

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016614.D
 Acq On : 30 Sep 2021 23:58
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_N
 LabSampleId :
 SSTDCCC0.4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016614.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	21	rBV	9910	12752	2.64%	0.174%
2	3.290	21	23	46	rVB	5018	24386	5.05%	0.332%
3	3.585	51	55	86	rVB2	6492	31977	6.62%	0.435%
4	5.254	231	236	252	rVB2	15231	57127	11.83%	0.778%
5	6.822	401	406	418	rBV	23765	61166	12.67%	0.833%
6	6.978	419	423	429	rVV	15902	35610	7.37%	0.485%
7	7.080	429	434	440	rVV	34849	72084	14.93%	0.982%
8	7.200	441	447	459	rVB	12149	32314	6.69%	0.440%
9	7.522	478	482	490	rVB	6557	14579	3.02%	0.199%
10	7.642	490	495	514	rVB2	49514	120789	25.01%	1.645%
11	7.956	524	529	539	rVB2	47348	107706	22.30%	1.467%
12	8.168	547	552	557	rBV	3289	7982	1.65%	0.109%
13	8.429	571	577	591	rVB3	19744	50706	10.50%	0.691%
14	8.696	595	598	601	rBV	4828	9089	1.88%	0.124%
15	8.784	601	605	607	rBV	34009	72139	14.94%	0.982%
16	8.822	607	608	613	rVB	25945	37964	7.86%	0.517%
17	9.342	646	649	656	rBV	48386	78834	16.32%	1.074%
18	9.532	661	664	666	rVV	3577	6786	1.41%	0.092%
19	9.595	666	669	679	rVB	8772	15604	3.23%	0.213%
20	9.836	685	688	694	rBV	15981	26781	5.55%	0.365%
21	10.064	702	706	709	rBV	3978	8283	1.72%	0.113%
22	10.407	729	733	735	rBV	105917	189198	39.18%	2.577%
23	10.457	735	737	741	rVV	111096	180994	37.48%	2.465%
24	10.584	743	747	756	rVV	24274	58197	12.05%	0.793%
25	10.749	757	760	763	rVB	33521	55205	11.43%	0.752%
26	11.306	801	804	815	rVB	2184	5341	1.11%	0.073%
27	11.709	853	865	893	rBV	13350	24947	5.17%	0.340%
28	12.003	921	931	940	rBV2	55157	91313	18.91%	1.244%
29	12.078	940	948	971	rVV	125935	203591	42.16%	2.773%
30	12.301	988	998	1020	rVV	124259	196359	40.66%	2.674%
31	12.695	1056	1059	1062	rBV	16752	28202	5.84%	0.384%
32	12.771	1062	1065	1071	rVB	12517	24258	5.02%	0.330%
33	12.898	1071	1075	1078	rBV	107563	190587	39.47%	2.596%
34	13.139	1091	1094	1097	rVB	81143	123136	25.50%	1.677%
35	13.736	1138	1141	1143	rBV	11356	15865	3.29%	0.216%
36	13.850	1147	1150	1153	rVB	17446	26079	5.40%	0.355%

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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	96737	149031	30.86%	2.030%
38	14.269	1180	1183	1186	rBV	129893	192199	39.80%	2.618%
39	14.332	1186	1188	1191	rVB	162544	228986	47.42%	3.119%
40	14.649	1209	1213	1220	rBV3	15219	40878	8.46%	0.557%
41	14.814	1224	1226	1230	rVV	4955	9152	1.90%	0.125%
42	14.903	1230	1233	1244	rVB	7628	12155	2.52%	0.166%
43	15.106	1246	1249	1252	rBV	8048	10501	2.17%	0.143%
44	15.322	1263	1266	1270	rBV2	201444	329297	68.19%	4.485%
45	15.410	1270	1273	1280	rVV2	4361	10534	2.18%	0.143%
46	15.537	1280	1283	1287	rVV	31646	58079	12.03%	0.791%
47	15.613	1287	1289	1298	rVV2	38156	61676	12.77%	0.840%
48	15.766	1298	1301	1311	rVB2	12781	21522	4.46%	0.293%
49	16.226	1335	1338	1341	rBV2	57588	84391	17.48%	1.149%
50	16.324	1343	1346	1350	rVB	43191	68055	14.09%	0.927%
51	16.506	1358	1361	1372	rBV	21086	32072	6.64%	0.437%
52	16.677	1372	1375	1384	rBV	21124	35347	7.32%	0.481%
53	17.017	1400	1403	1405	rBV	84700	144091	29.84%	1.962%
54	17.066	1405	1407	1410	rVV	141944	200748	41.57%	2.734%
55	17.151	1411	1414	1434	rVV	100243	171518	35.52%	2.336%
56	17.431	1434	1437	1453	rVV	77500	125832	26.06%	1.714%
57	18.020	1483	1486	1499	rVB	5051	6644	1.38%	0.090%
58	19.068	1686	1697	1699	rBV	106229	144996	30.02%	1.975%
59	19.093	1699	1702	1741	rVB	168246	234450	48.55%	3.193%
60	19.460	1767	1776	1813	rBV	168279	233016	48.25%	3.173%
61	19.678	1813	1820	1852	rVB	100377	128209	26.55%	1.746%
62	20.378	1918	1921	1924	rBV	46498	55246	11.44%	0.752%
63	21.164	1992	1995	1997	rBV	46970	61216	12.68%	0.834%
64	21.217	1997	2000	2003	rVV2	189340	377408	78.15%	5.140%
65	21.270	2003	2005	2017	rVB	179040	240958	49.90%	3.282%
66	22.056	2076	2079	2082	rBV	58843	75304	15.59%	1.026%
67	22.803	2216	2228	2235	rBV	114625	196598	40.71%	2.677%
68	22.848	2235	2241	2284	rVB	122383	217488	45.04%	2.962%
69	23.382	2384	2397	2415	rBV	81252	172780	35.78%	2.353%
70	23.481	2415	2426	2472	rVB	87936	183552	38.01%	2.500%
71	24.083	2594	2602	2620	rVB	5415	10137	2.10%	0.138%
72	24.853	2817	2827	2845	rVB2	5268	11962	2.48%	0.163%
73	25.771	3066	3095	3182	rBV4	126774	482920	100.00%	6.577%
74	26.452	3270	3294	3345	rBV	69293	225732	46.74%	3.074%

Sum of corrected areas: 7342610

Instrument :

BNA_N

LabSampleId :

