

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016654.D
 Acq On : 02 Oct 2021 03:59
 Operator : CG/JU
 Sample : PB139433BSD
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139433BSD

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: BN016654.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	5937	8695	1.94%	0.122%
2	3.281	20	22	39	rVB	4890	23067	5.16%	0.323%
3	3.594	51	56	87	rVB	5931	29554	6.60%	0.414%
4	5.263	231	237	254	rVB	13343	51186	11.44%	0.716%
5	6.821	401	406	418	rBV	21729	55629	12.43%	0.779%
6	6.978	418	423	429	rVV	15462	33966	7.59%	0.475%
7	7.080	429	434	440	rVV	32254	66829	14.94%	0.935%
8	7.200	440	447	460	rVB	11114	29693	6.64%	0.416%
9	7.522	478	482	488	rVB	6347	13921	3.11%	0.195%
10	7.642	490	495	509	rVB2	43891	108726	24.30%	1.522%
11	7.956	524	529	538	rVB2	43412	99114	22.15%	1.387%
12	8.168	547	552	557	rBV	2846	6934	1.55%	0.097%
13	8.429	571	577	591	rVB3	19510	45530	10.18%	0.637%
14	8.695	594	598	601	rBV	4298	8184	1.83%	0.115%
15	8.784	601	605	606	rBV	29605	56640	12.66%	0.793%
16	8.822	606	608	617	rVB	24369	45801	10.24%	0.641%
17	9.342	645	649	652	rBV	41728	70175	15.68%	0.982%
18	9.519	660	663	666	rBV	2859	5680	1.27%	0.079%
19	9.595	666	669	679	rVB	7804	14125	3.16%	0.198%
20	9.836	685	688	702	rVB	14088	25454	5.69%	0.356%
21	10.052	702	705	718	rVB	3688	8318	1.86%	0.116%
22	10.406	729	733	735	rBV	95979	177548	39.68%	2.485%
23	10.457	735	737	741	rVV	97723	162332	36.28%	2.272%
24	10.571	743	746	756	rVV	25226	55776	12.46%	0.781%
25	10.749	756	760	763	rVB	28624	51449	11.50%	0.720%
26	11.709	852	865	901	rBV	12295	23410	5.23%	0.328%
27	12.002	920	931	939	rBV	53080	85224	19.05%	1.193%
28	12.074	939	947	972	rVV	114477	190670	42.61%	2.668%
29	12.296	987	997	1021	rVV	116703	184175	41.16%	2.577%
30	12.695	1056	1059	1062	rBV	15505	26044	5.82%	0.364%
31	12.771	1062	1065	1071	rVB	10648	22516	5.03%	0.315%
32	12.886	1071	1074	1078	rBV	113544	181571	40.58%	2.541%
33	13.139	1089	1094	1097	rBV	71041	122236	27.32%	1.711%
34	13.736	1138	1141	1143	rBV	10766	15314	3.42%	0.214%
35	13.850	1147	1150	1153	rVB	17134	24608	5.50%	0.344%
36	13.939	1155	1157	1158	rBV	4785	7657	1.71%	0.107%

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

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37	13.989	1158	1161	1164	rVB	83817	139133	31.09%	1.947%
38	14.268	1180	1183	1185	rBV	122747	177564	39.68%	2.485%
39	14.332	1185	1188	1191	rVB	154027	223271	49.90%	3.125%
40	14.636	1209	1212	1220	rBV3	14451	38819	8.68%	0.543%
41	14.814	1224	1226	1230	rVV	4792	8377	1.87%	0.117%
42	14.903	1230	1233	1243	rVB	6944	11469	2.56%	0.161%
43	15.106	1246	1249	1252	rBV	7748	10019	2.24%	0.140%
44	15.322	1263	1266	1270	rBV2	212893	324247	72.46%	4.538%
45	15.410	1271	1273	1280	rVV2	2163	5699	1.27%	0.080%
46	15.537	1280	1283	1287	rVV	34090	57310	12.81%	0.802%
47	15.613	1287	1289	1298	rVV2	37860	57963	12.95%	0.811%
48	15.766	1298	1301	1311	rVB2	12160	20607	4.61%	0.288%
49	16.226	1334	1338	1341	rBV2	52694	84505	18.89%	1.183%
50	16.324	1343	1346	1350	rVB	44553	67096	14.99%	0.939%
51	16.506	1358	1361	1372	rVB	17864	30712	6.86%	0.430%
52	16.677	1372	1375	1384	rBV	16545	30304	6.77%	0.424%
53	17.017	1400	1403	1405	rBV	93920	148689	33.23%	2.081%
54	17.066	1405	1407	1410	rVV	136280	199641	44.62%	2.794%
55	17.151	1411	1414	1434	rVB	105482	172050	38.45%	2.408%
56	17.431	1434	1437	1453	rBV	76361	127015	28.39%	1.778%
57	18.015	1482	1485	1507	rVB8	5070	6932	1.55%	0.097%
58	19.063	1686	1696	1699	rBV	109002	154639	34.56%	2.164%
59	19.092	1699	1702	1747	rVB	170007	242941	54.29%	3.400%
60	19.460	1766	1776	1808	rBV	168143	238766	53.36%	3.341%
61	19.678	1813	1820	1844	rBV	98883	130887	29.25%	1.832%
62	20.378	1918	1921	1924	rBV	46562	53770	12.02%	0.752%
63	21.163	1992	1995	1997	rBV	49055	57751	12.91%	0.808%
64	21.217	1997	2000	2003	rVV2	196321	389972	87.15%	5.458%
65	21.270	2003	2005	2017	rVB	179892	251449	56.19%	3.519%
66	22.056	2075	2079	2082	rBV	60018	85129	19.02%	1.191%
67	22.803	2216	2228	2234	rBV	116281	194841	43.54%	2.727%
68	22.848	2234	2241	2274	rVB	121919	229133	51.21%	3.207%
69	23.381	2384	2397	2415	rBV	79597	176252	39.39%	2.467%
70	23.481	2415	2426	2461	rVB	89088	185627	41.48%	2.598%
71	24.083	2593	2602	2616	rBV	4646	8615	1.93%	0.121%
72	24.850	2816	2826	2847	rVB2	4715	10653	2.38%	0.149%
73	25.767	3067	3094	3171	rBV3	113614	447463	100.00%	6.262%
74	26.452	3272	3294	3351	rBV	60703	208546	46.61%	2.919%

Sum of corrected areas: 7145607

Instrument :

BNA_N

ClientSampleId :

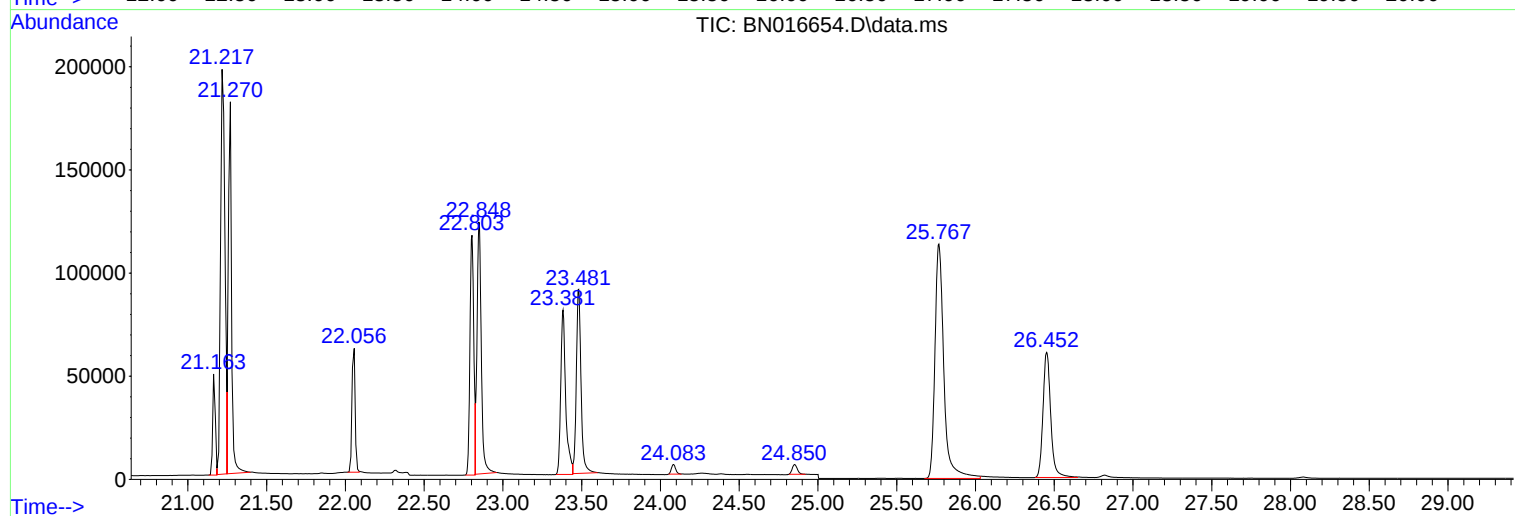
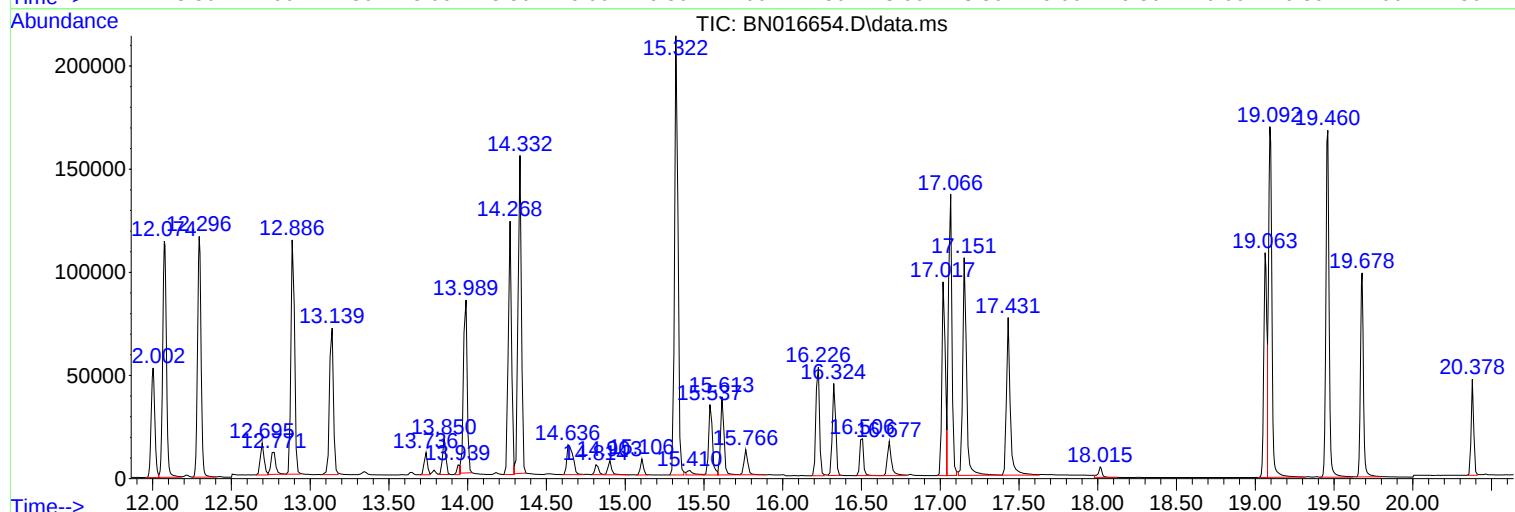
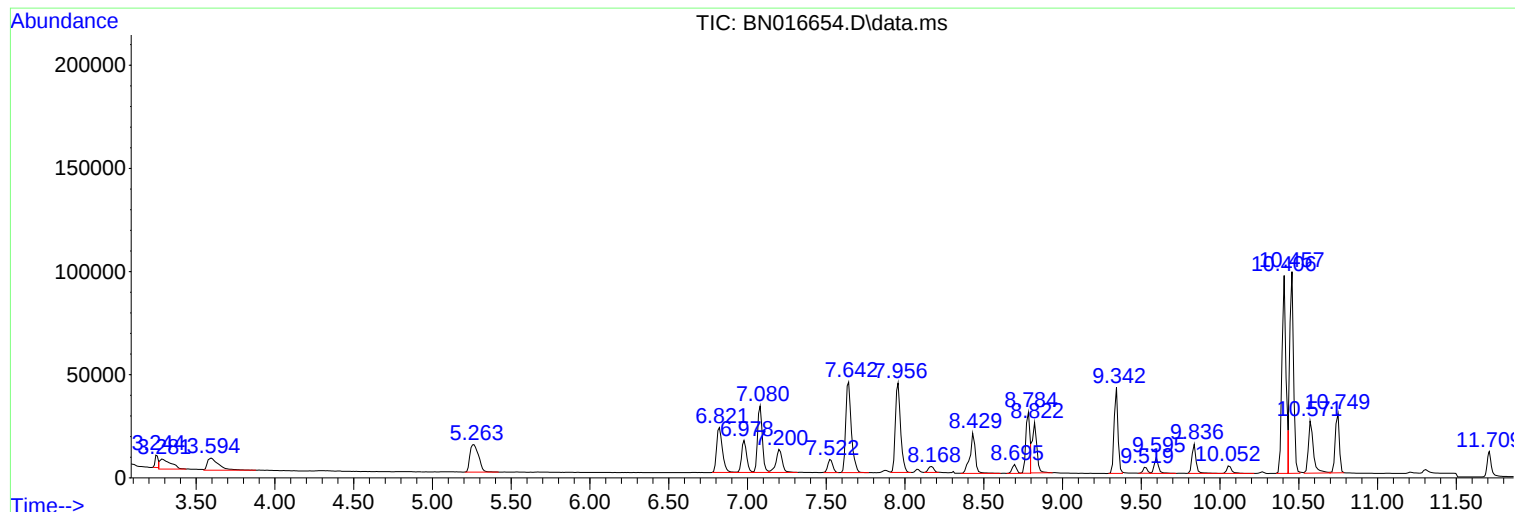
PB139433BSD

