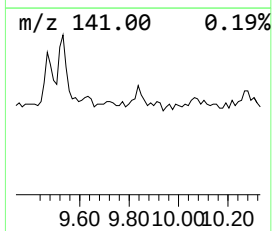
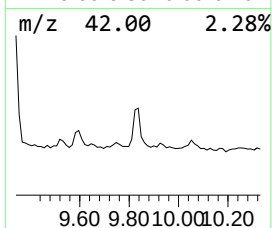
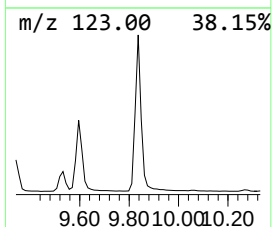
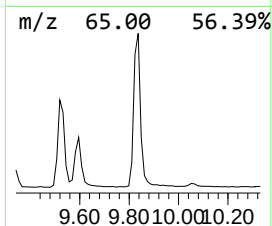
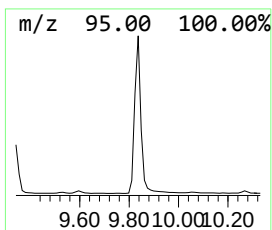
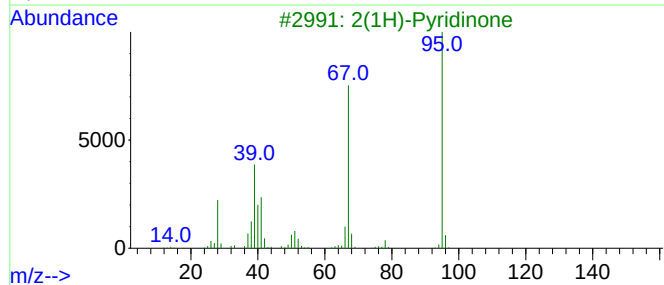
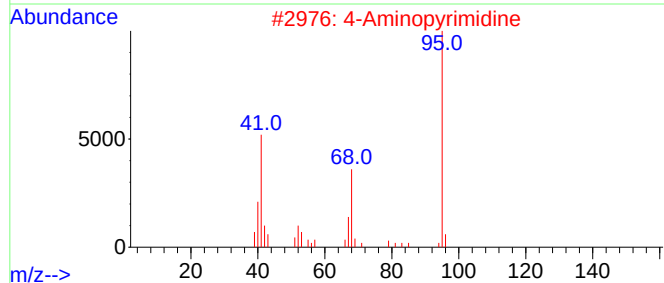
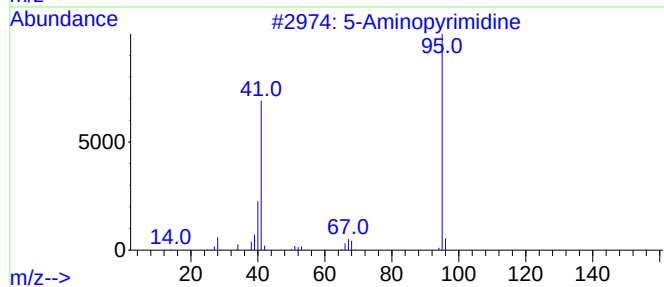
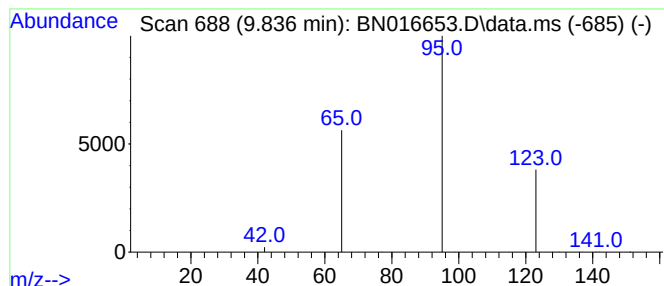
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Aminopyrimidine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	26338	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

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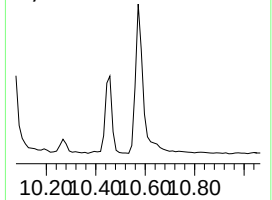
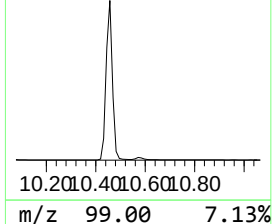
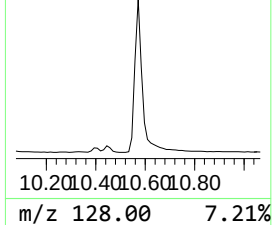
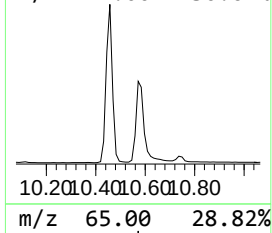
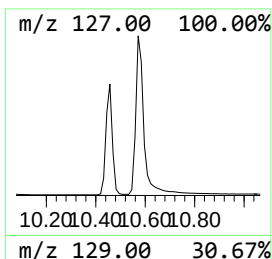
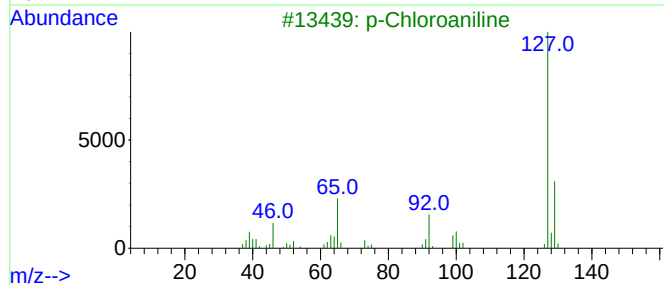
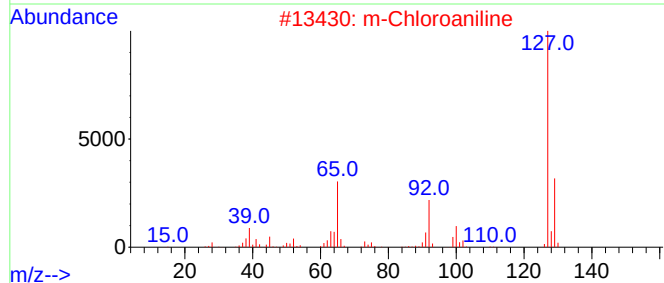
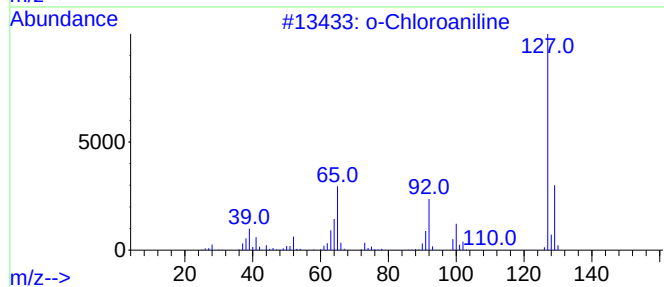
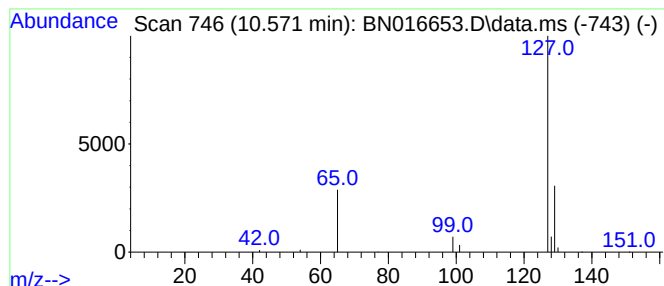
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	56814	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			Pyridine, 2-chloro-6-methyl-	127	C6H6ClN	018368-63-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