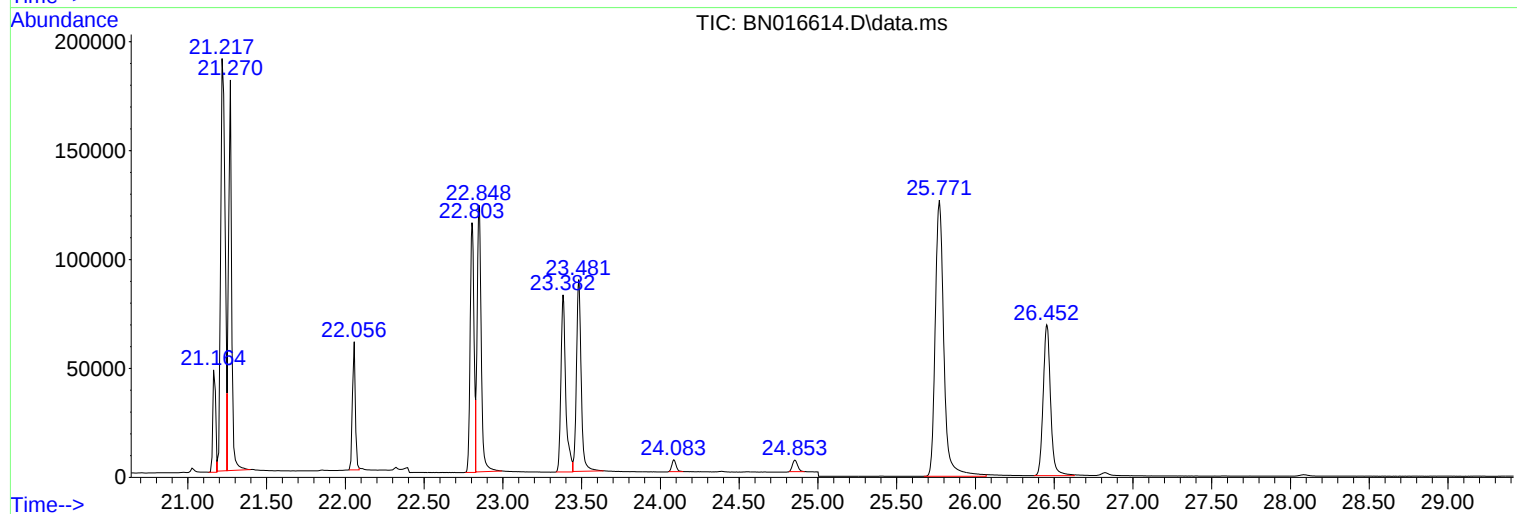
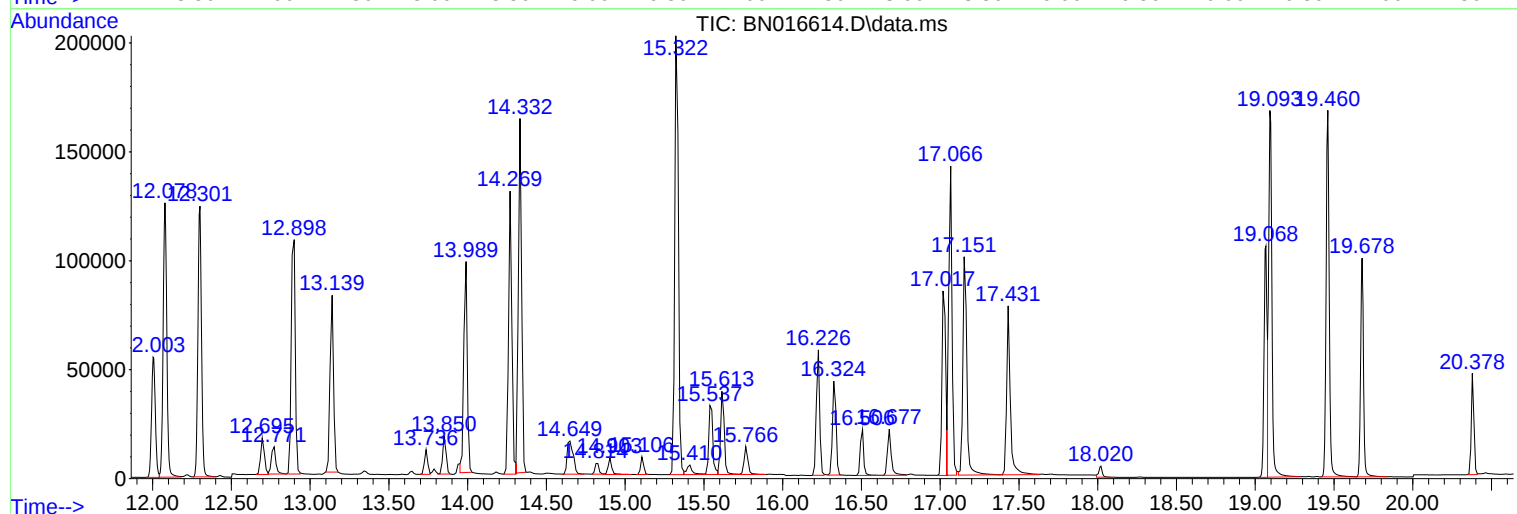
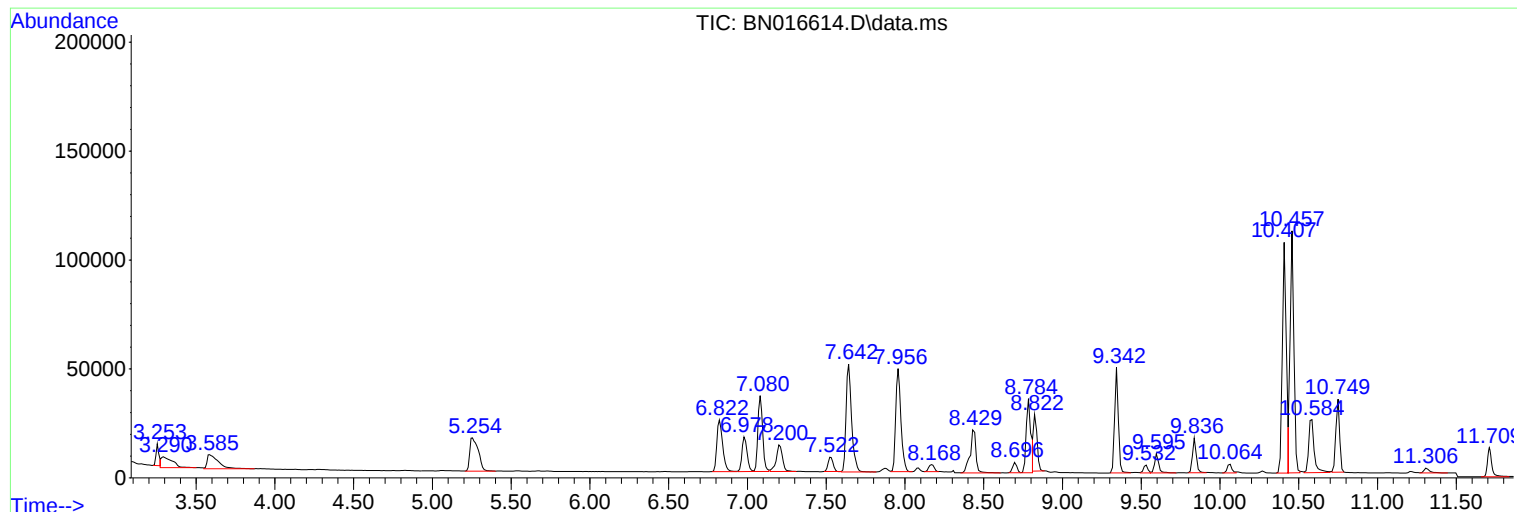
SSTDCCC0.4

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Instrument :
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LabSampleId :
SSTDCCC0.4

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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Data File : BN016614.D
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Operator : CG/JU
Sample : SSTDCCC0.4
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Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