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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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Operator : CG/JU
Sample : PB139433BSD
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Instrument :
BNA_N
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PB139433BSD

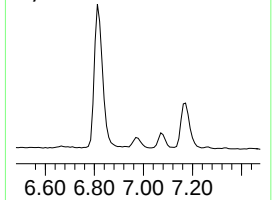
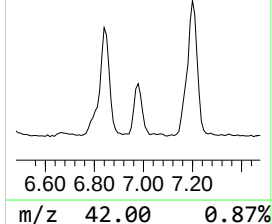
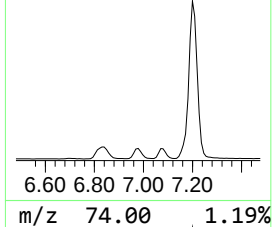
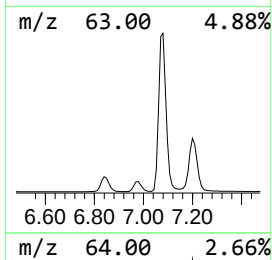
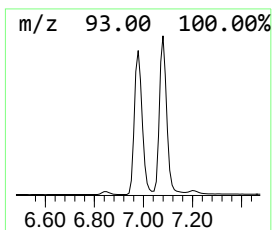
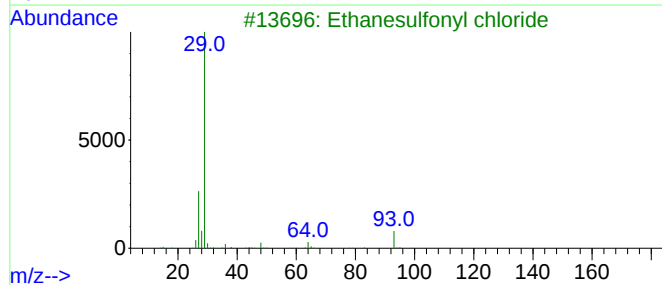
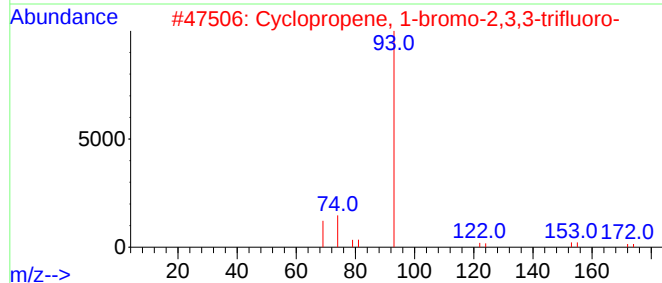
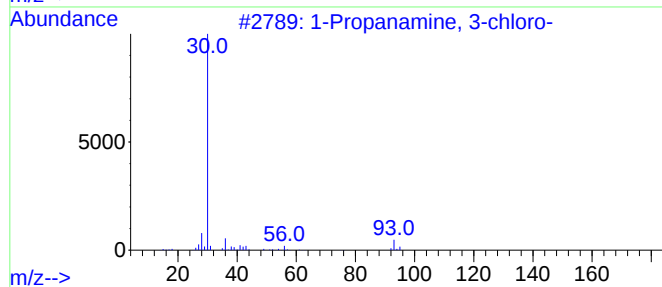
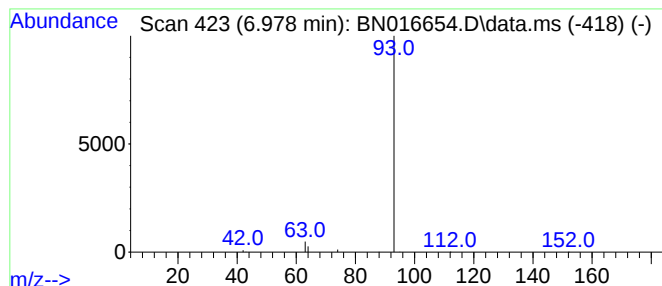
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	33966	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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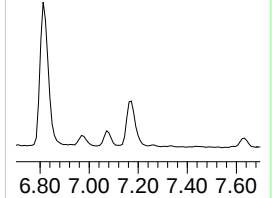
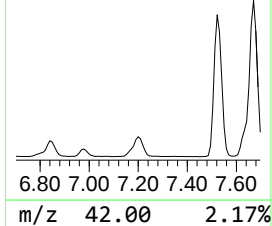
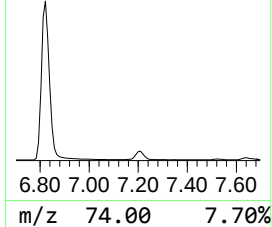
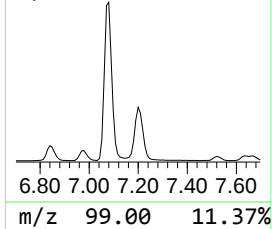
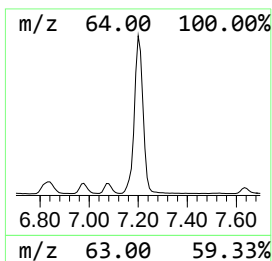
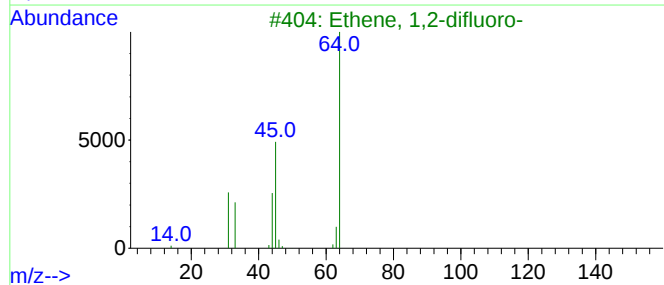
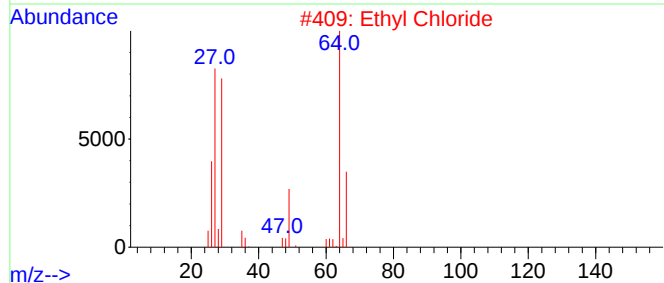
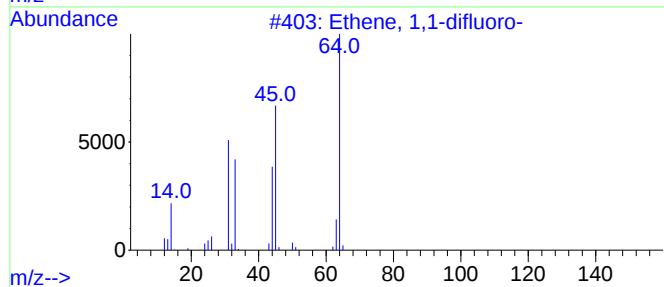
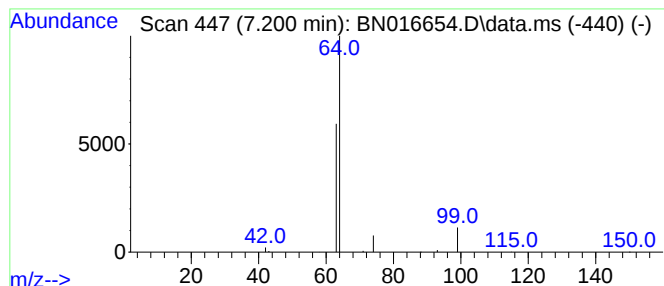
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	29693	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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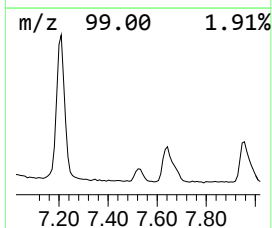
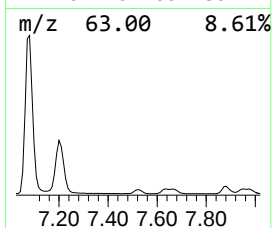
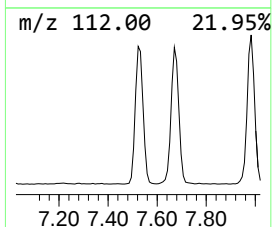
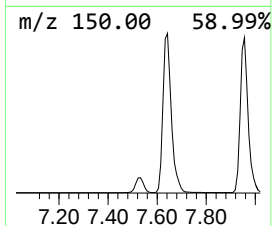
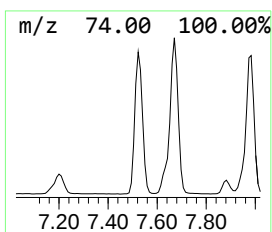
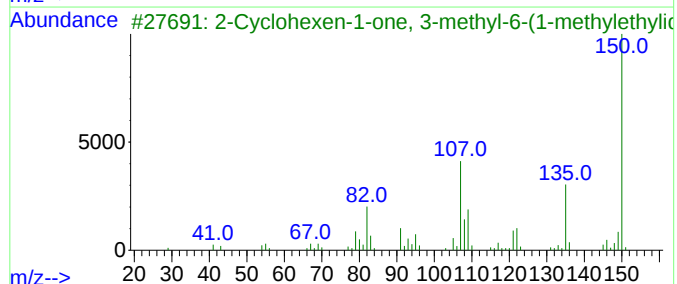
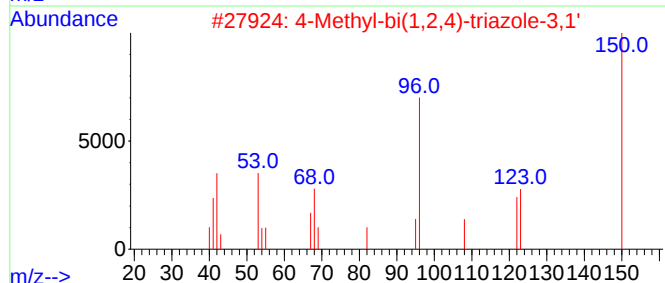
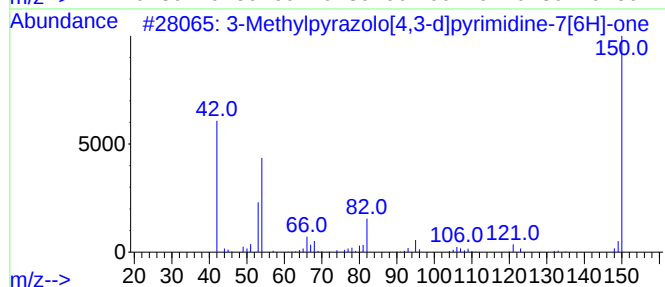
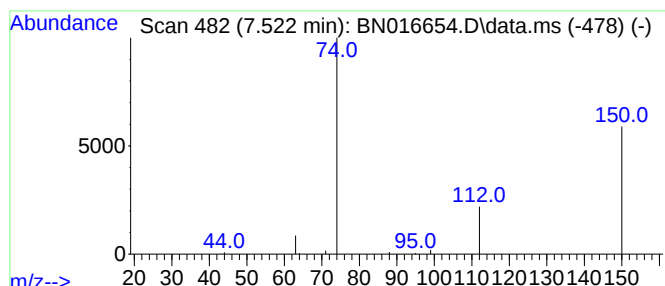
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Methylpyrazolo[4,3-d]pyri... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	13921	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
2			4-Methyl-bi(1,2,4)-triazole-3,1'	150	C5H6N6	063523-89-7	2
3			2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
4			Hexa-1,3,5-triyne	74	C6H2	1010383-52-7	2
5			N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2