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Misc :
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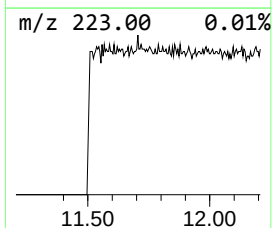
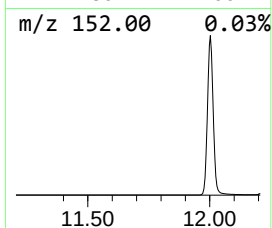
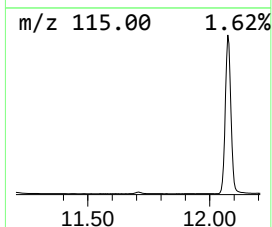
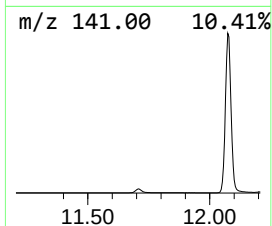
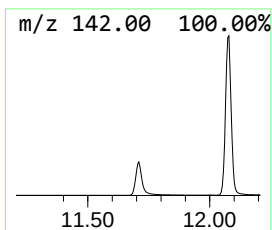
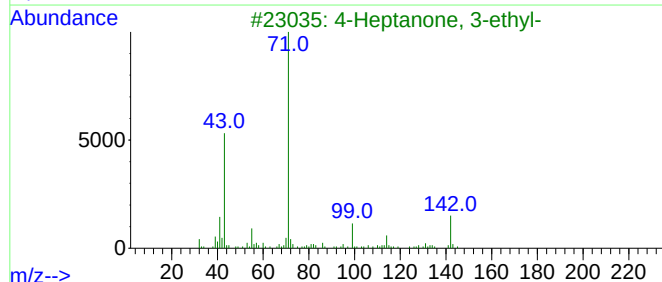
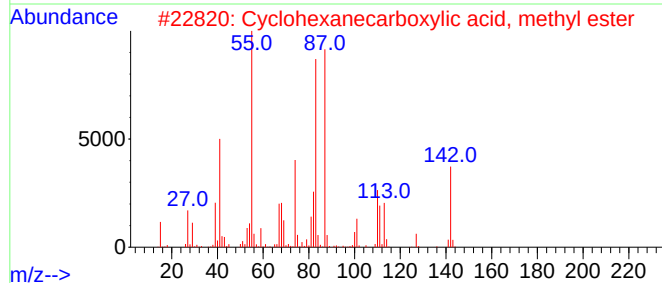
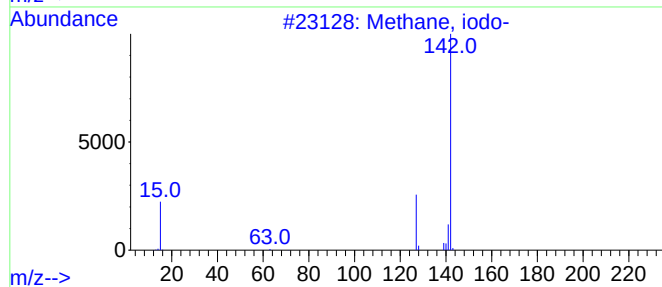
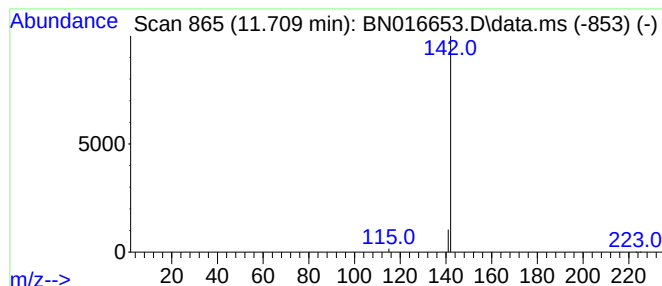
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	23613	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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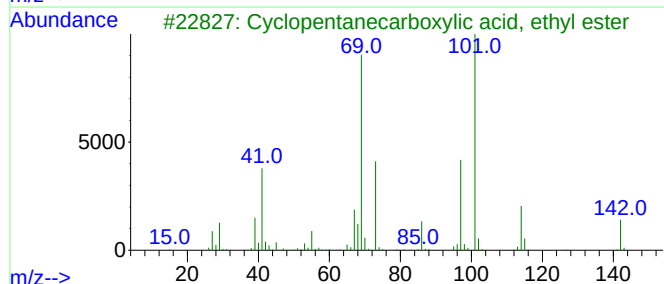
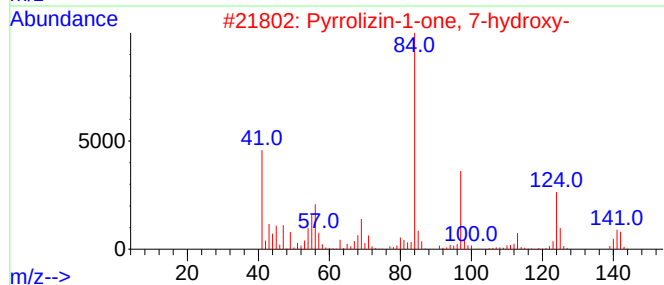
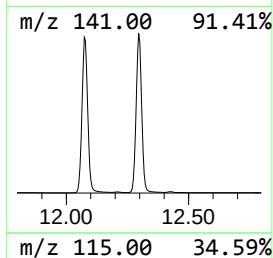
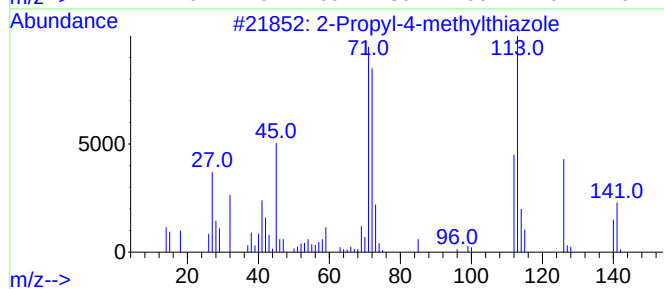
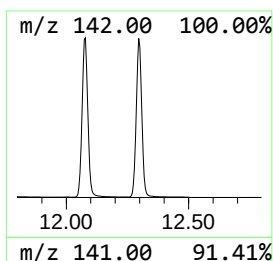
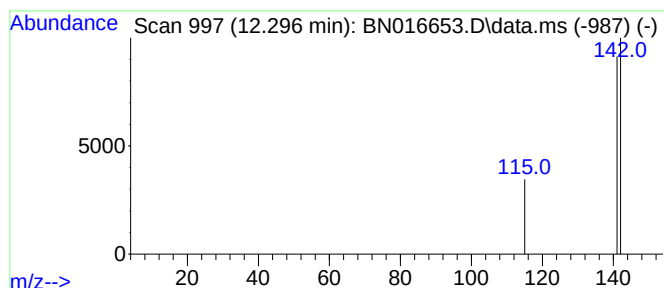
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	192089	Naphthalene-d8	10.407	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
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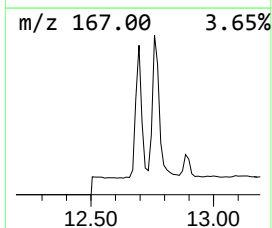
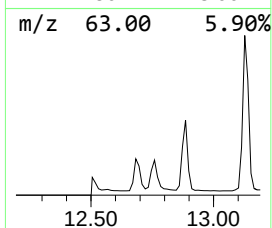
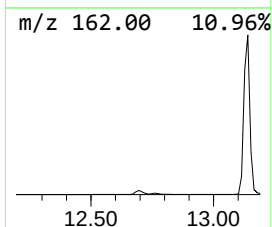