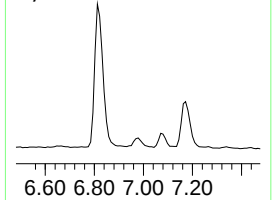
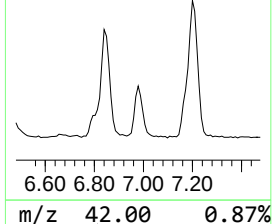
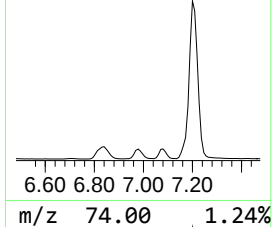
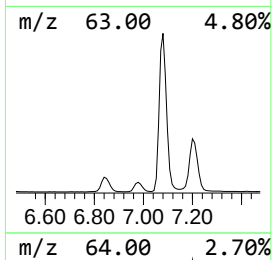
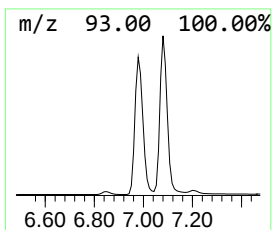
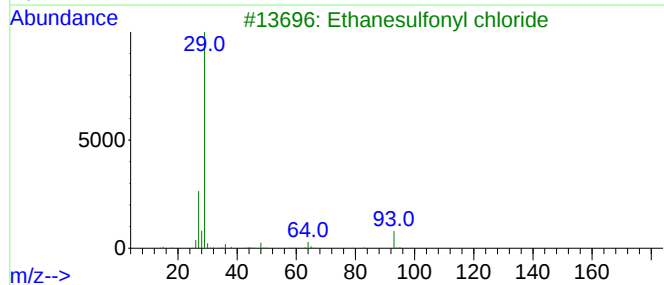
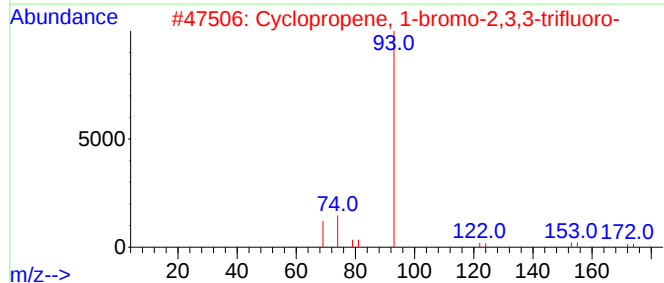
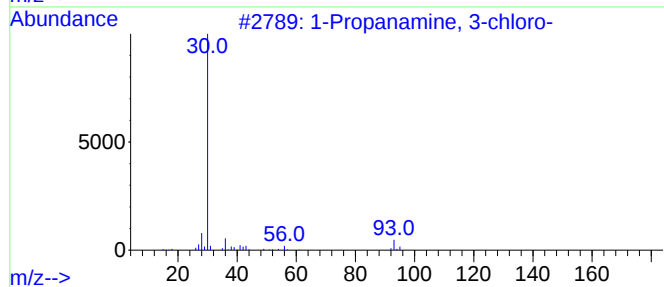
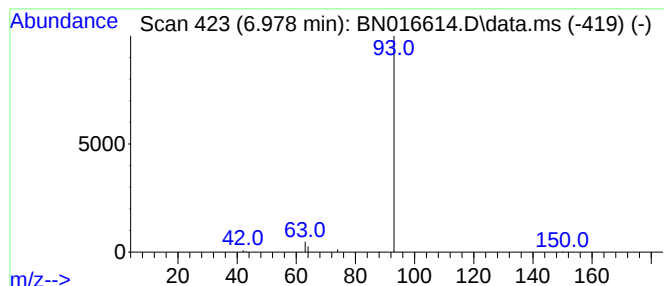
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	35610	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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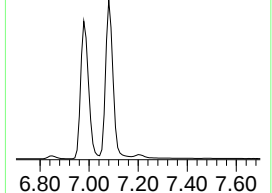
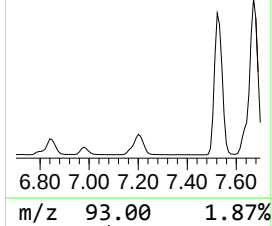
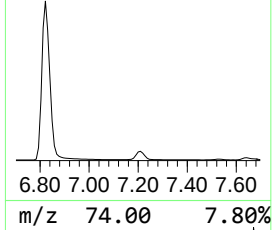
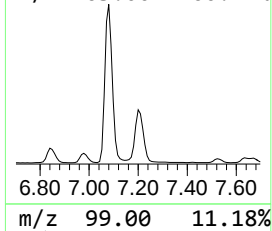
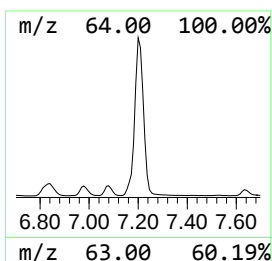
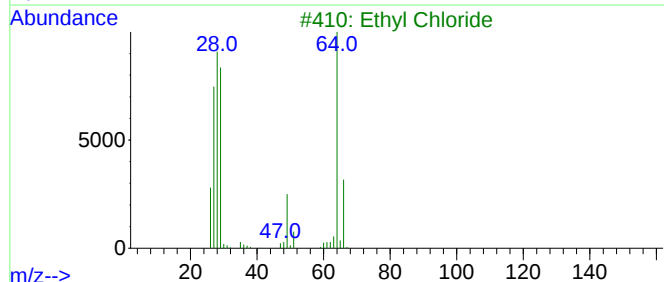
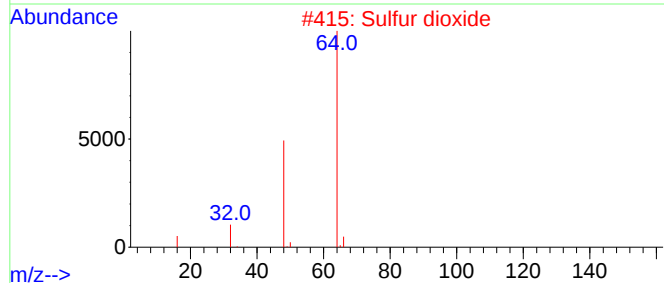
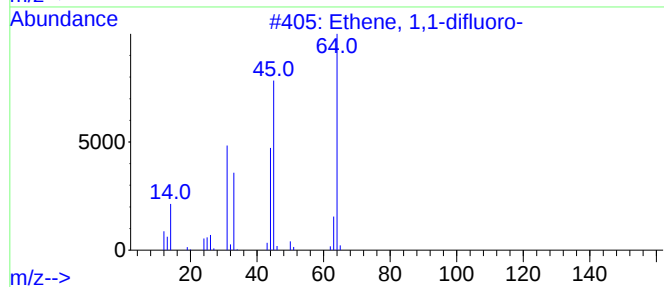
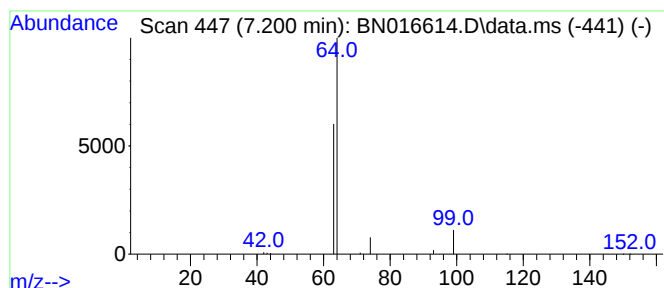
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	32314	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			Sulfur dioxide	64	O2S	007446-09-5	3
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
5			(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2



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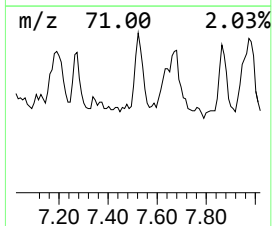
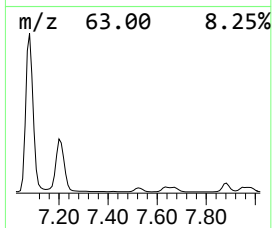
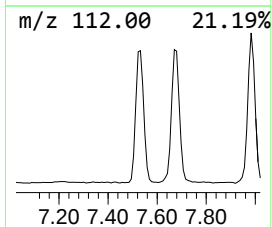
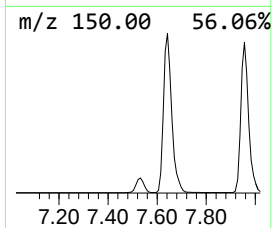
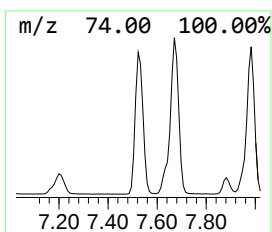
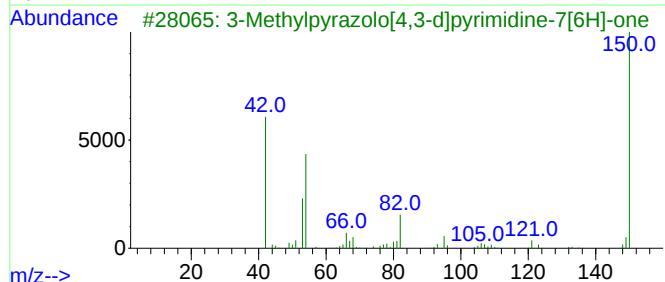
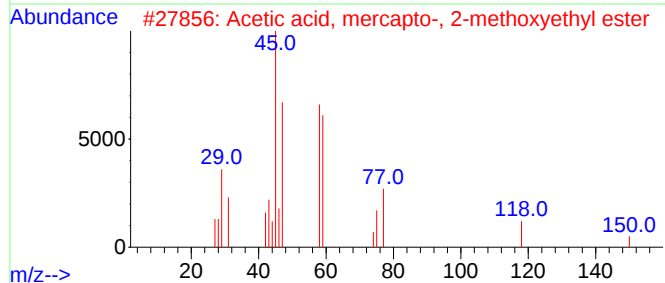
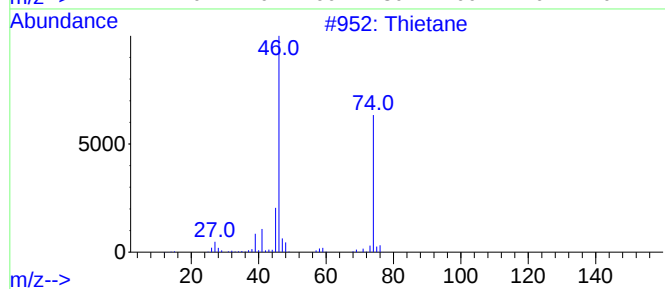
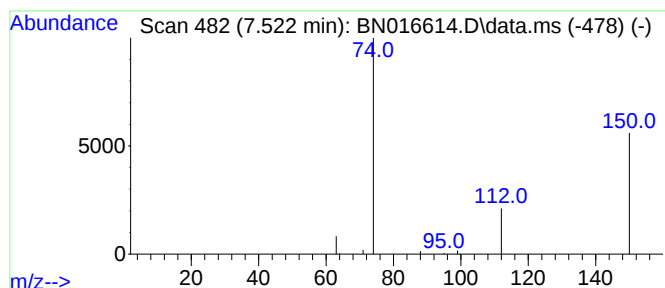
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Thietane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	14579	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thietane	74	C3H6S	000287-27-4	3
2			Acetic acid, mercapto-, 2-methox...	150	C5H10O3S	019788-48-8	3
3			3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
4			3-Cyano-2,6-dihydroxy-4-methylpy...	150	C7H6N2O2	005444-02-0	2
5			3-Methyl-4,4'-bi(1,2,4-triazole)	150	C5H6N6	063523-91-1	2