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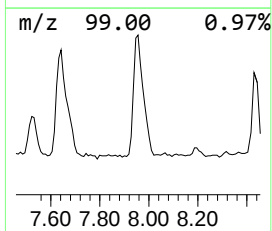
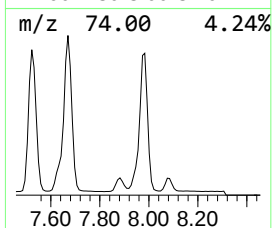
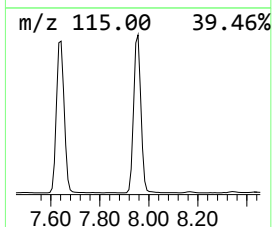
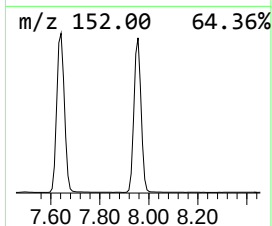
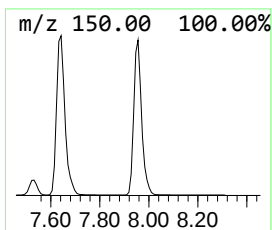
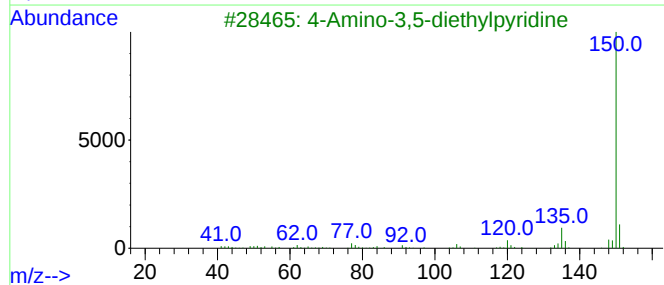
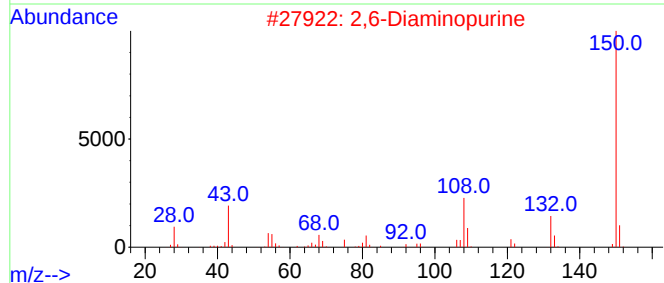
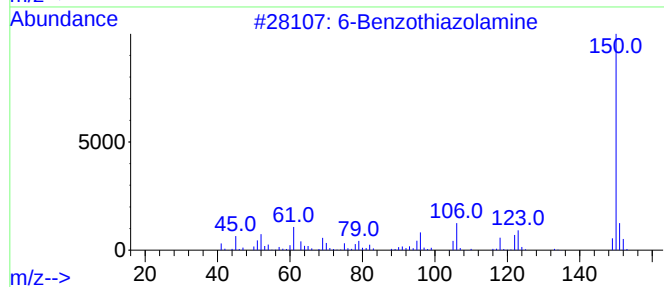
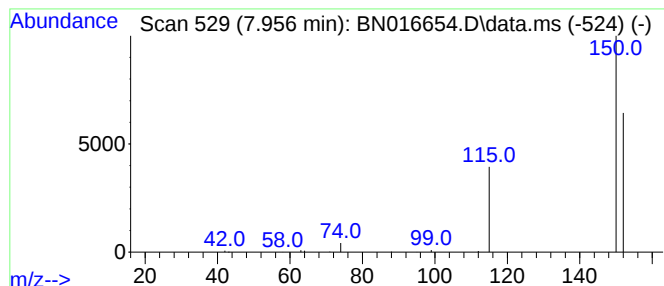
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	99114	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 : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

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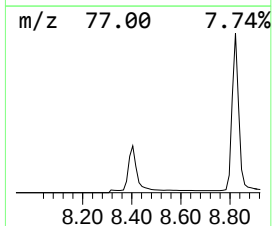
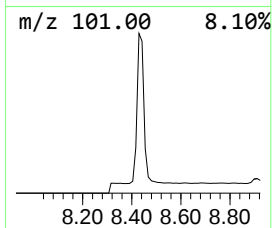
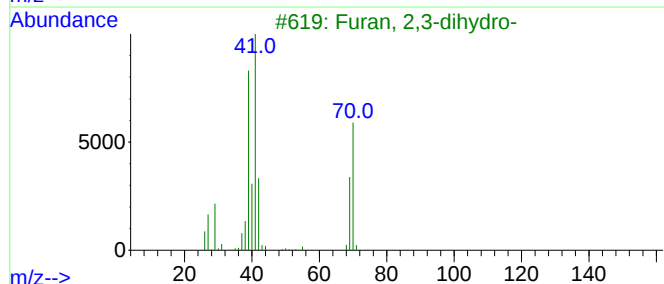
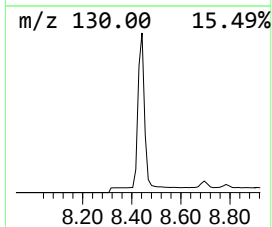
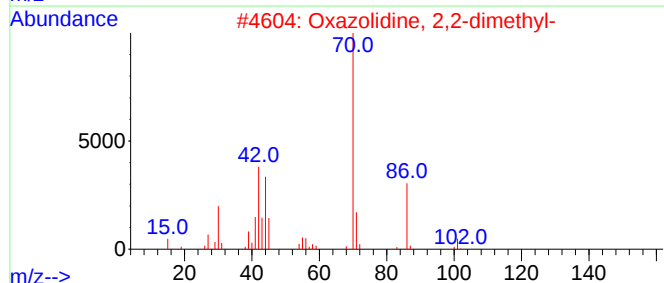
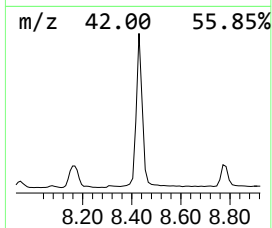
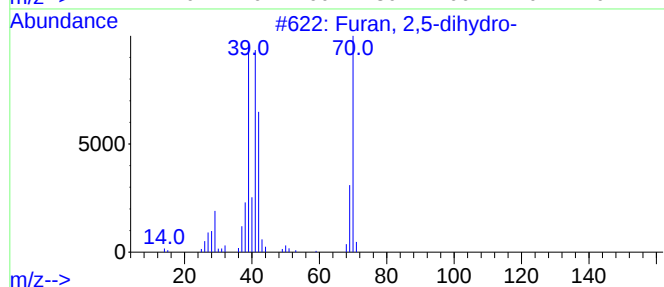
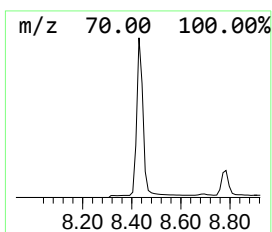
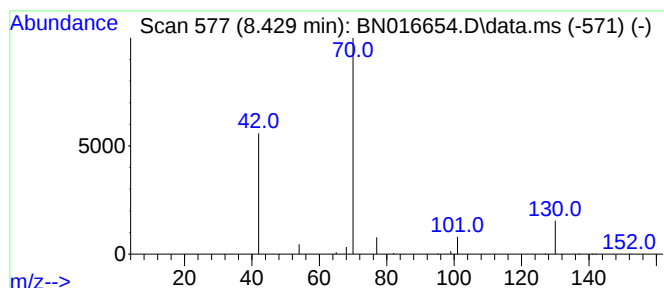
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.17 ng	45530	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2			Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4			Dimethylketene	70	C4H6O	000598-26-5	5
5			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4



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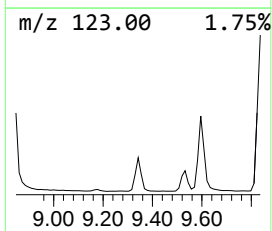
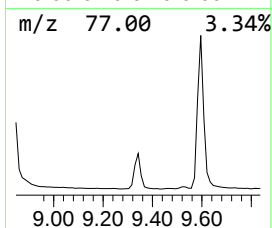
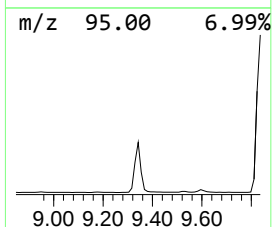
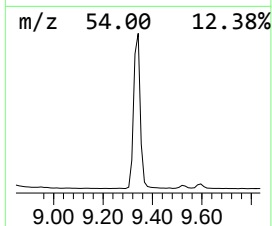
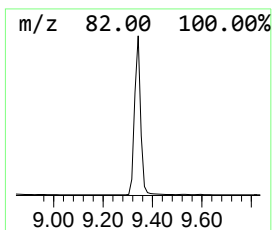
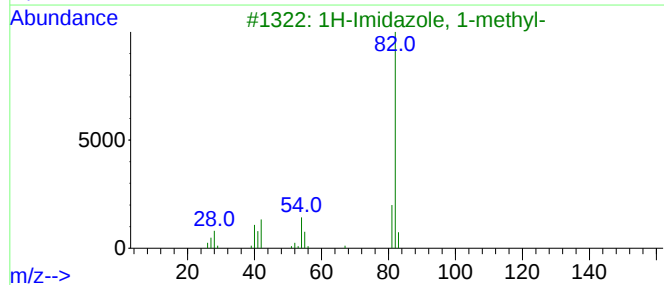
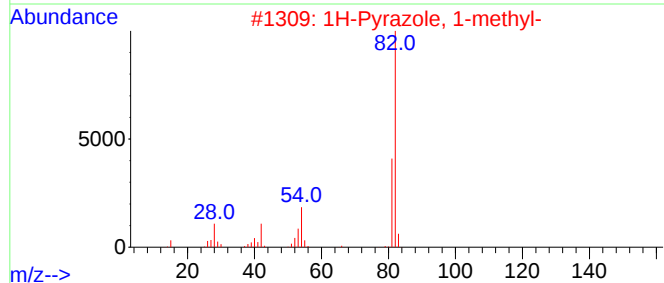
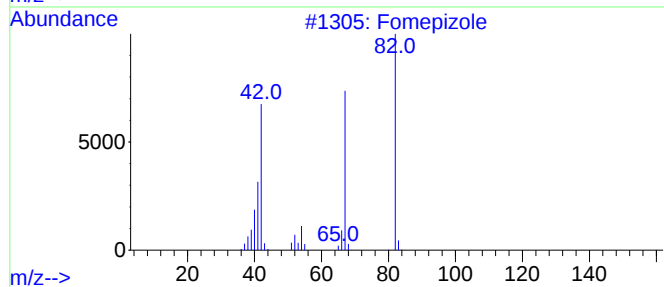
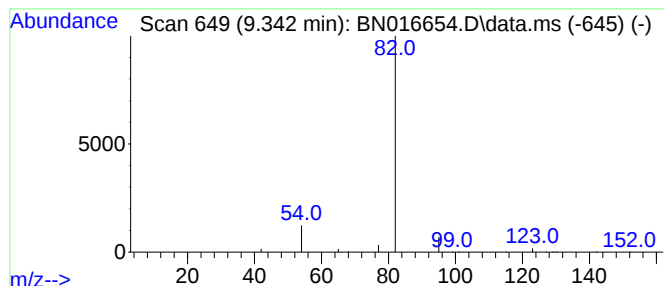
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	70175	Naphthalene-d8	10.406