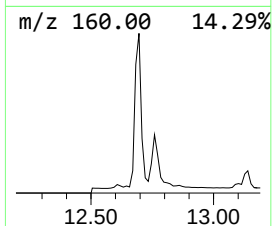
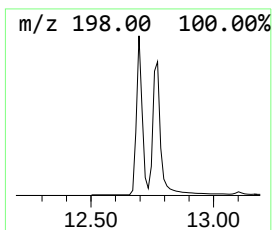
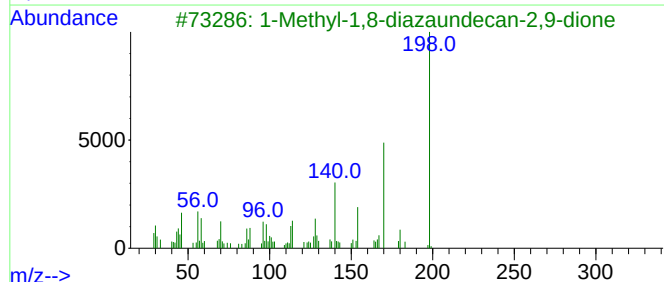
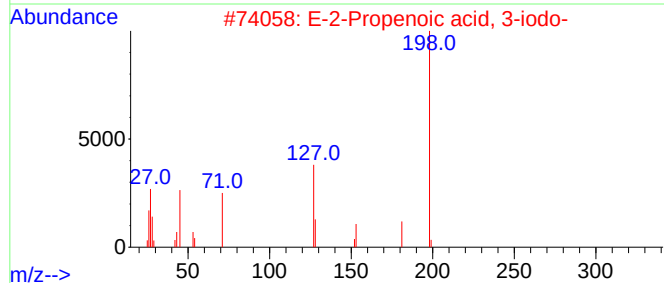
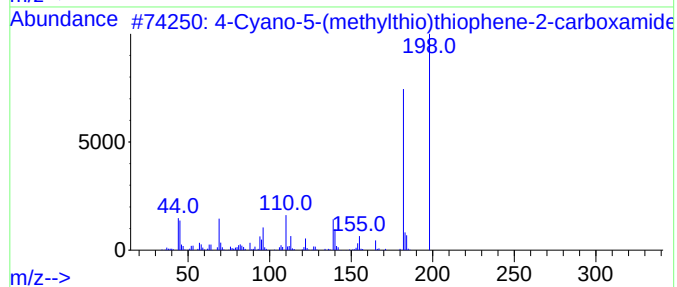
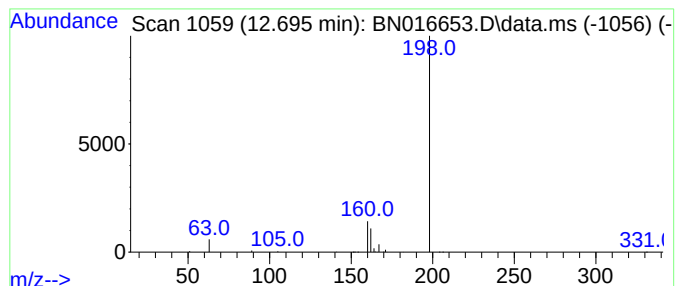
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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	27083	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

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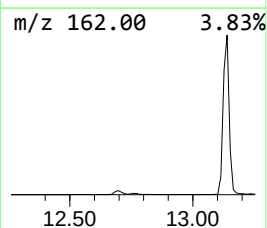
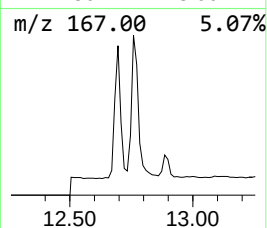
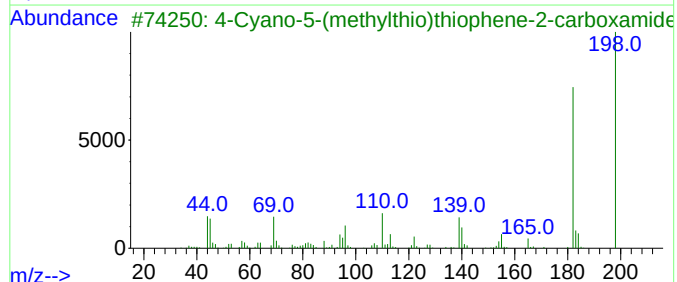
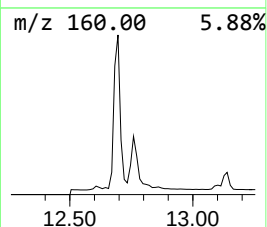
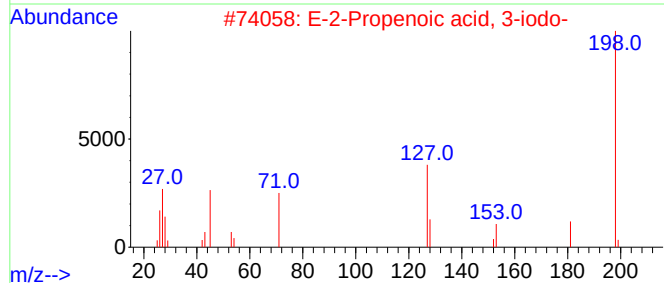
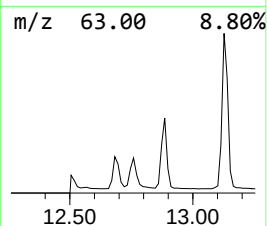
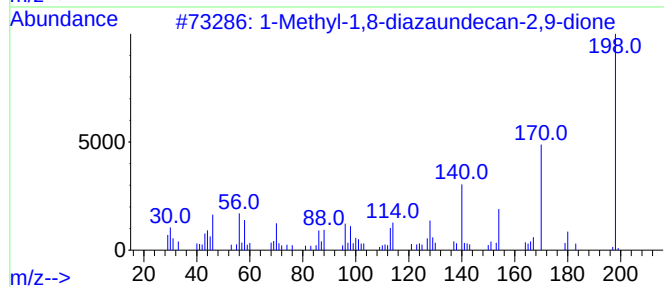
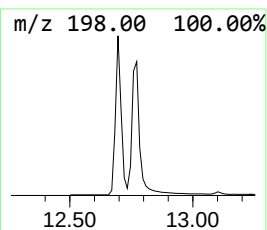
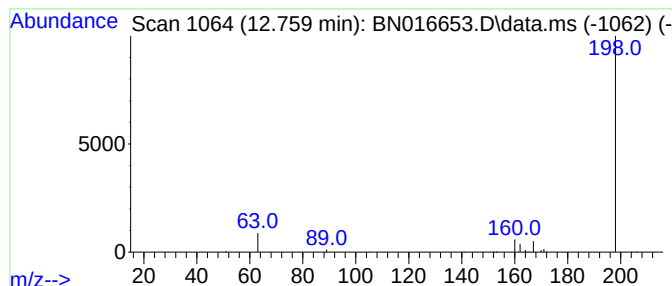
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Methyl-1,8-diazaundecan-2... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	23752	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

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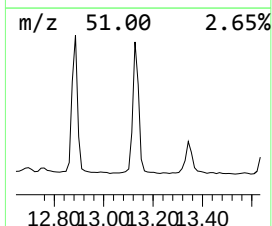
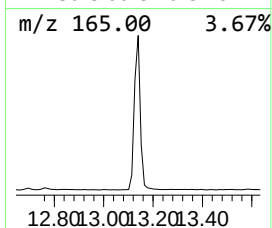
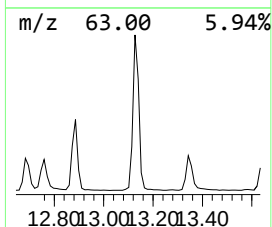