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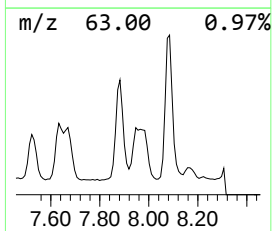
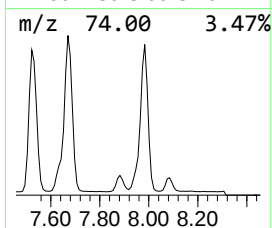
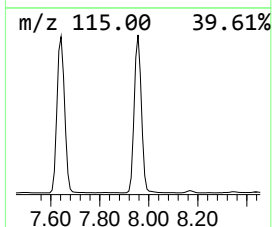
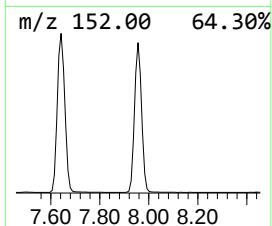
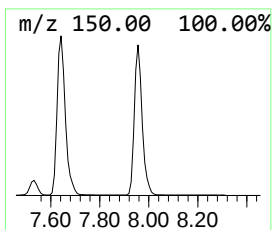
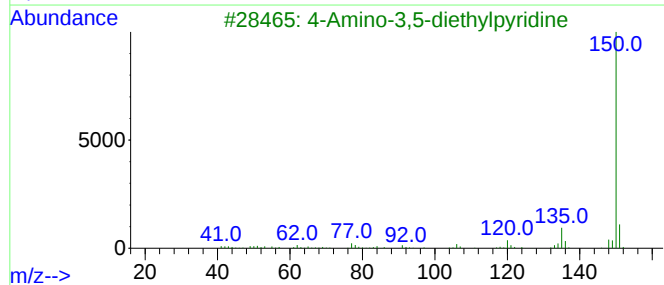
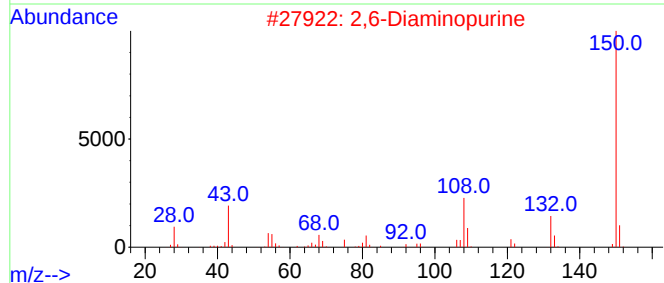
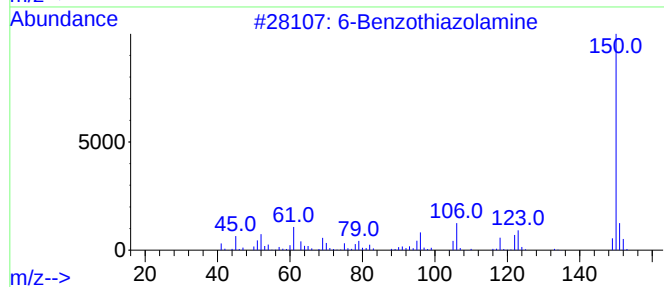
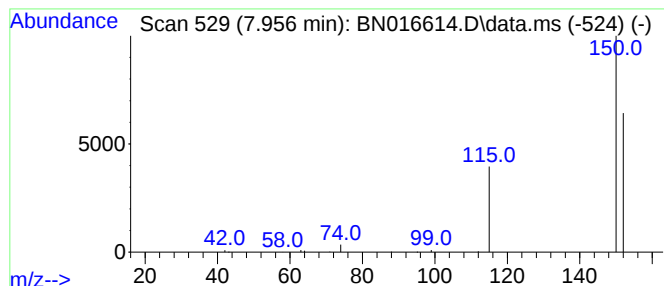
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	107706	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 : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