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
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Sample : PB139433BSD
Misc :
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ClientSampleId :
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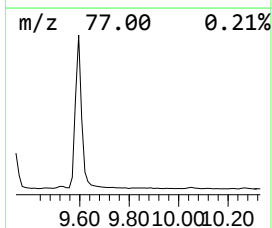
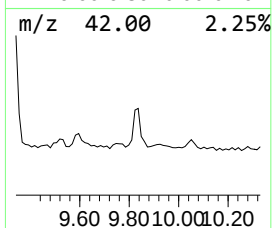
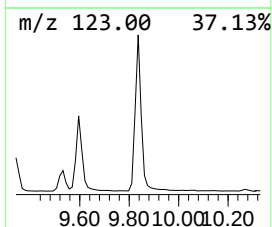
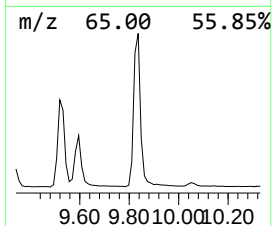
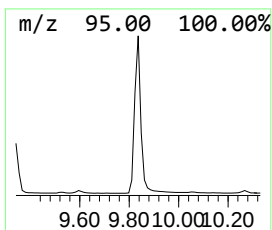
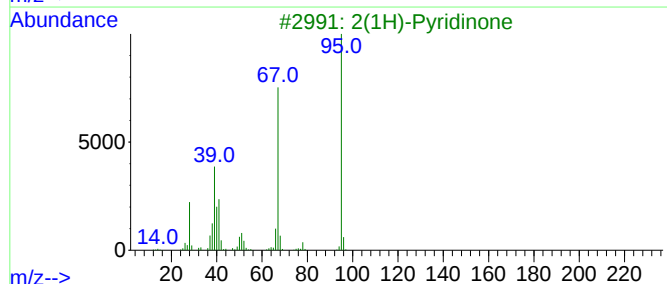
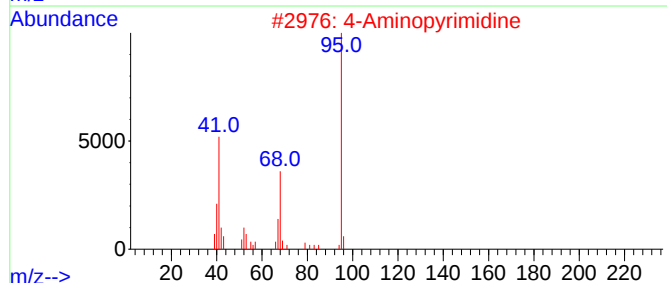
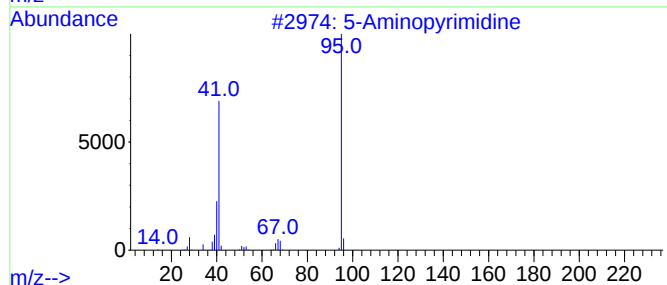
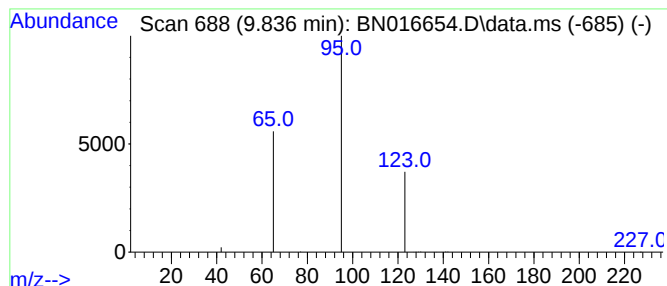
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Aminopyrimidine Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	25454	Naphthalene-d8	10.406

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 : BN016654.D
Acq On : 02 Oct 2021 03:59
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Misc :
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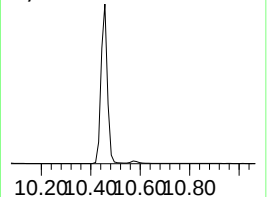
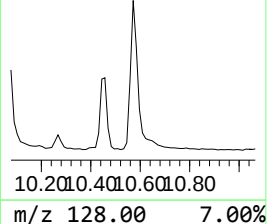
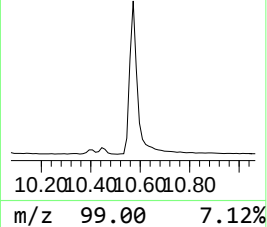
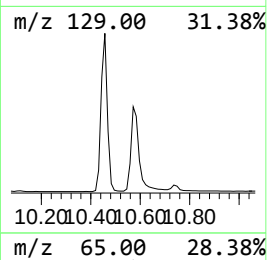
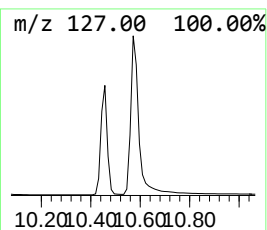
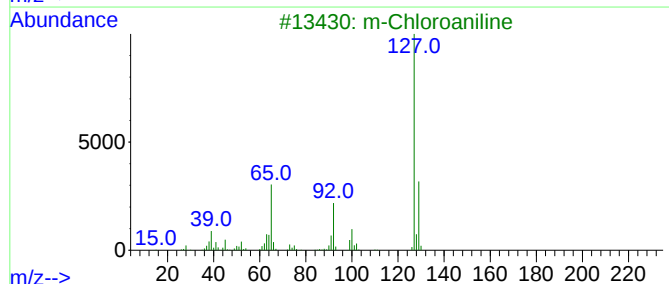
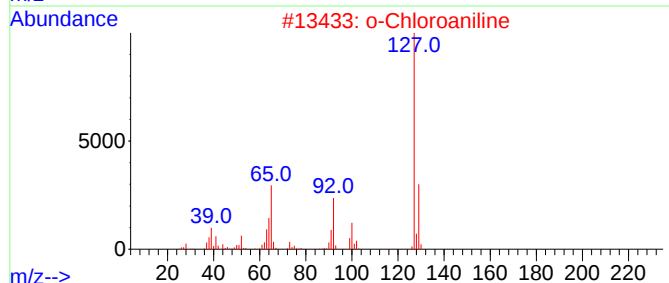
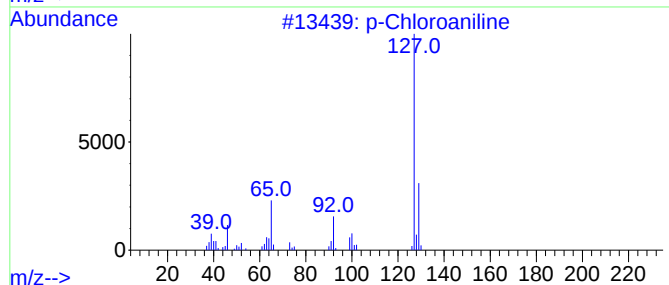
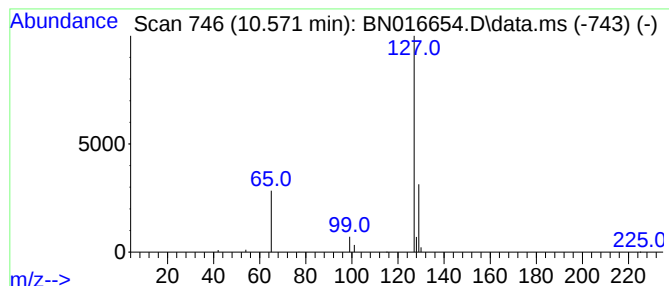
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.13 ng	55776	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Chloroaniline	127	C6H6ClN	000106-47-8	90
2		o-Chloroaniline	127	C6H6ClN	000095-51-2	90
3		m-Chloroaniline	127	C6H6ClN	000108-42-9	90
4		4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5		Pyridine, 2-chloro-6-methyl-	127	C6H6ClN	018368-63-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
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ALS Vial : 22 Sample Multiplier: 1

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BNA_N
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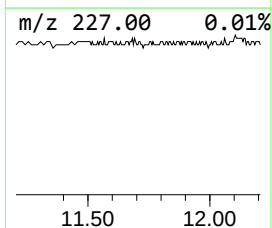
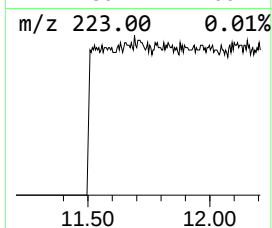
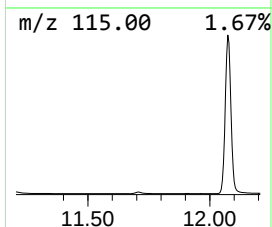
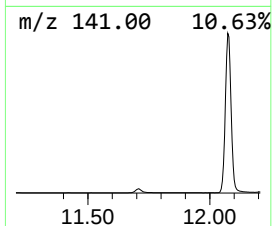
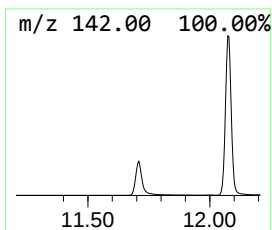
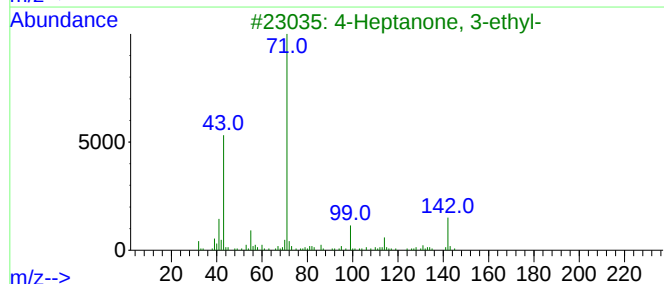
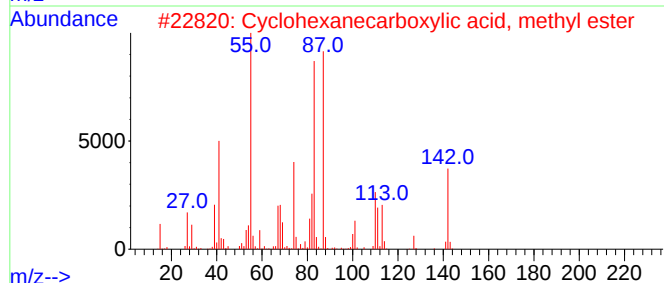
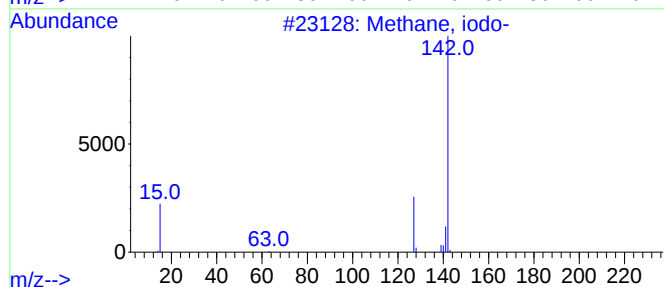
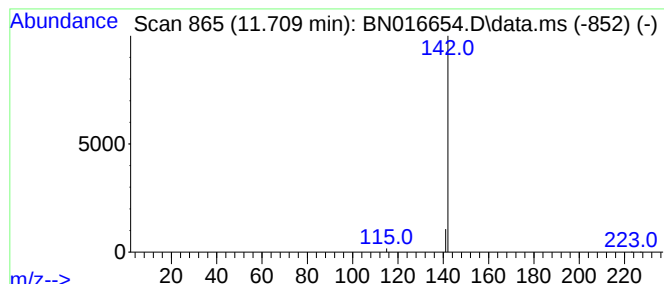
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	23410	Naphthalene-d8	10.406