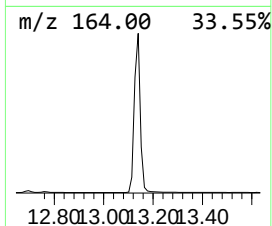
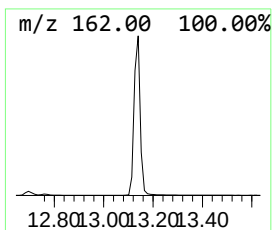
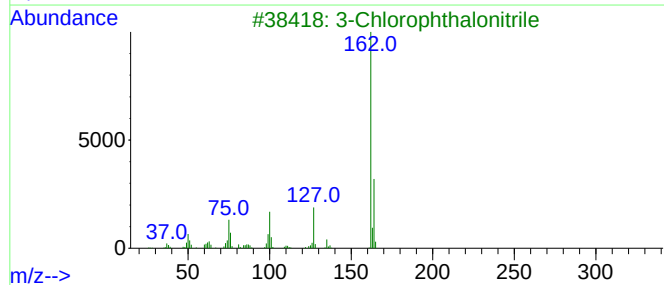
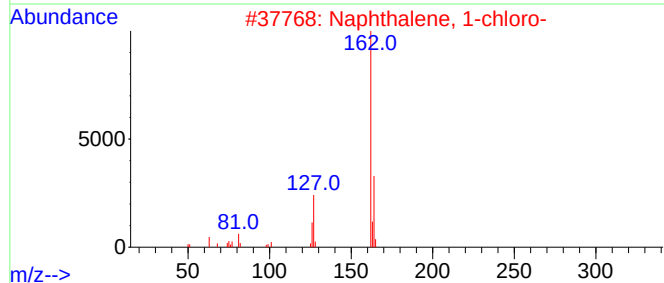
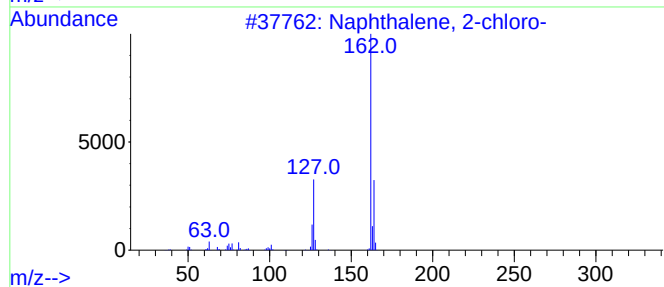
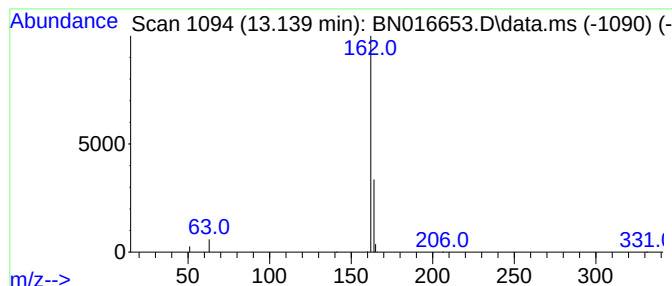
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.26 ng	124429	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

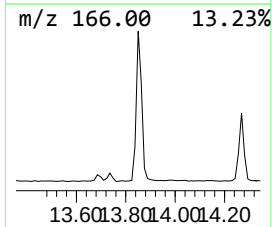
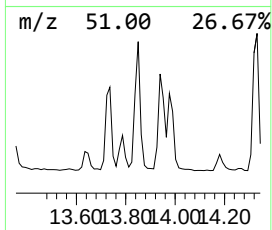
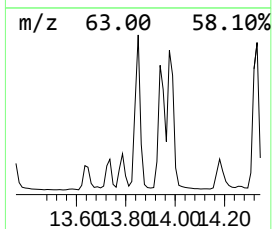
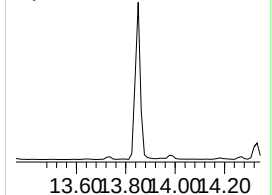
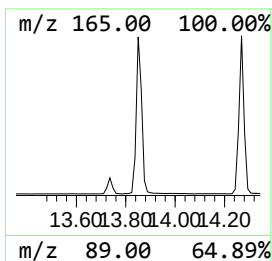
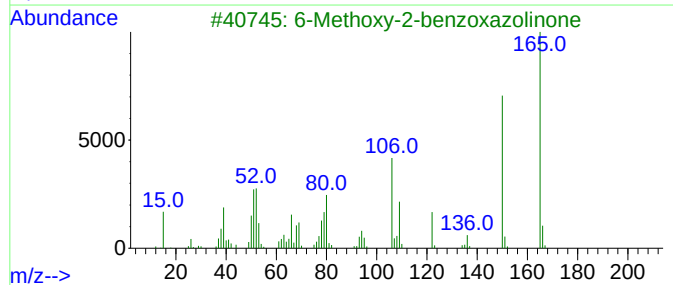
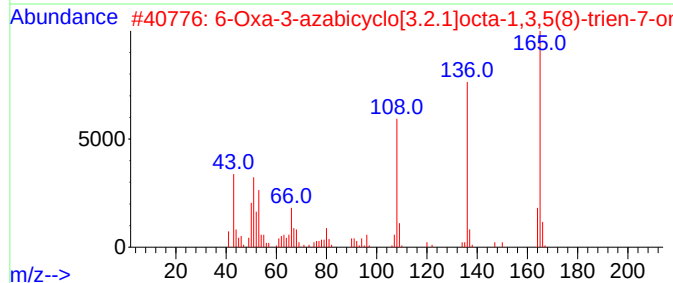
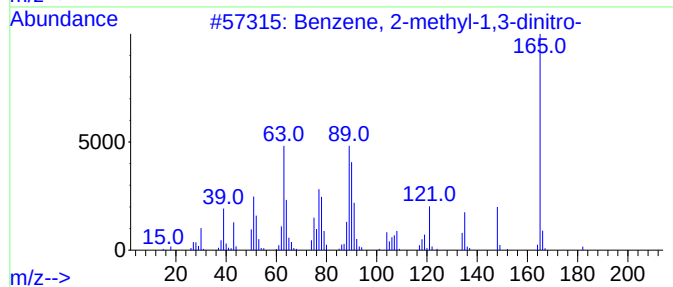
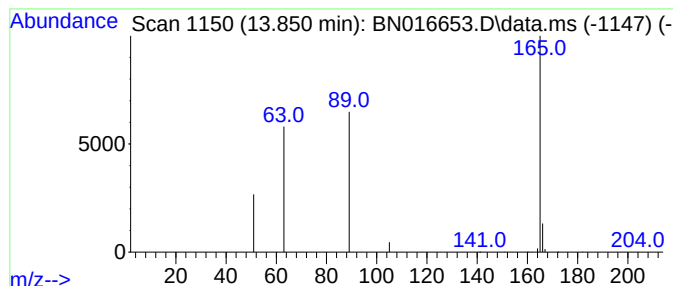
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	0.05 ng	25693	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-Oxa-3-azabicyclo[3.2.1]octa-1,...		165	C8H7NO3	055255-96-4	9
3	6-Methoxy-2-benzoxazolinone		165	C8H7NO3	000532-91-2	9
4	Furo[3,4-c]pyridin-1(3H)-one, 7-...		165	C8H7NO3	004753-19-9	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

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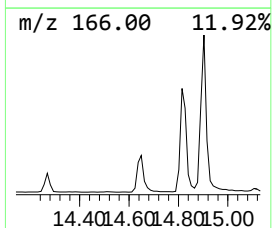
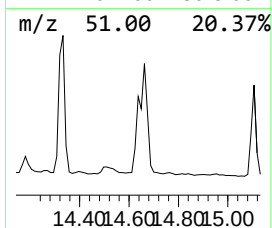