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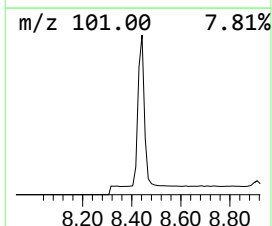
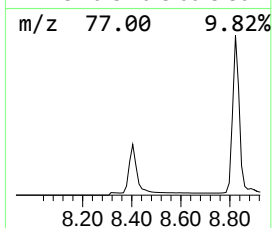
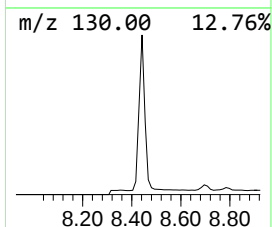
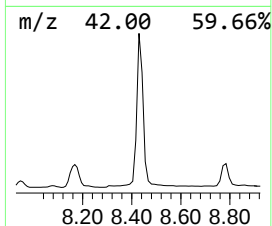
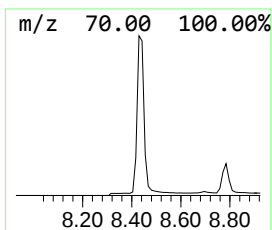
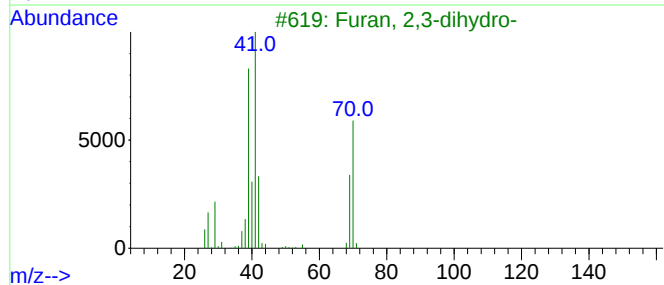
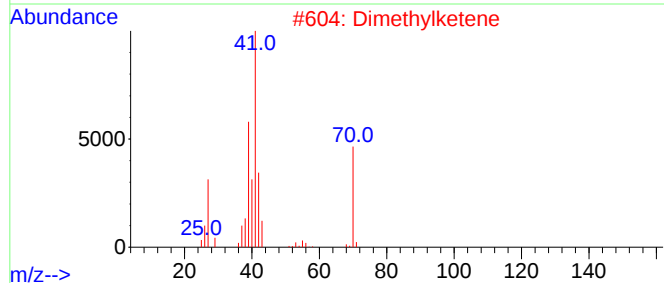
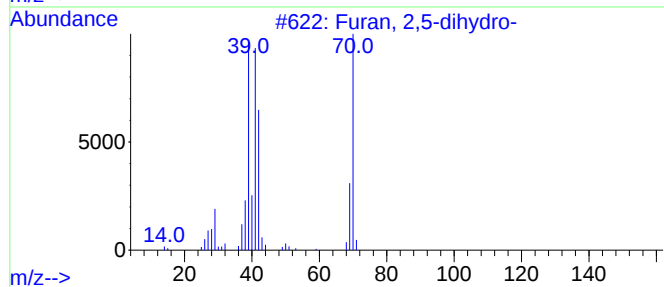
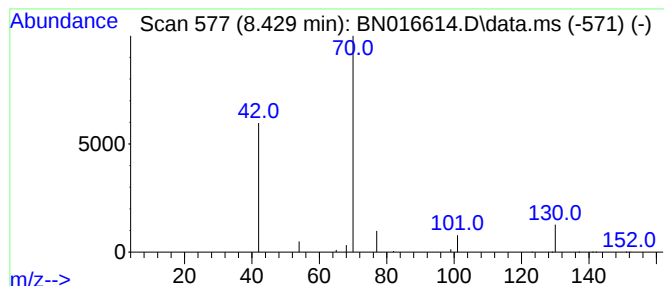
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.17 ng	50706	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			Dimethylketene	70	C4H6O	000598-26-5	5
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4			1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4
5			Ethoxyacetylene	70	C4H6O	000927-80-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
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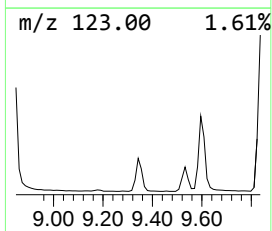
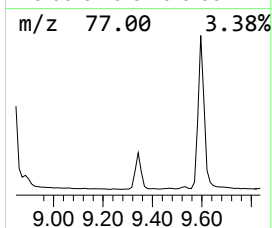
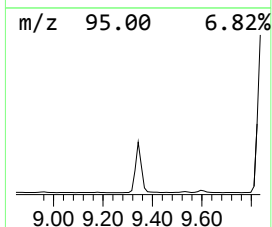
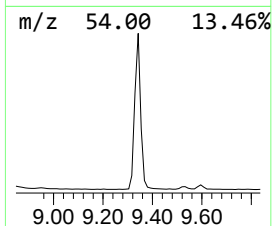
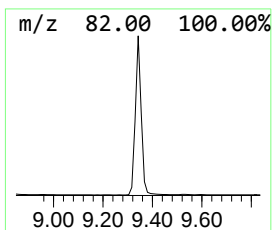
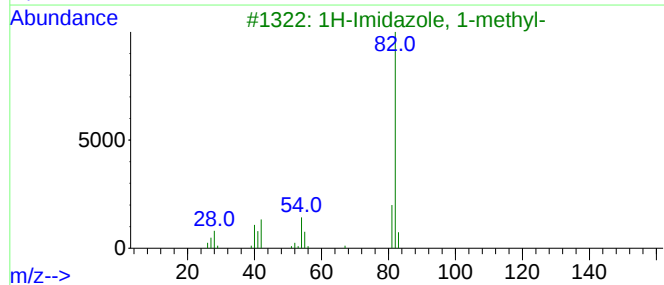
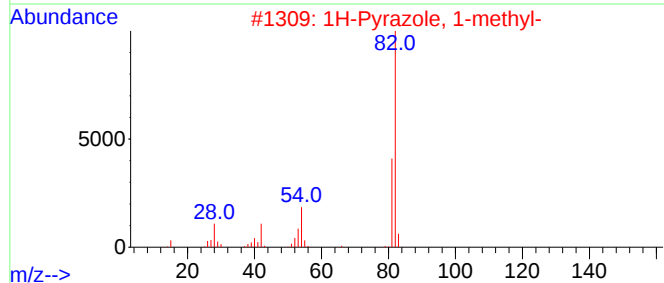
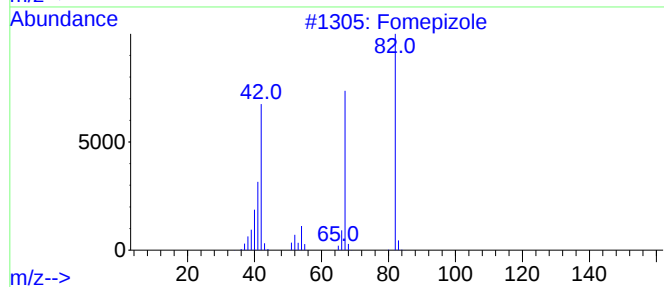
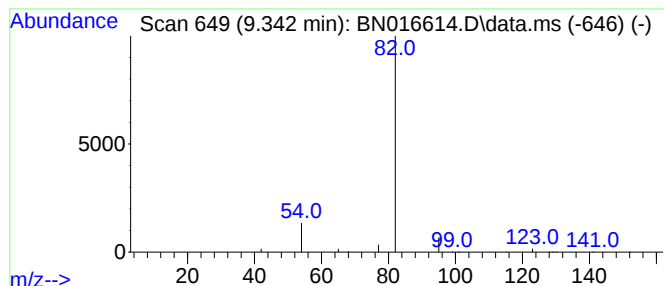
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.17 ng	78834	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 : BN016614.D
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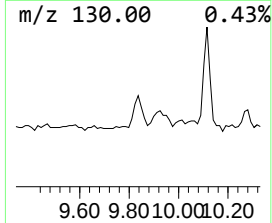
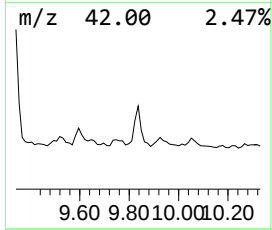
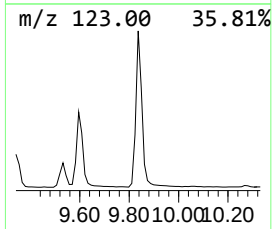
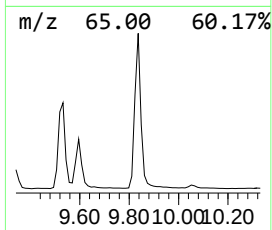
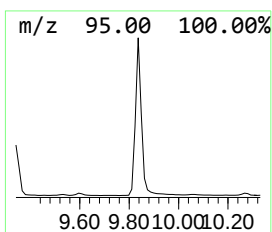
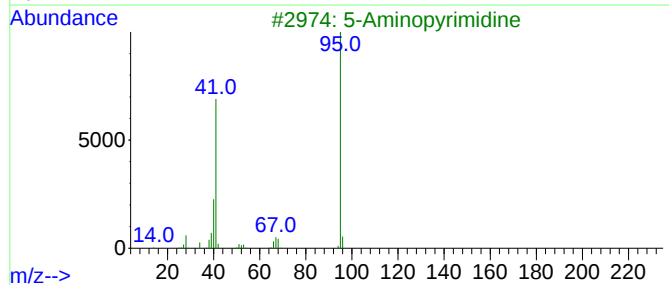
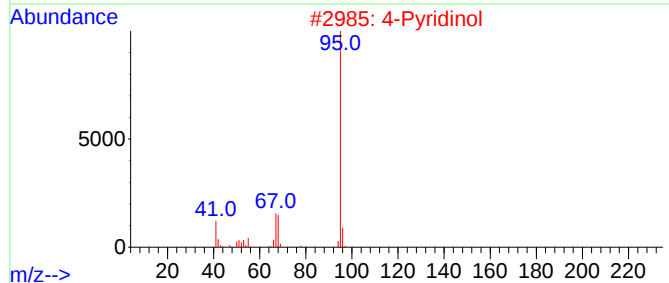
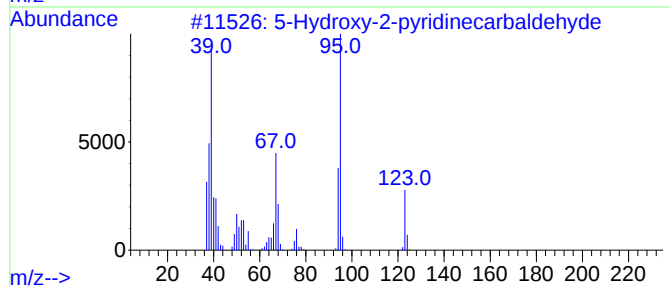
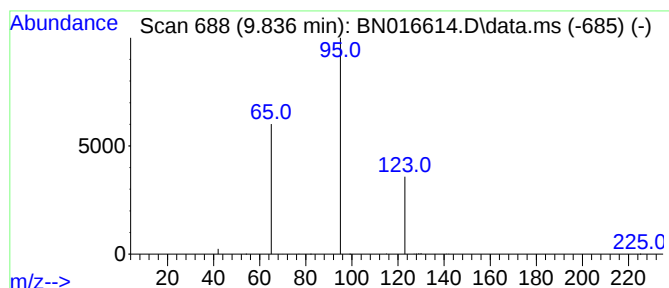
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Hydroxy-2-pyridinecarbal... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	26781	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2		4-Pyridinol	95	C5H5NO	000626-64-2	4
3		5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
4		3-Pyridinol	95	C5H5NO	000109-00-2	2
5		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
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Operator : CG/JU
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Misc :
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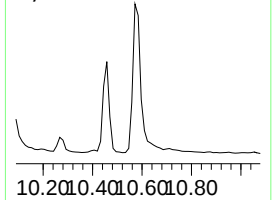
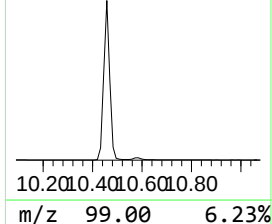
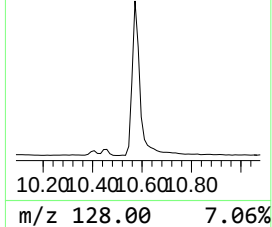
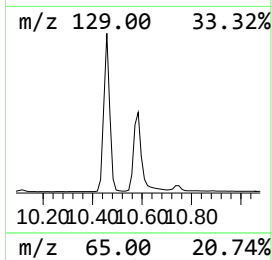
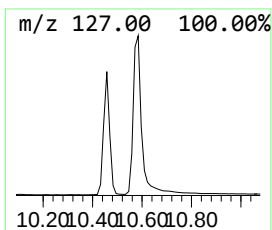
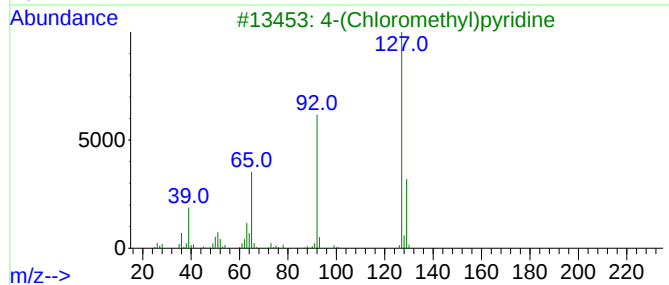
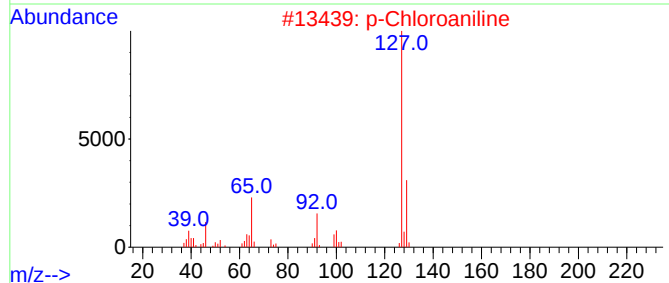
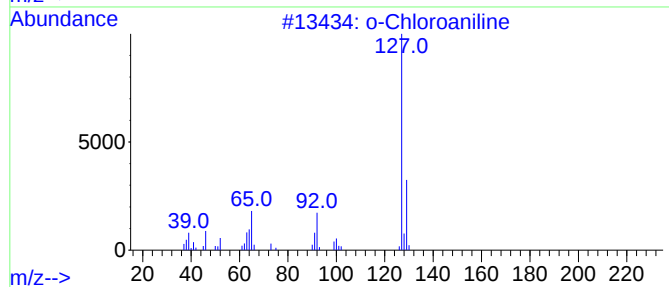
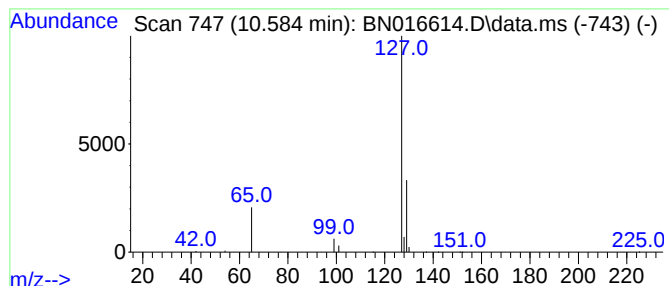
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.584	0.12 ng	58197	Naphthalene-d8	10.406