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



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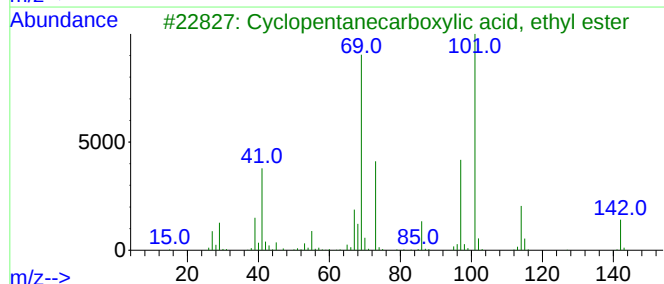
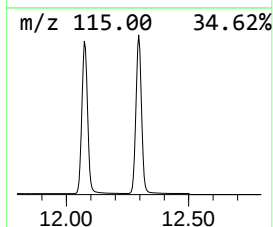
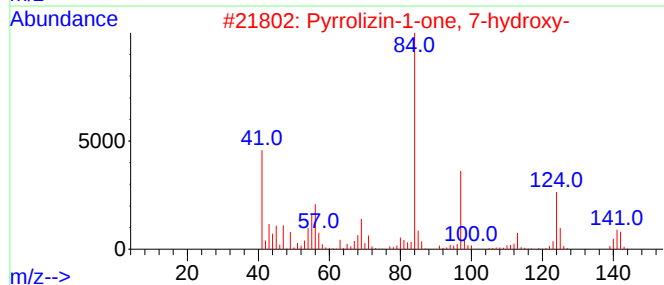
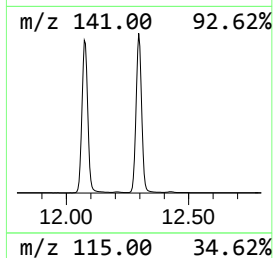
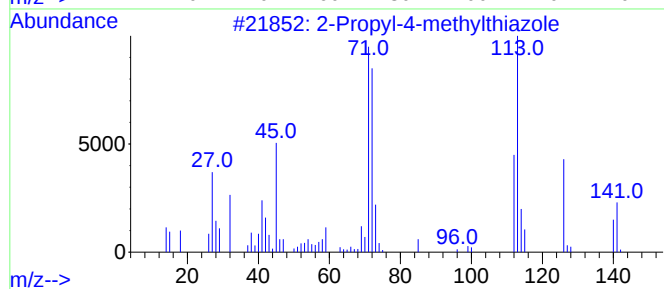
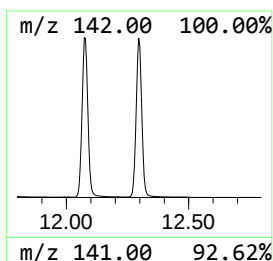
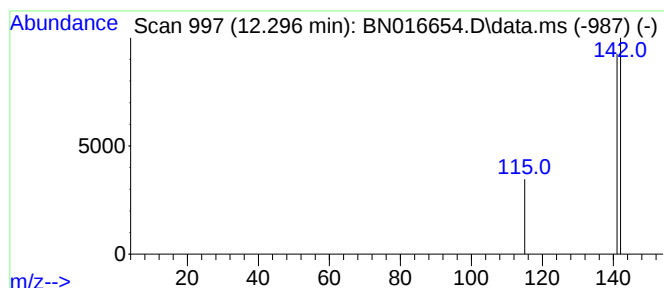
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	184175	Naphthalene-d8	10.406

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



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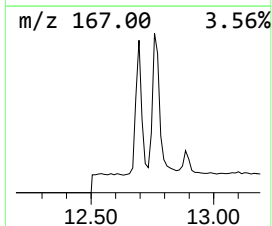
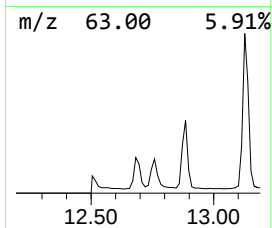
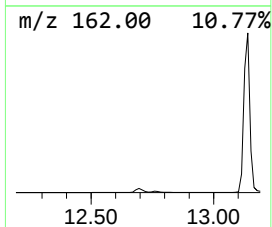
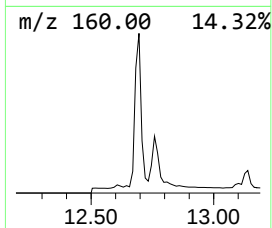
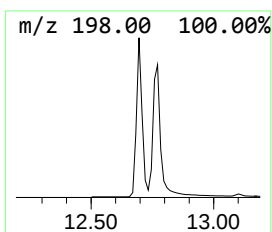
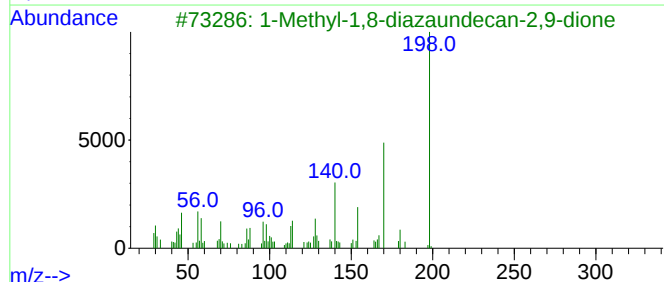
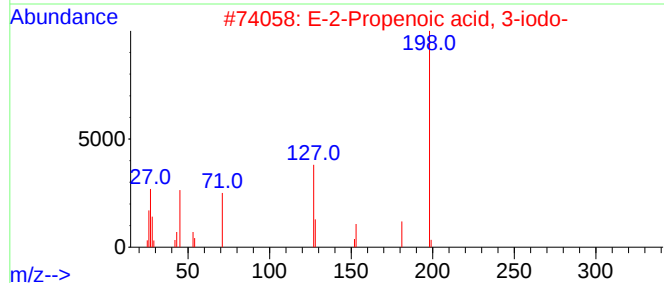
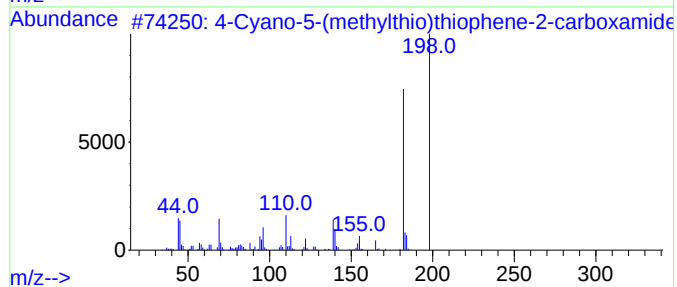
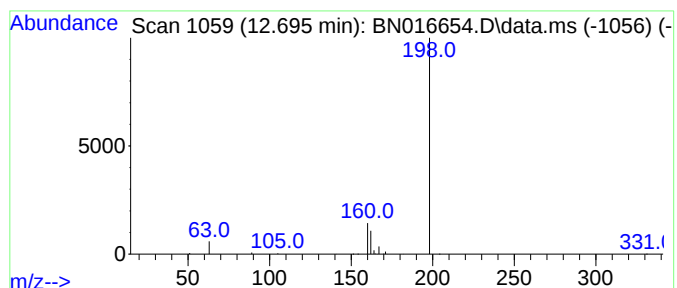
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	26044	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 : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

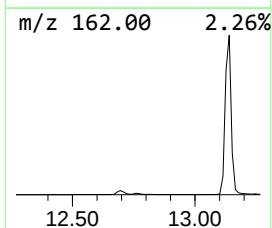
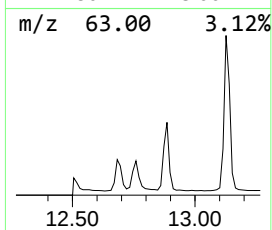
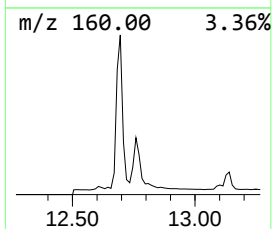
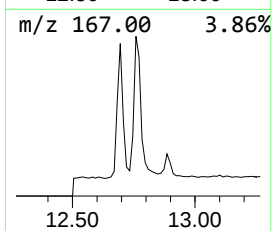
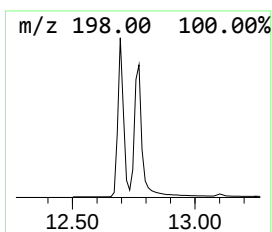
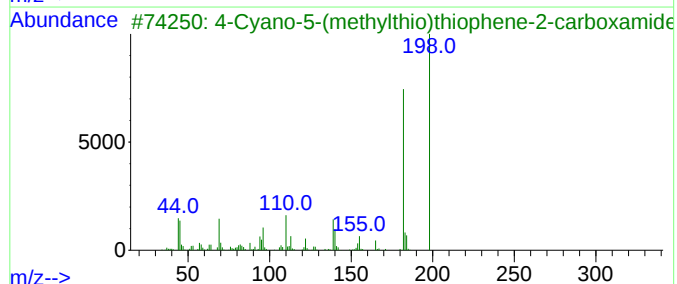
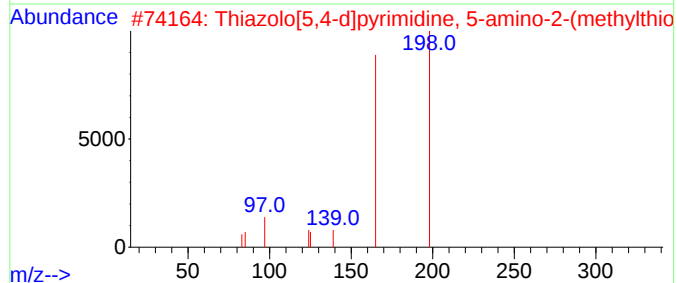
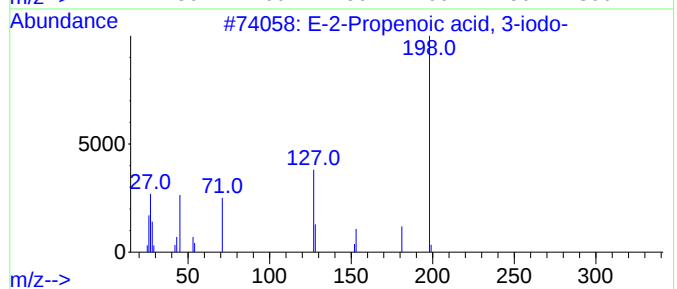
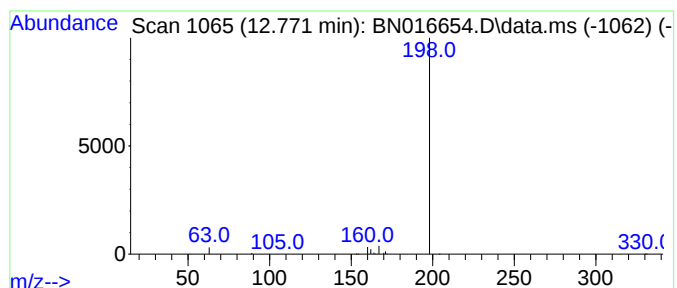
Instrument :
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ClientSampleId :
PB139433BSD