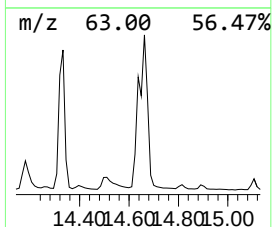
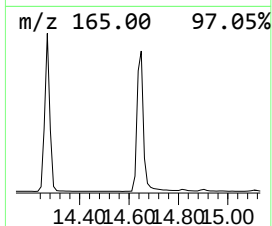
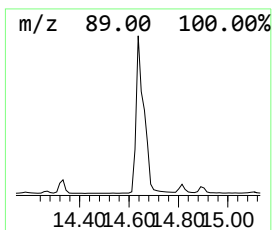
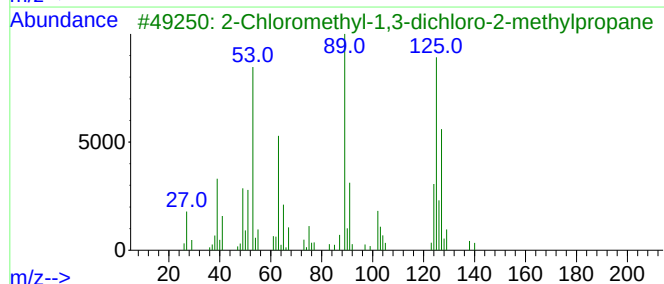
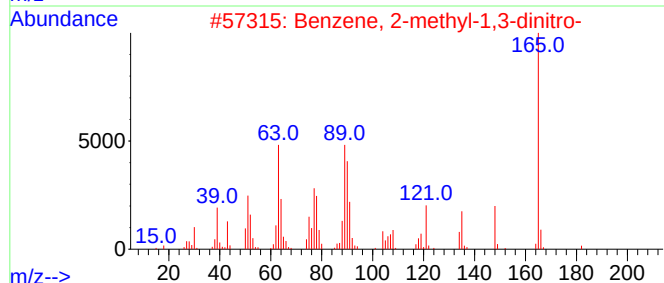
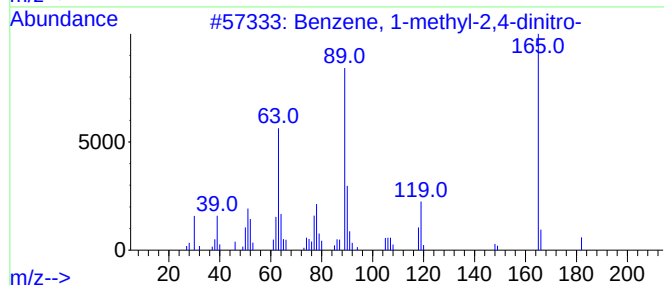
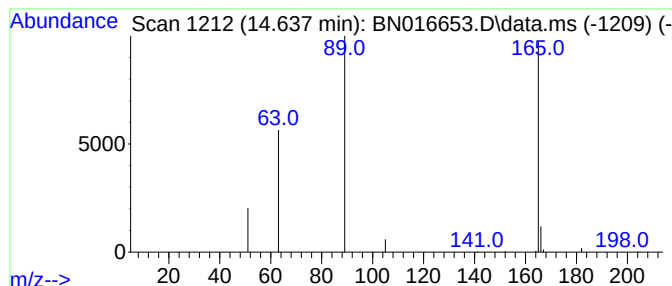
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	40299	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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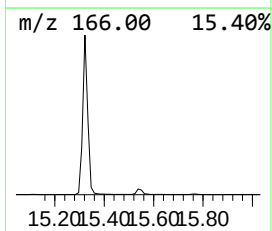
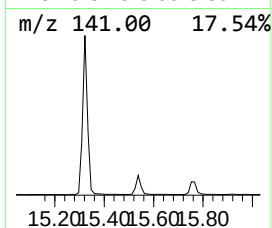
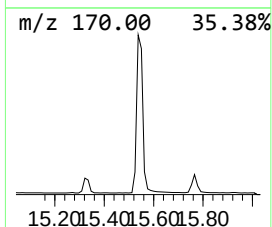
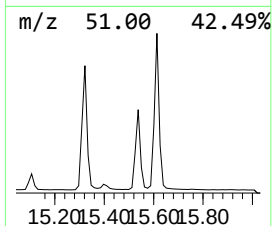
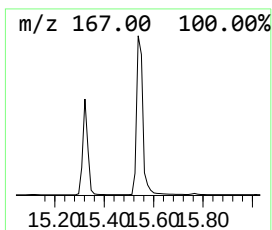
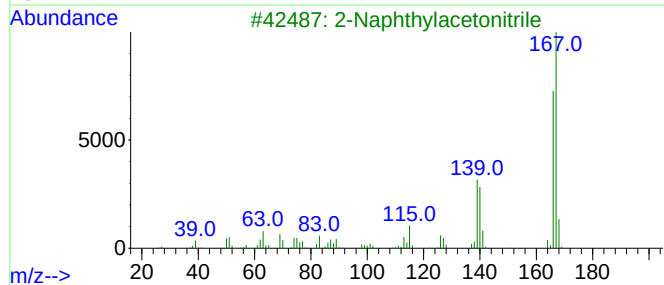
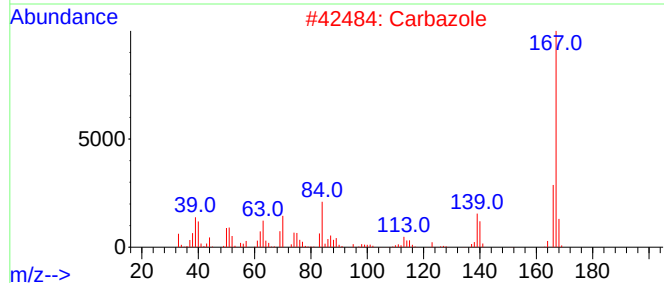
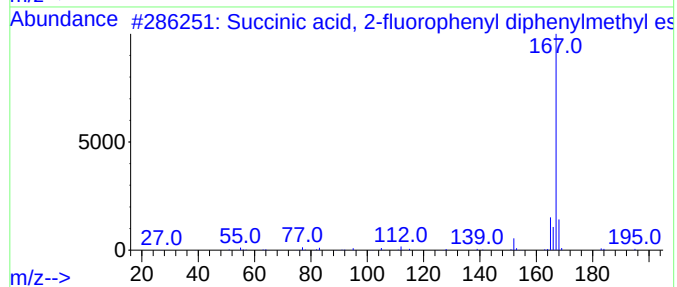
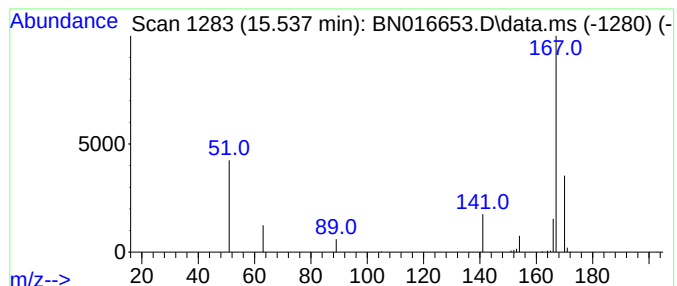
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	58343	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			2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5N04	000097-51-8	5
5			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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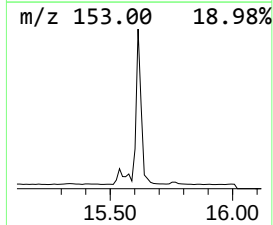
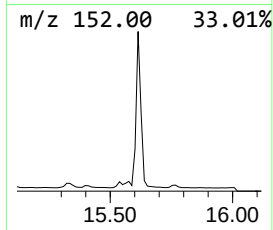