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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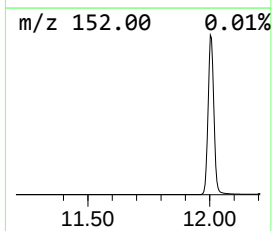
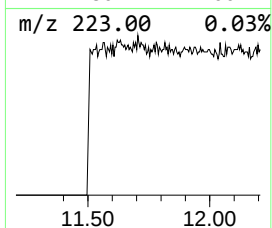
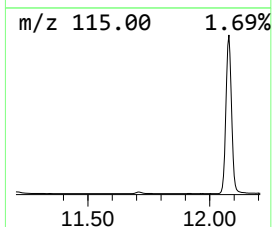
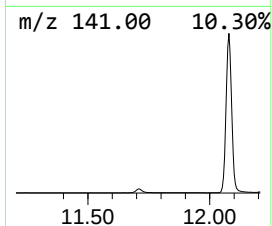
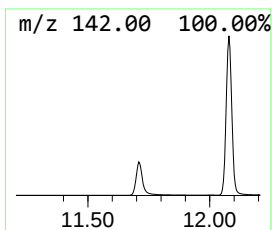
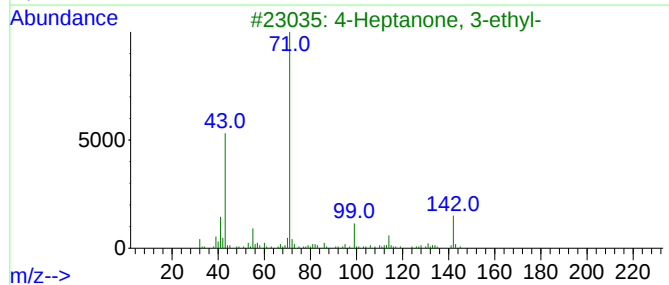
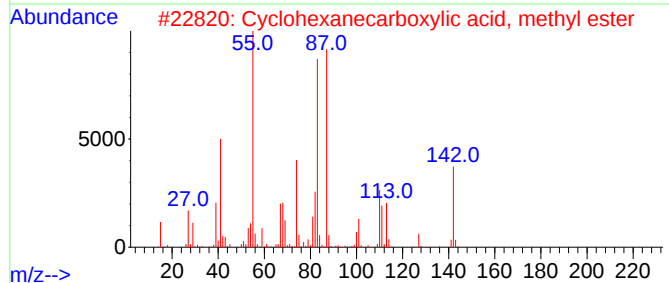
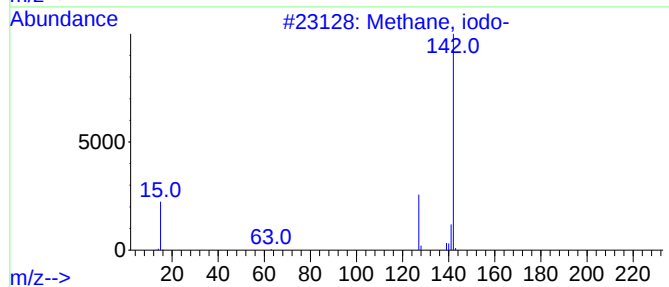
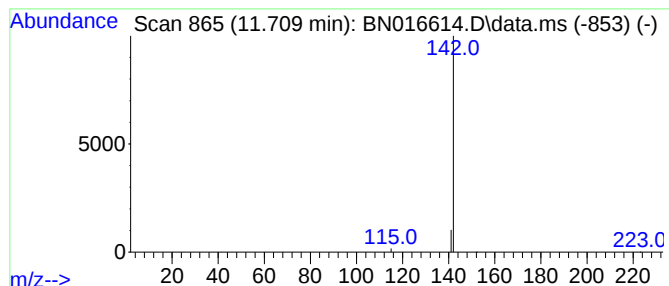
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	24947	Naphthalene-d8	10.406

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



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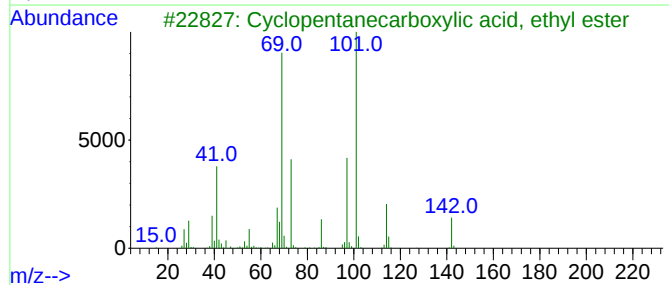
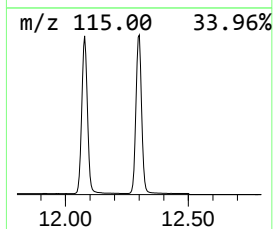
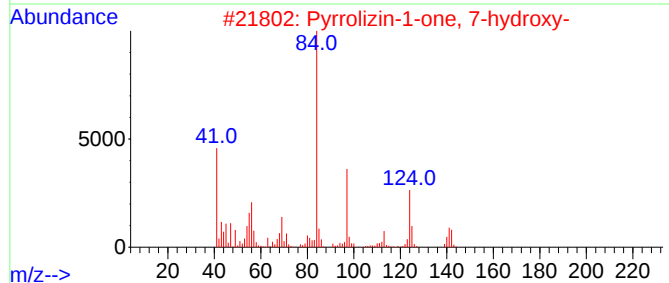
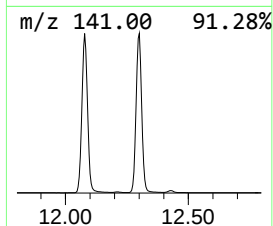
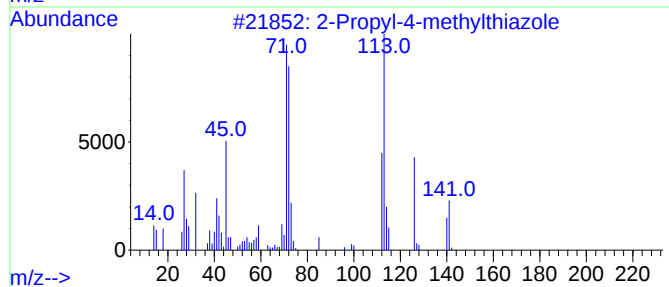
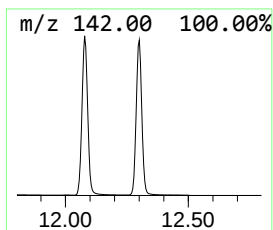
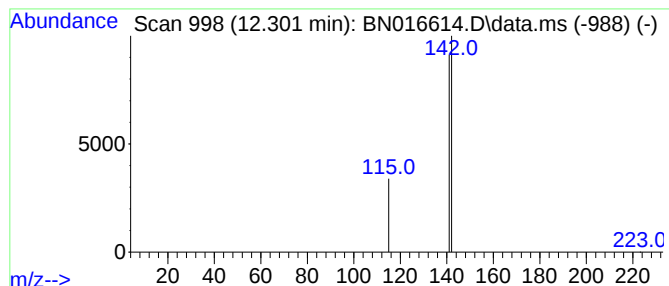
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.42 ng	196359	Naphthalene-d8	10.406
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2-Propyl-4-methylthiazole	141 C7H11NS	052414-87-6 4
2		Pyrrolizin-1-one, 7-hydroxy-	141 C7H11NO2	1000125-96-2 3
3		Cyclopentanecarboxylic acid, eth...	142 C8H14O2	1000375-86-4 3
4		2-Propionylthiazole	141 C6H7NOS	043039-98-1 3
5		2,4(1H,3H)-Pyrimidinedione, 6-am...	141 C5H7N3O2	002434-53-9 2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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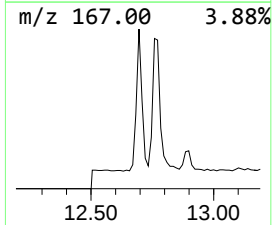
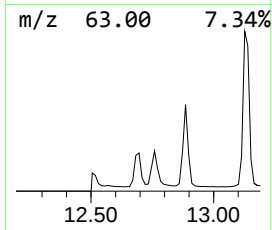
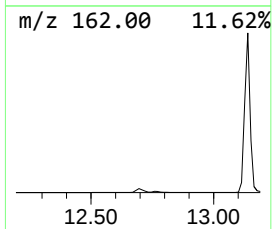
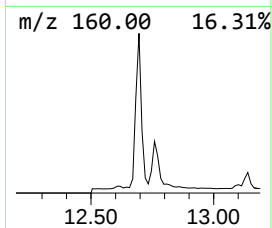
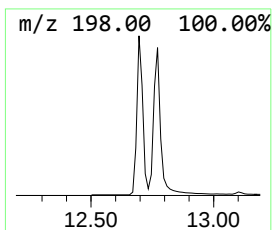
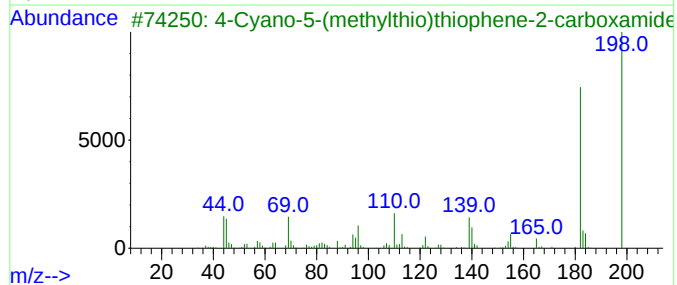
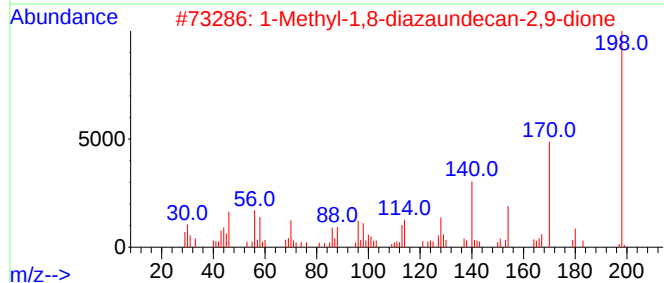
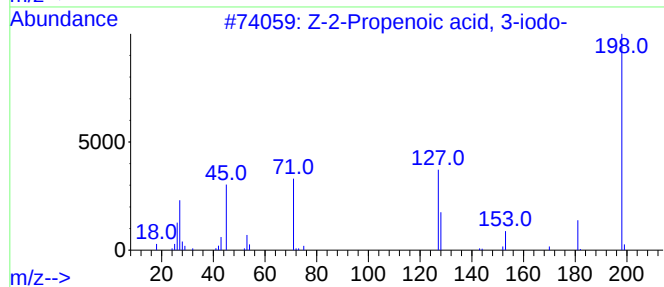
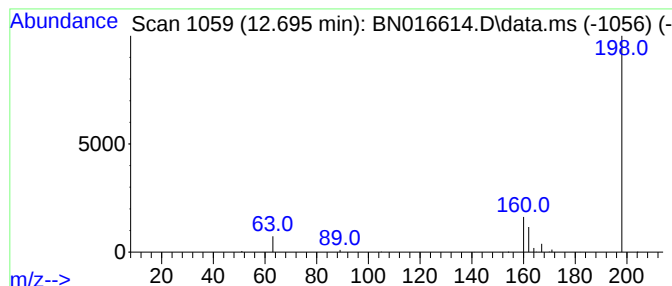
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Z-2-Propenoic acid, 3-iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	28202	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
2			1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	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			E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