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 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.771	0.05 ng	22516	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	E-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-7	3
2	Thiazolo[5,4-d]pyrimidine, 5-ami...		198	C6H6N4S2	019835-31-5	3
3	4-Cyano-5-(methylthio)thiophene-...		198	C7H6N2OS2	1000267-39-2	3
4	Z-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-8	3
5	Imidazolidine-2,4,5-trione, 1,3-...		198	C7H6N2O5	115083-04-0	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

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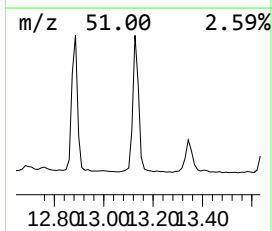
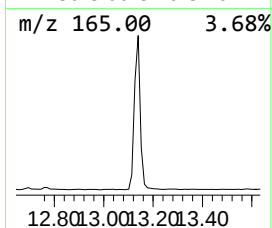
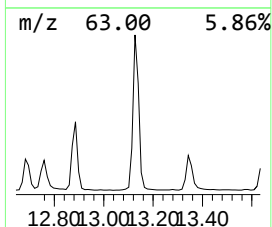
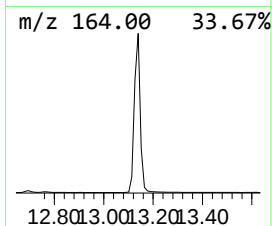
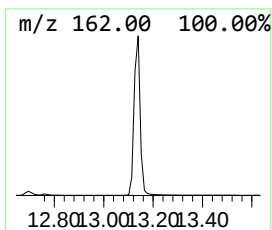
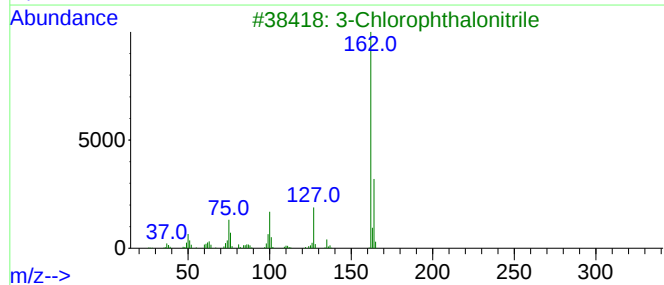
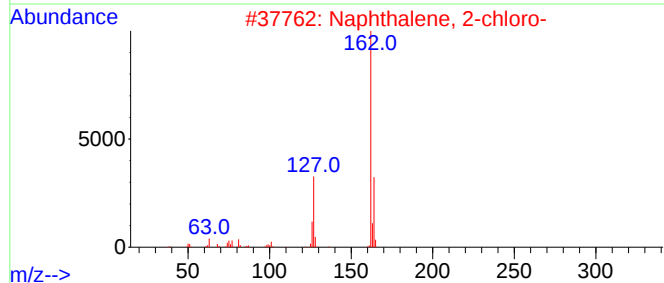
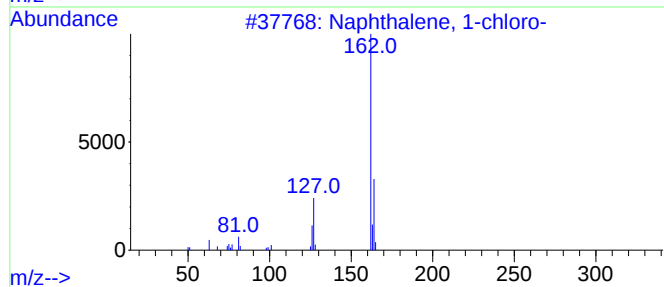
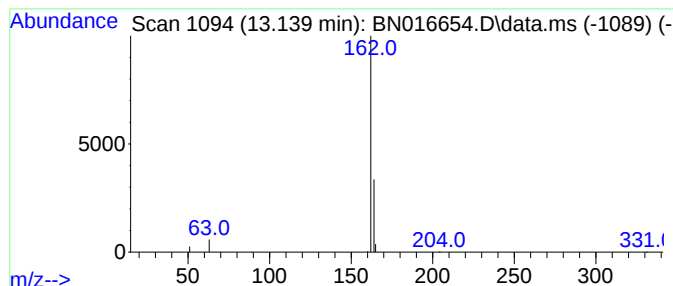
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Naphthalene, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.28 ng	122236	Acenaphthene-d10	14.269

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

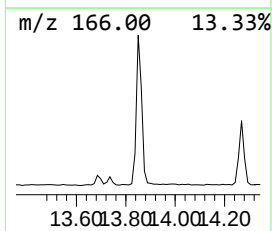
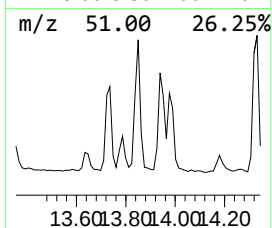
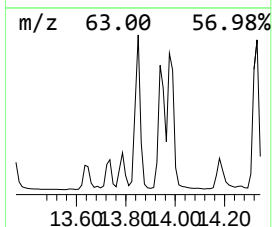
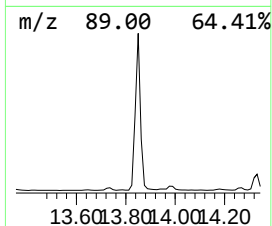
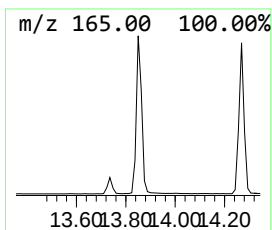
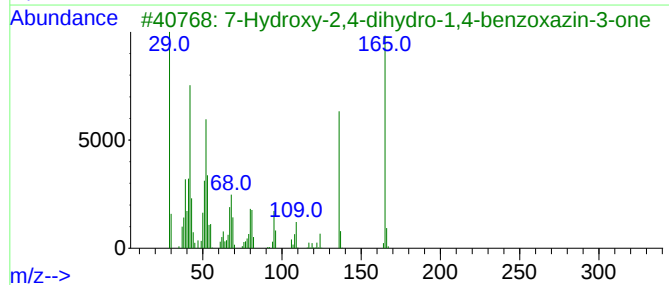
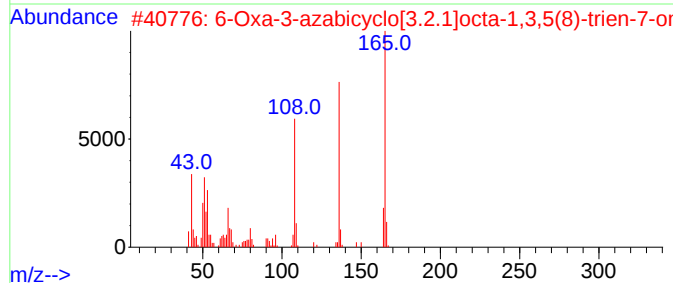
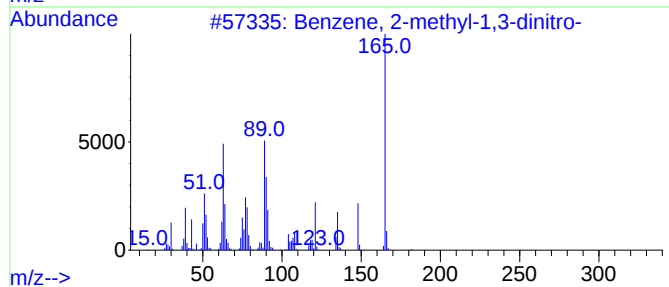
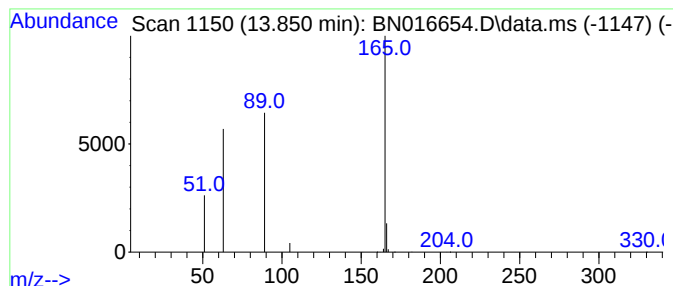
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.850	0.06 ng	24608	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	7-Hydroxy-2,4-dihydro-1,4-benzox...	165	C8H7NO3	067193-97-9	9
4	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
5	5,6-Dimethoxy-3-pyridazinecarbon...	165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

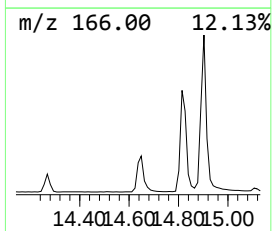
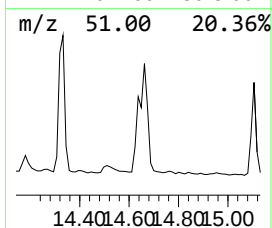
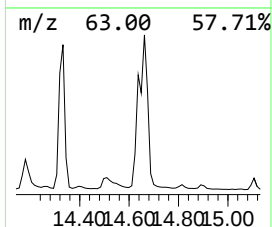
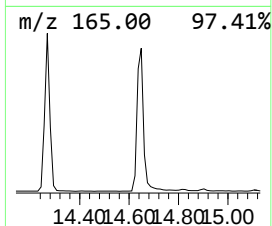
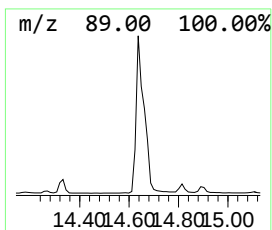
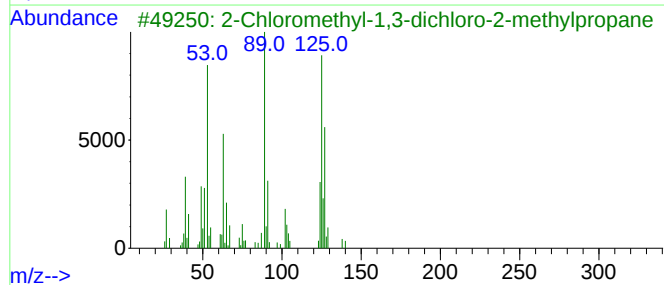
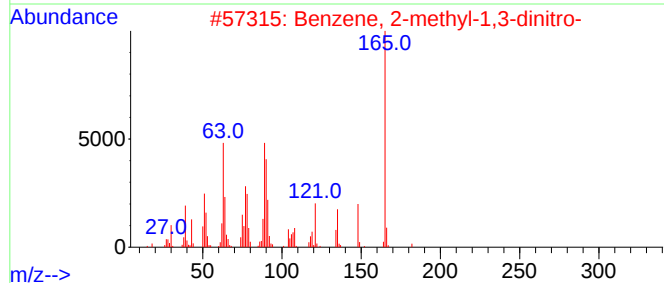
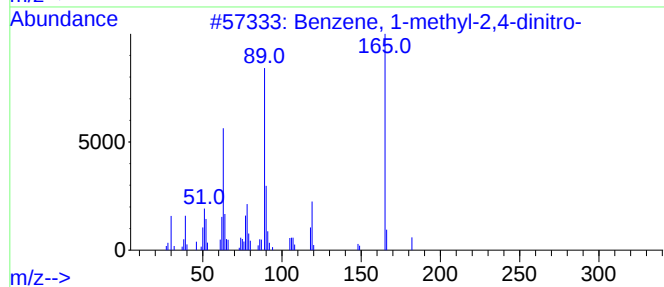
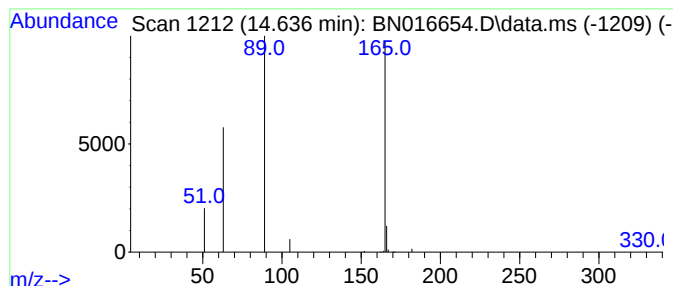
Instrument :
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ClientSampleId :
PB139433BSD