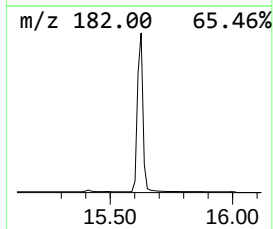
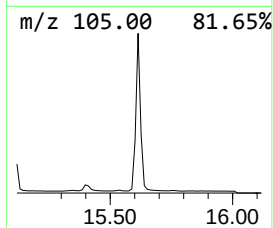
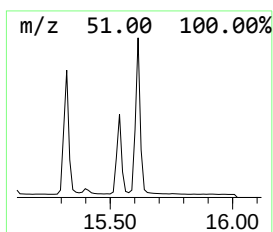
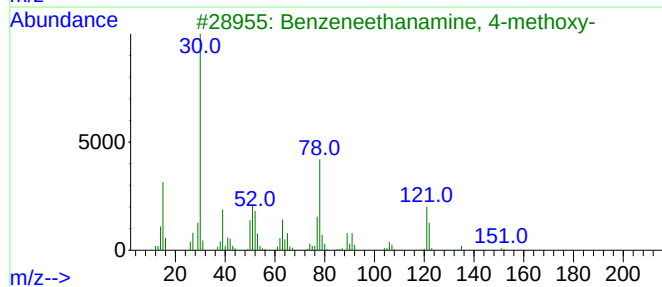
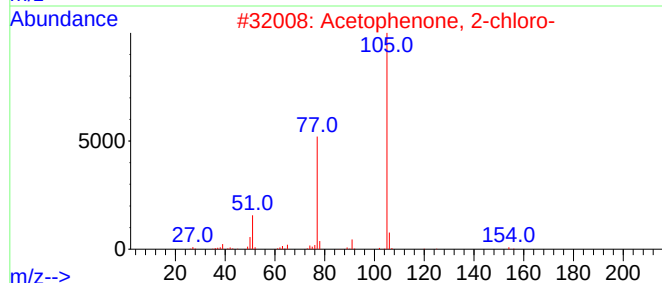
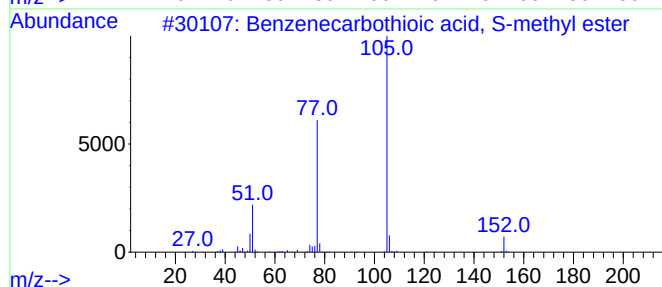
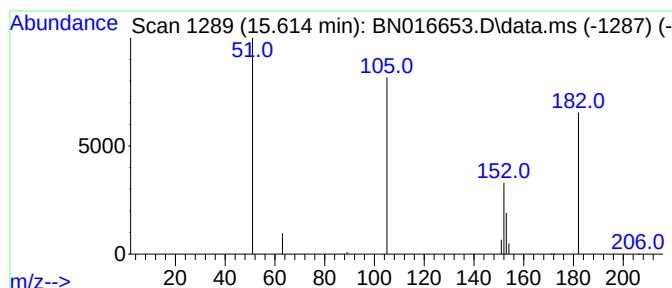
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzenecarbothioic acid, S-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.12 ng	56217	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016653.D
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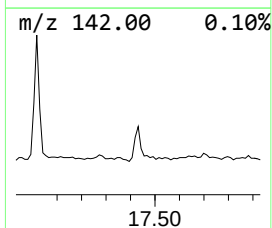
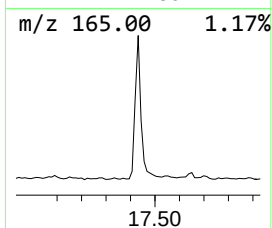
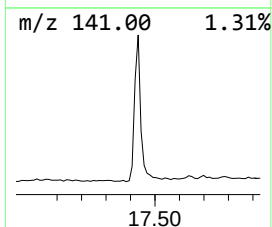
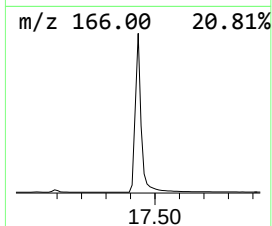
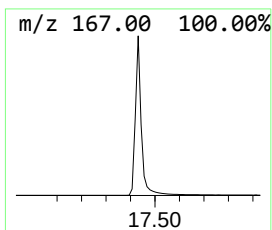
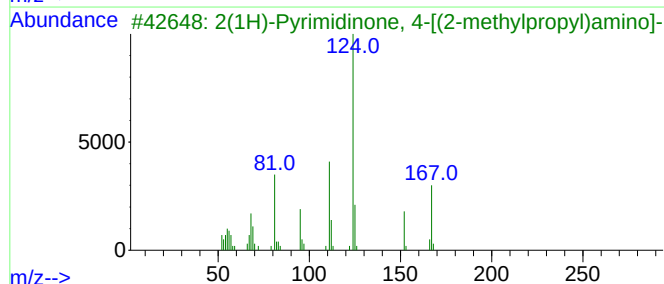
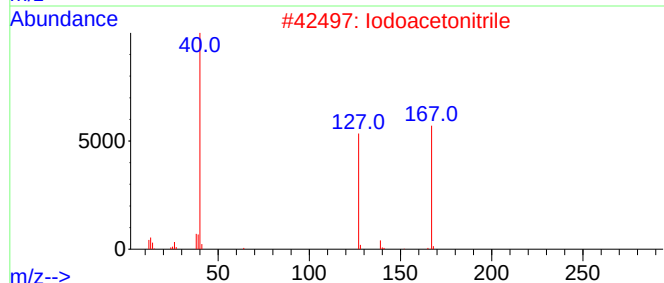
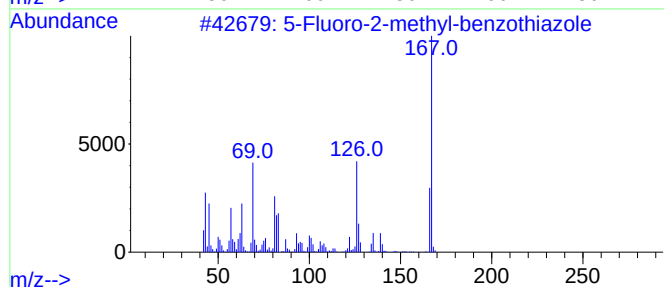
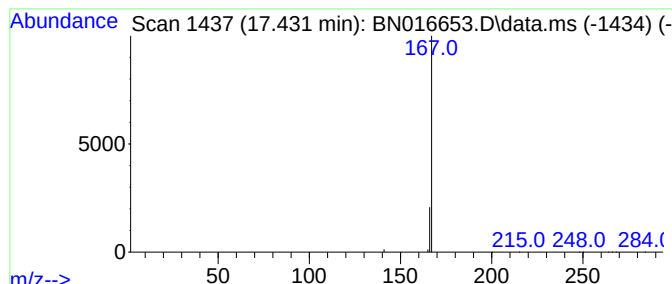
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.33 ng	129969	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 : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139433BS

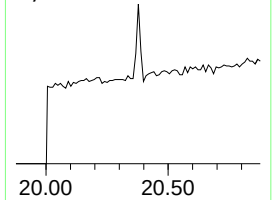
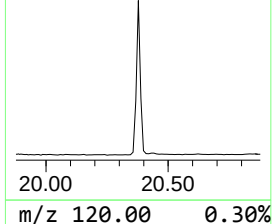
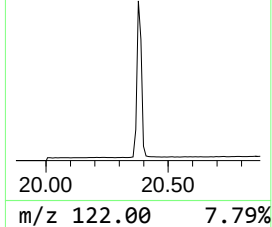