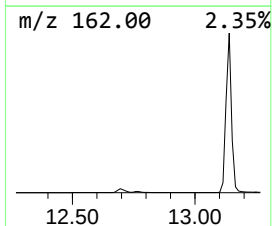
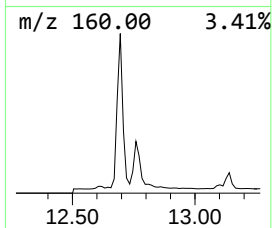
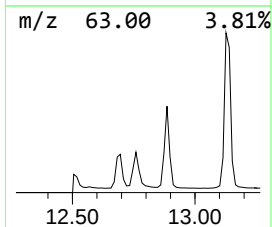
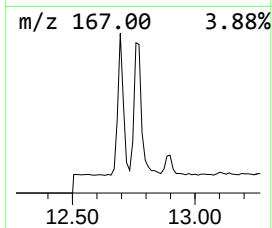
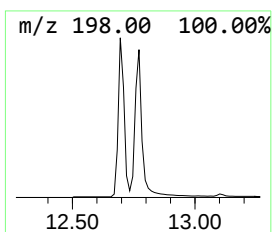
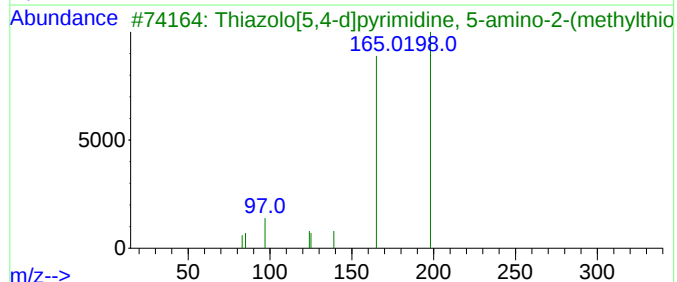
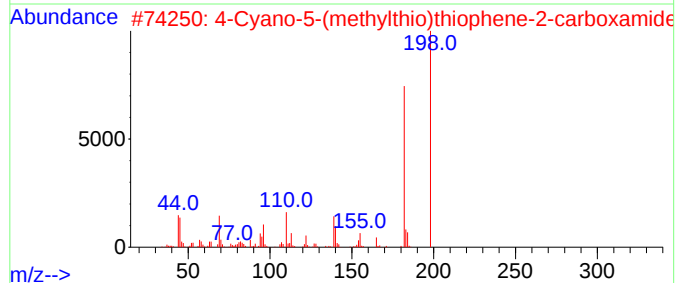
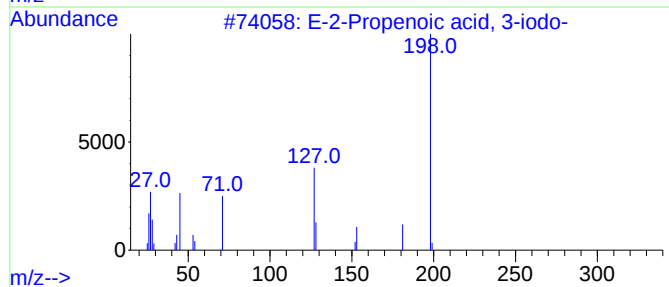
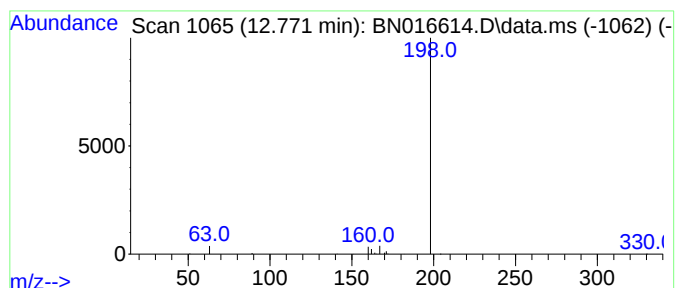
Instrument :
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.772	0.05 ng	24258	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	E-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-7	3
2	4-Cyano-5-(methylthio)thiophene-...		198	C7H6N2OS2	1000267-39-2	3
3	Thiazolo[5,4-d]pyrimidine, 5-ami...		198	C6H6N4S2	019835-31-5	3
4	Z-2-Propenoic acid, 3-iodo-		198	C3H3IO2	1000308-86-8	3
5	Methyl 2-(dimethylhydrazono)-3,3...		198	C6H9F3N2O2	1000489-35-4	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