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.636	0.09 ng	38819	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2,4-dinitro-		182	C7H6N2O4	000121-14-2	74
2	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	38
3	2-Chloromethyl-1,3-dichloro-2-me...		174	C5H9Cl3	001067-09-0	9
4	Ethanol, 1-(4-nitrophenyl)-2-[1-...		304	C17H24N2O3	1000264-75-7	9
5	5-[2-Chlorophenyl]tetraazole		180	C7H5ClN4	050907-46-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

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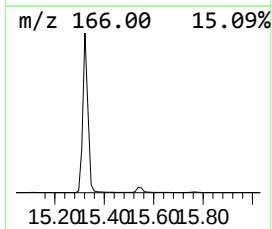
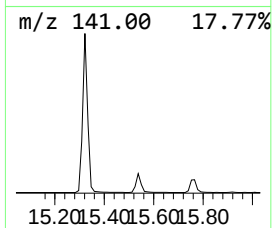
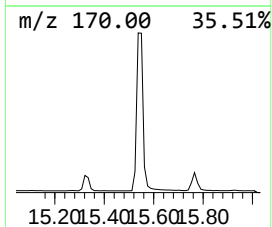
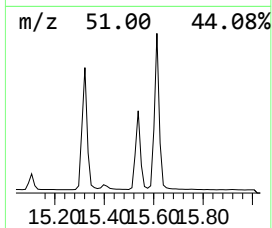
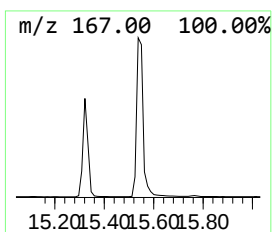
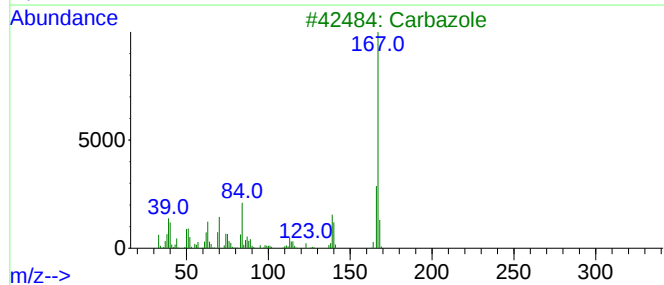
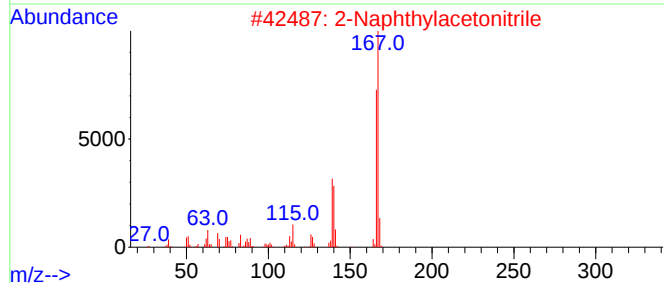
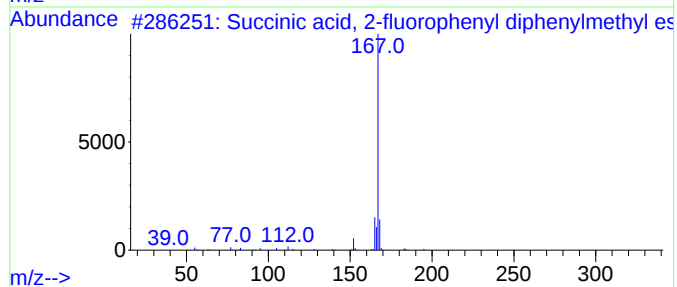
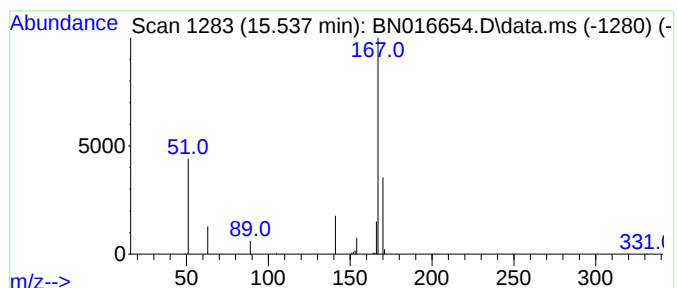
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.13 ng	57310	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19F04	1000390-17-0	9
2			2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
3			Carbazole	167	C12H9N	000086-74-8	7
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
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Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

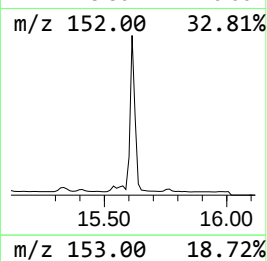
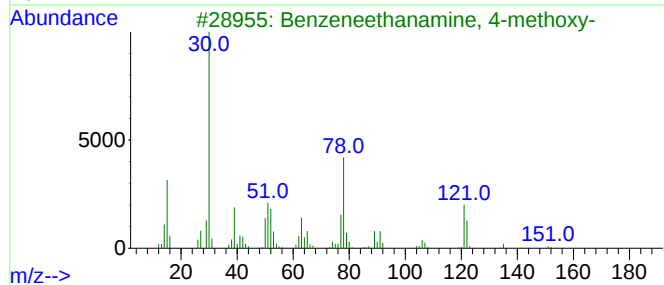
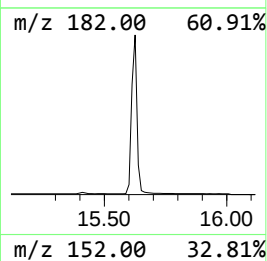
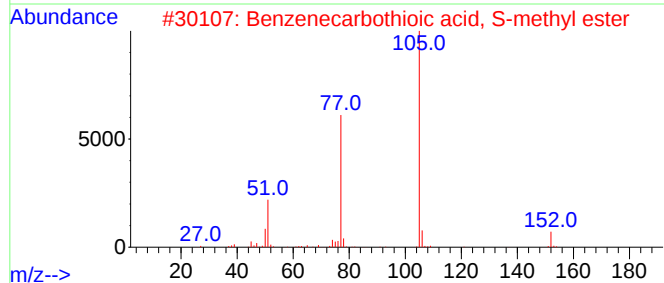
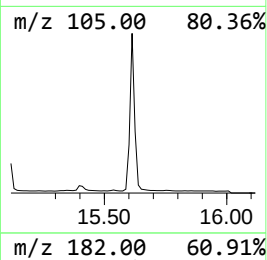
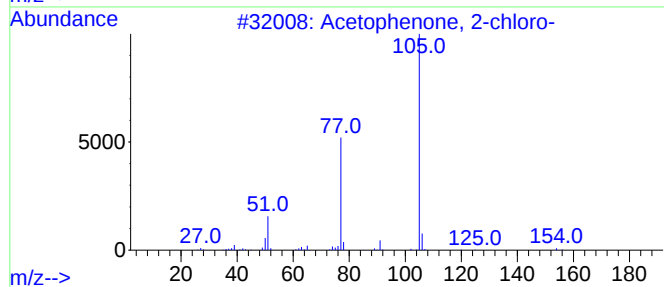
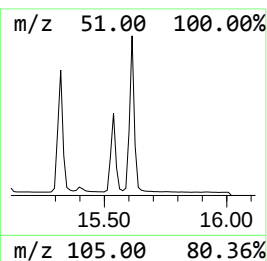
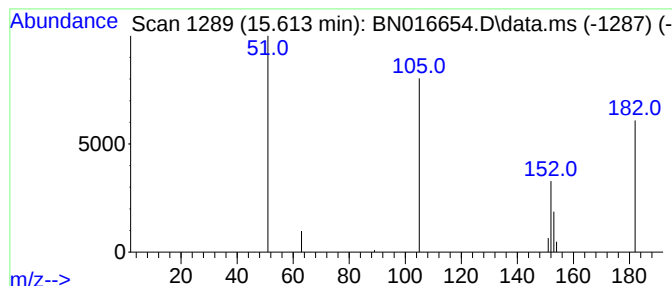
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
15.613	0.13 ng	57963	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Acetophenone, 2-chloro-		154	C8H7ClO	000532-27-4	3
2	Benzenecarbothioic acid, S-methy...		152	C8H8OS	005925-68-8	3
3	Benzenethanamine, 4-methoxy-		151	C9H13NO	000055-81-2	3
4	Propiolonitrile		51	C3HN	001070-71-9	3
5	Propanal, 2-(benzoyloxy)-, (R)-		178	C10H10O3	078871-04-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139433BSD