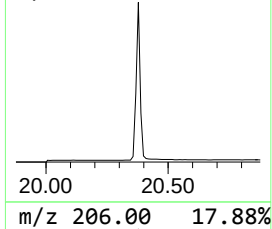
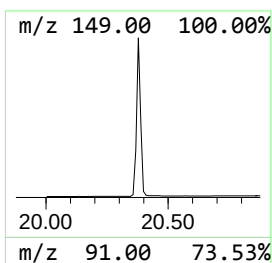
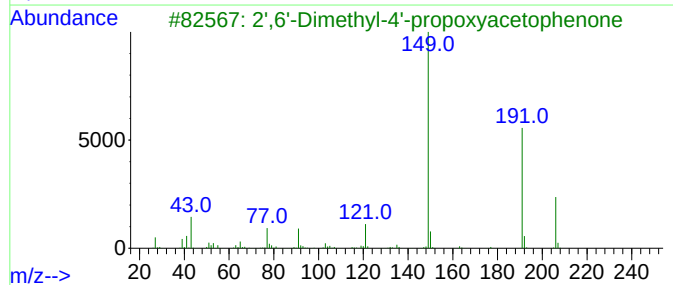
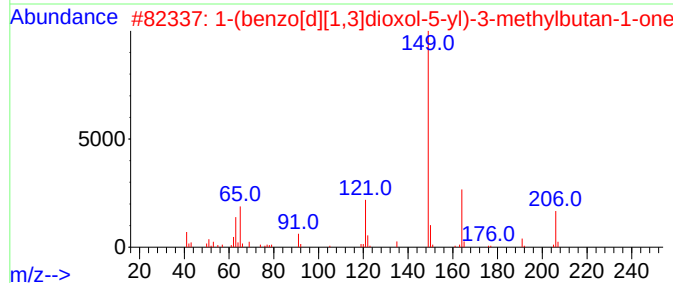
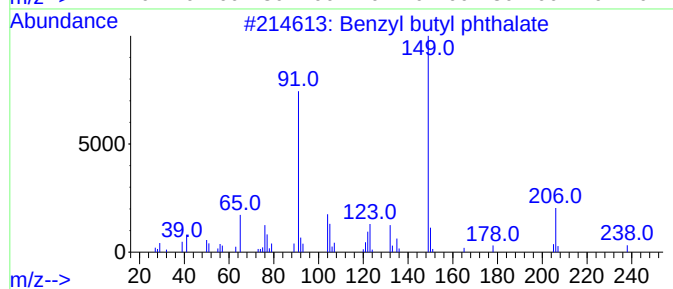
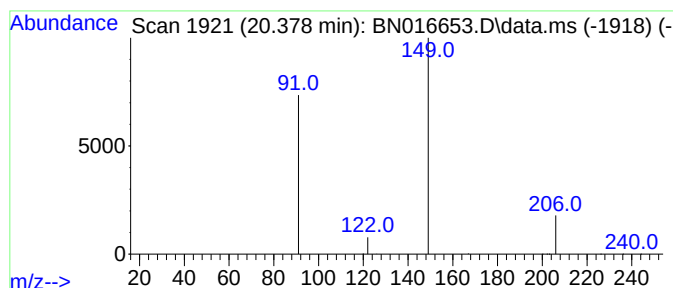
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	59203	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\
Data File : BN016653.D
Acq On : 02 Oct 2021 03:23
Operator : CG/JU
Sample : PB139433BS
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139433BS

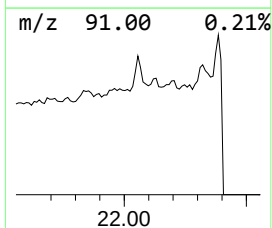
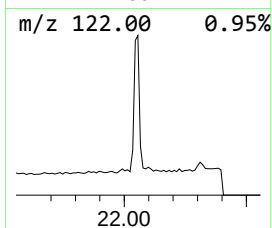
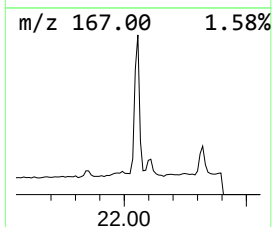
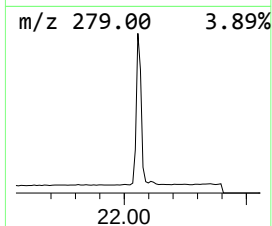
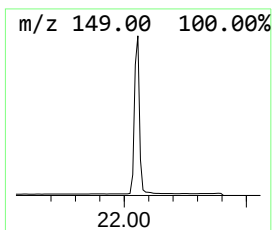
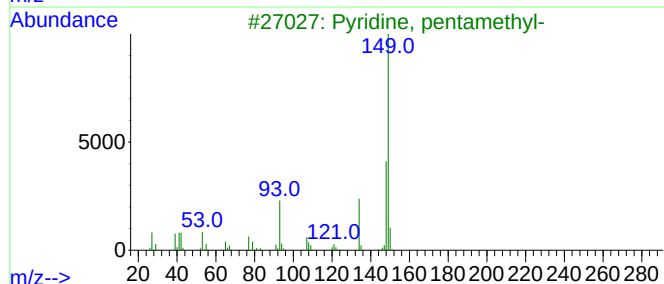
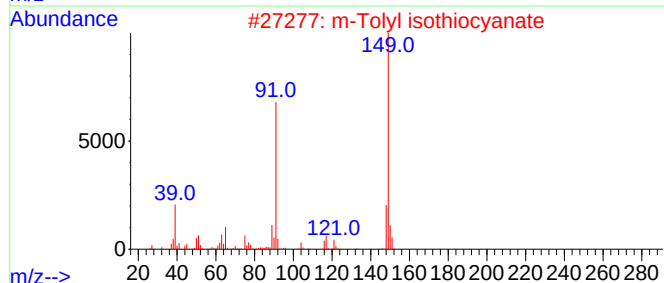
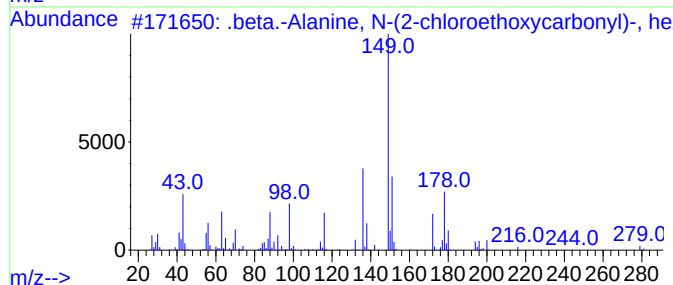
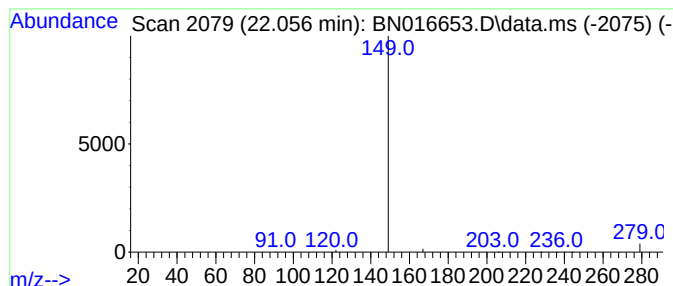
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	80040	Chrysene-d12	21.227

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016653.D
 Acq On : 02 Oct 2021 03:23
 Operator : CG/JU
 Sample : PB139433BS
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139433BS