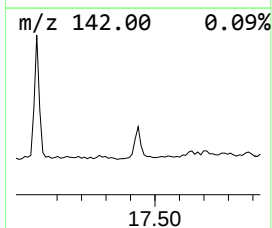
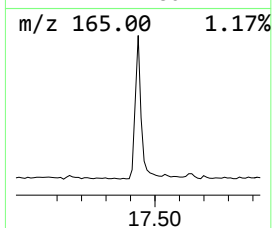
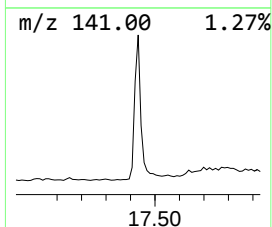
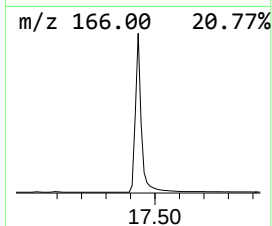
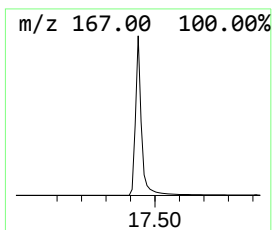
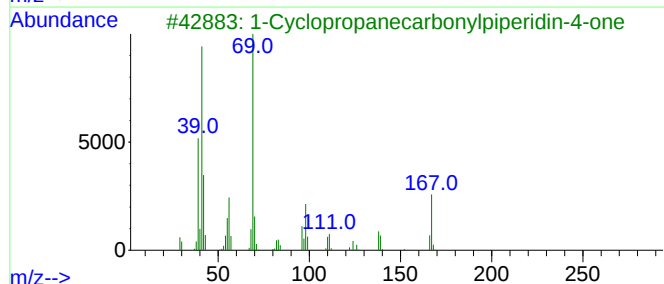
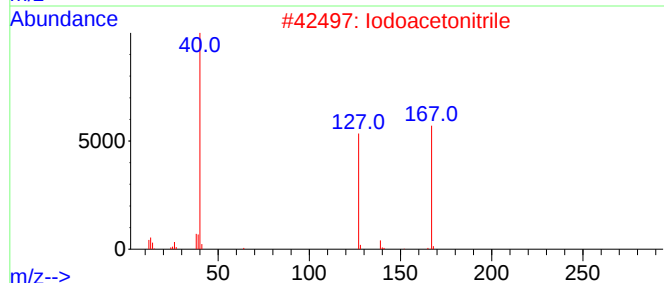
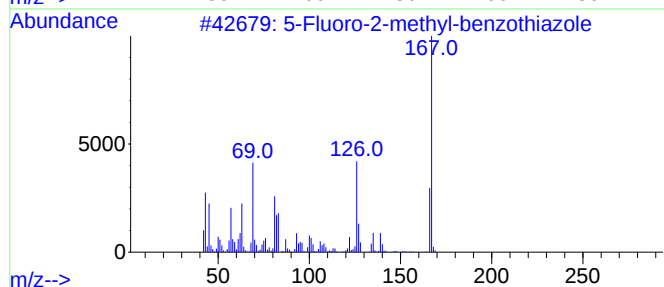
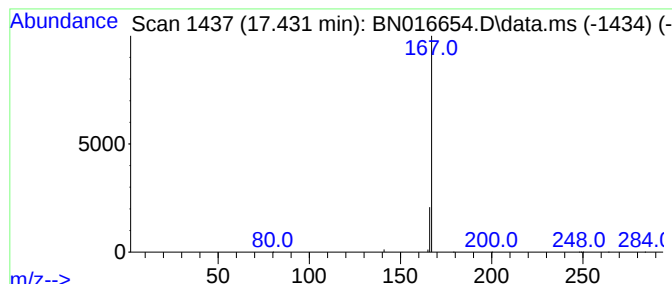
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.34 ng	127015	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			1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
4			1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
5			2-propenoic acid, 2-methyl-, 2-(...	167	C7H9N3O2	1000404-53-2	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139433BSD

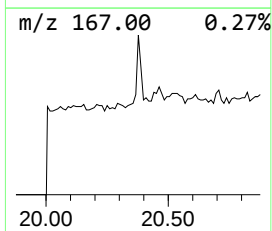
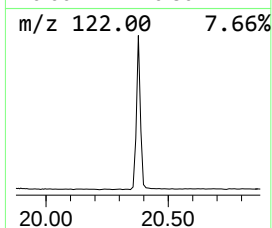
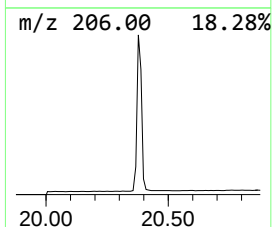
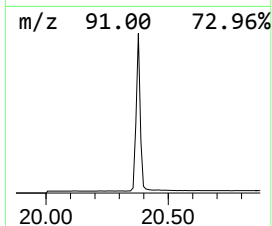
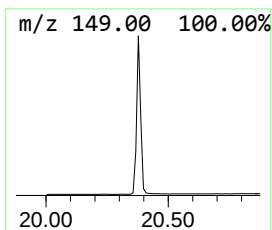
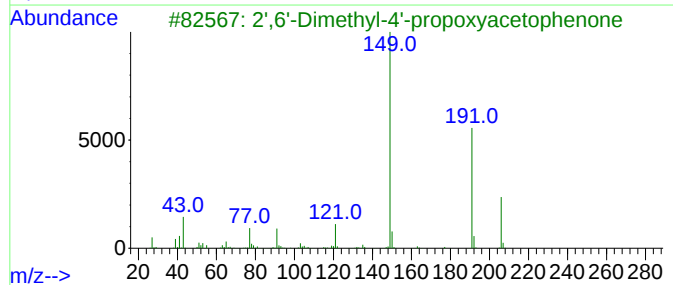
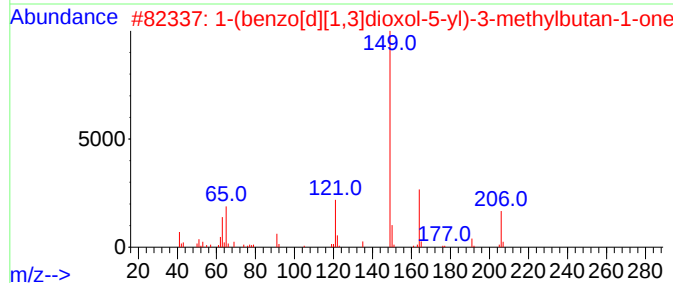
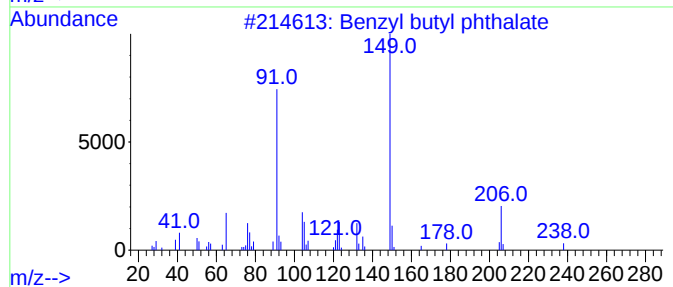
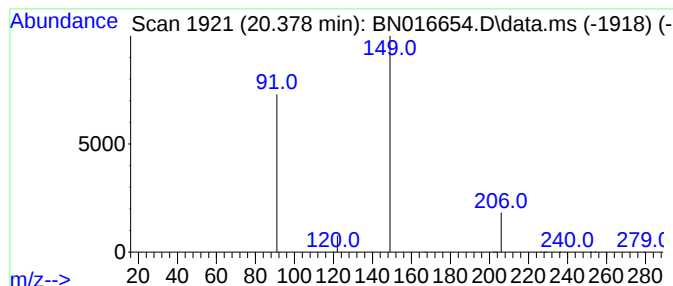
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	53770	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl butyl phthalate	312	C19H20O4	000085-68-7	40
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 : BN016654.D
Acq On : 02 Oct 2021 03:59
Operator : CG/JU
Sample : PB139433BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139433BSD

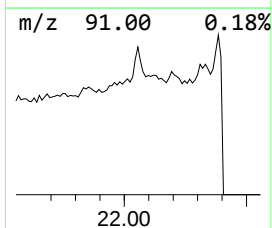
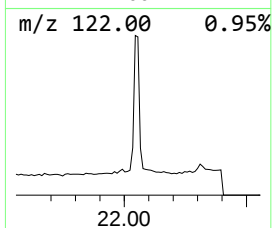
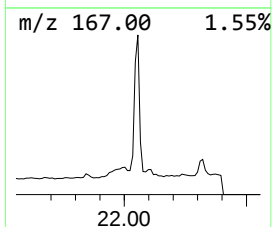
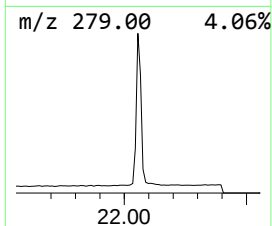
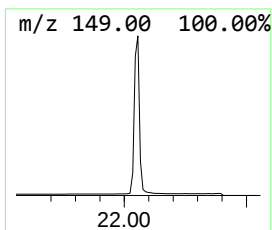
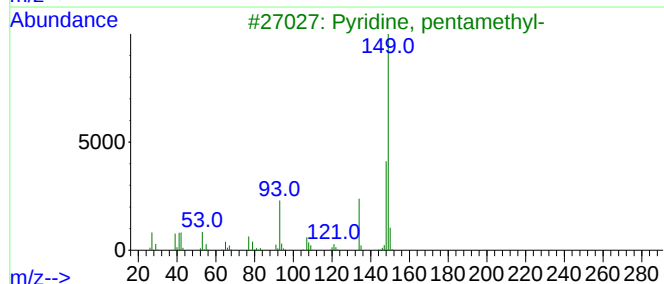
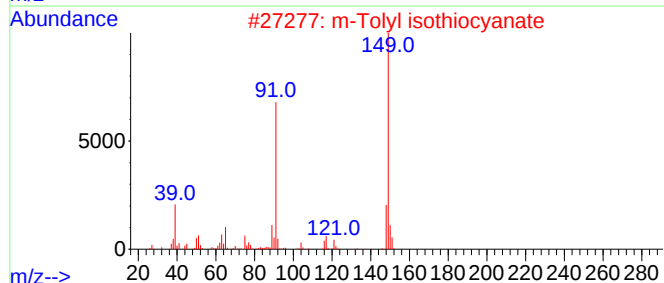
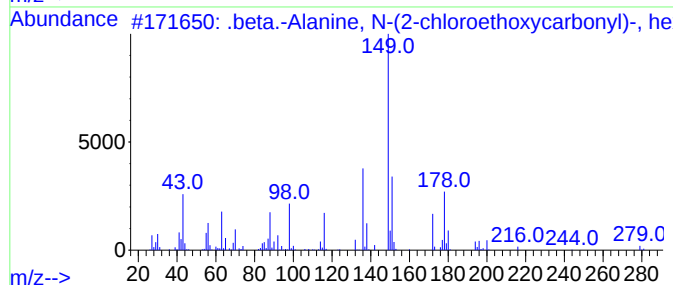
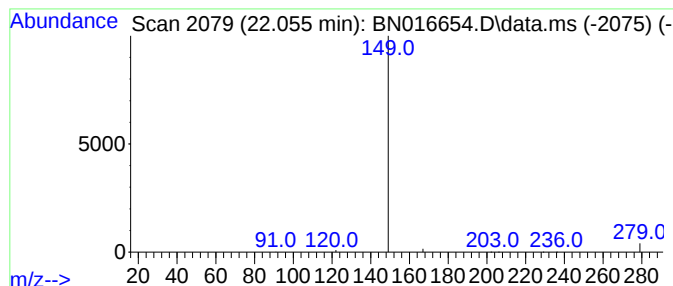
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.055	0.09 ng	85129	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 : BN016654.D
 Acq On : 02 Oct 2021 03:59
 Operator : CG/JU
 Sample : PB139433BSD
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139433BSD

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	33966	1	7.642	108726	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	29693	1	7.642	108726	0.4
3-Methylpyrazol...	7.522	0.1	ng	13921	1	7.642	108726	0.4
6-Benzothiazola...	7.956	0.4	ng	99114	1	7.642	108726	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	45530	1	7.642	108726	0.4
Fomepizole	9.342	0.2	ng	70175	2	10.406	177548	0.4
5-Aminopyrimidine	9.836	0.1	ng	25454	2	10.406	177548	0.4
p-Chloroaniline	10.571	0.1	ng	55776	2	10.406	177548	0.4
Methane, iodo-	11.709	0.1	ng	23410	2	10.406	177548	0.4
2-Propyl-4-meth...	12.296	0.4	ng	184175	2	10.406	177548	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	26044	3	14.269	177564	0.4
E-2-Propenoic a...	12.771	0.1	ng	22516	3	14.269	177564	0.4
Naphthalene, 1-...	13.139	0.3	ng	122236	3	14.269	177564	0.4
Benzene, 2-meth...	13.850	0.1	ng	24608	3	14.269	177564	0.4
Benzene, 1-meth...	14.636	0.1	ng	38819	3	14.269	177564	0.4
Succinic acid, ...	15.537	0.1	ng	57310	3	14.269	177564	0.4
Acetophenone, 2...	15.613	0.1	ng	57963	3	14.269	177564	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	127015	4	17.017	148689	0.4
Benzyl butyl ph...	20.378	0.1	ng	53770	5	21.227	389972	0.4
.beta.-Alanine,...	22.055	0.1	ng	85129	5	21.227	389972	0.4