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	34299	1	7.642	115747	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	30600	1	7.642	115747	0.4
2-Cyclohexen-1-...	7.522	0.0	ng	14466	1	7.642	115747	0.4
6-Benzothiazola...	7.956	0.4	ng	103394	1	7.642	115747	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	46950	1	7.642	115747	0.4
Fomepizole	9.342	0.2	ng	71940	2	10.407	188018	0.4
5-Aminopyrimidine	9.836	0.1	ng	26338	2	10.407	188018	0.4
o-Chloroaniline	10.571	0.1	ng	56814	2	10.407	188018	0.4
Methane, iodo-	11.709	0.1	ng	23613	2	10.407	188018	0.4
2-Propyl-4-meth...	12.296	0.4	ng	192089	2	10.407	188018	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	27083	3	14.269	188650	0.4
1-Methyl-1,8-di...	12.759	0.1	ng	23752	3	14.269	188650	0.4
Naphthalene, 2-...	13.140	0.3	ng	124429	3	14.269	188650	0.4
Benzene, 2-meth...	13.850	0.1	ng	25693	3	14.269	188650	0.4
Benzene, 1-meth...	14.637	0.1	ng	40299	3	14.269	188650	0.4
Succinic acid, ...	15.537	0.1	ng	58343	3	14.269	188650	0.4
Benzenecarbothi...	15.614	0.1	ng	56217	3	14.269	188650	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	129969	4	17.017	156717	0.4
Benzyl butyl ph...	20.378	0.1	ng	59203	5	21.227	410773	0.4
.beta.-Alanine,...	22.056	0.1	ng	80040	5	21.227	410773	0.4