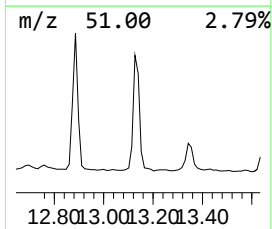
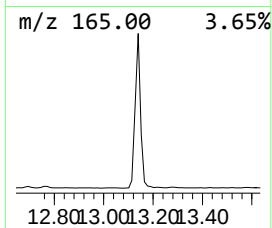
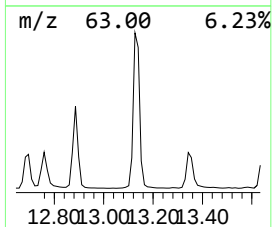
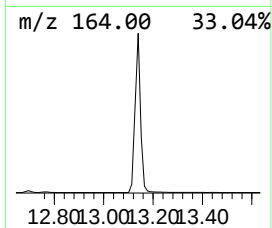
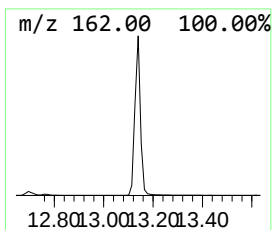
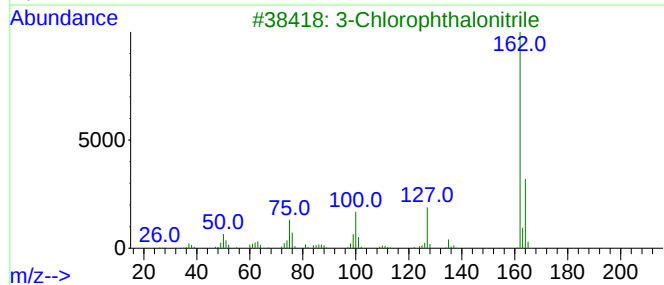
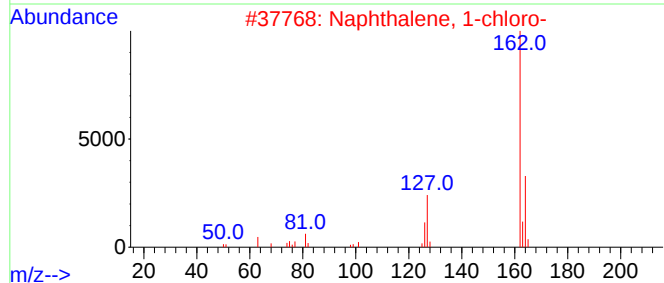
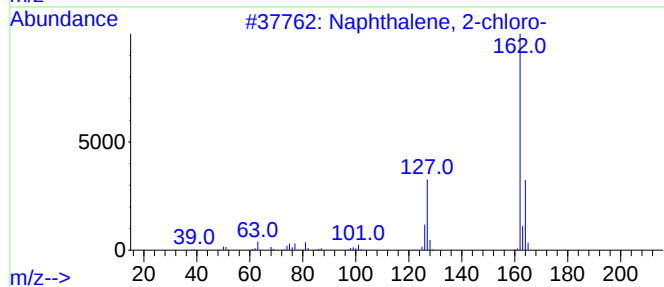
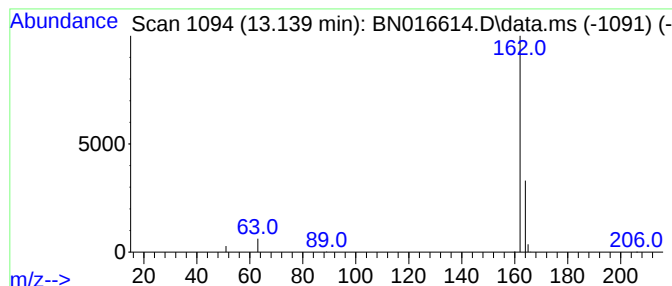
Instrument :
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LabSampleId :
SSTDCCC0.4

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

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.139	0.26 ng	123136	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 : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

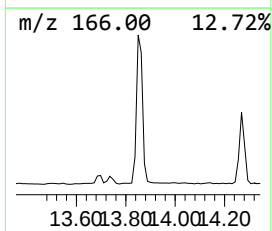
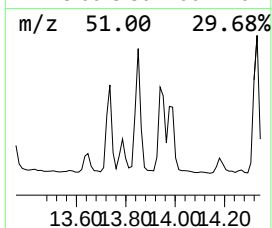
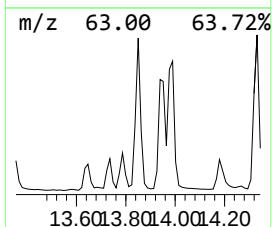
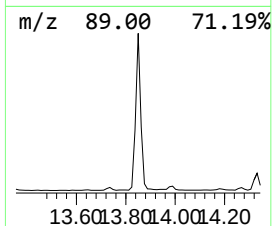
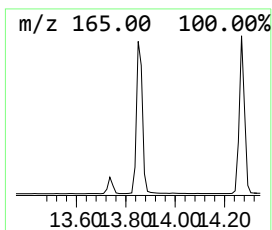
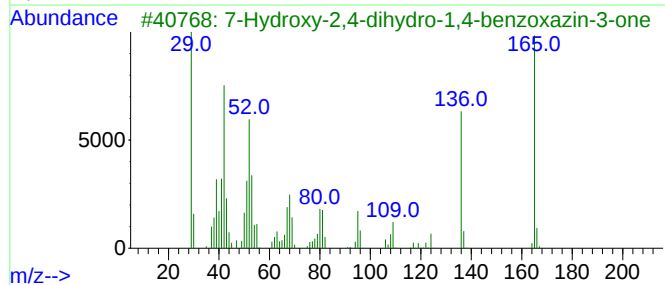
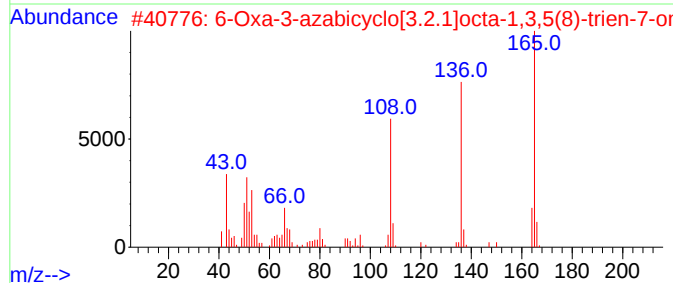
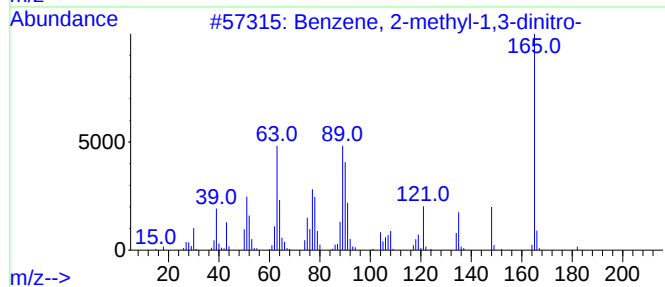
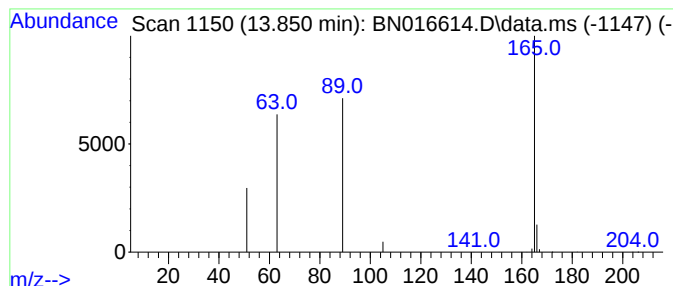
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.850	0.05 ng	26079	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-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9
5	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

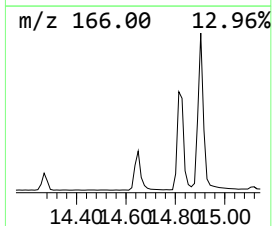
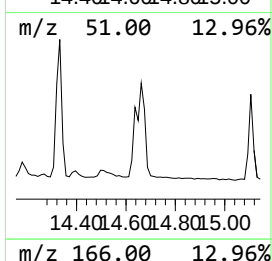
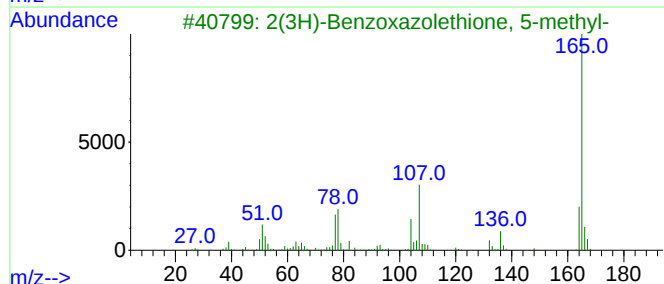
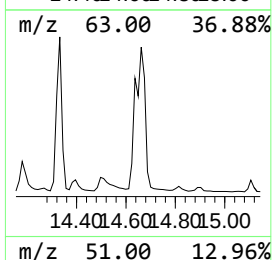
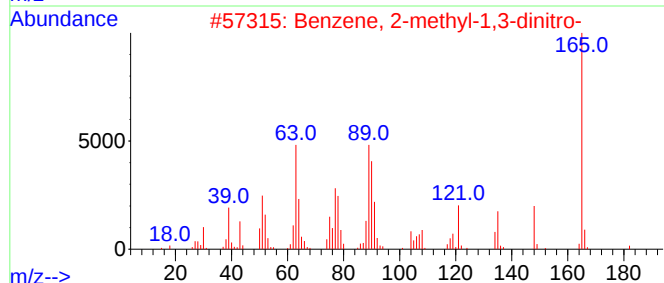
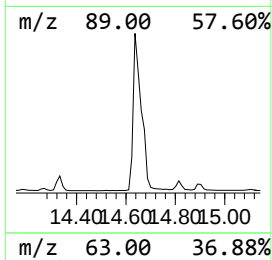
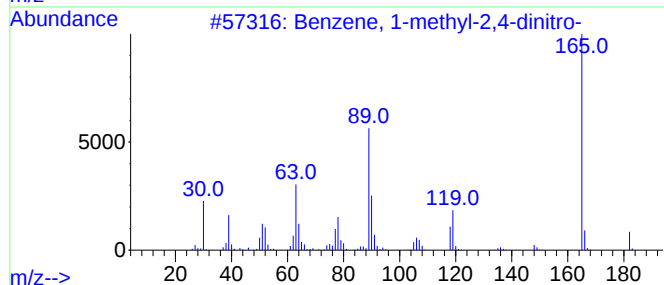
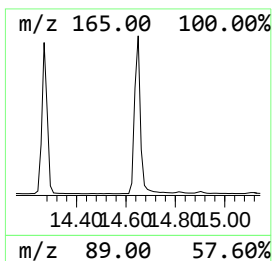
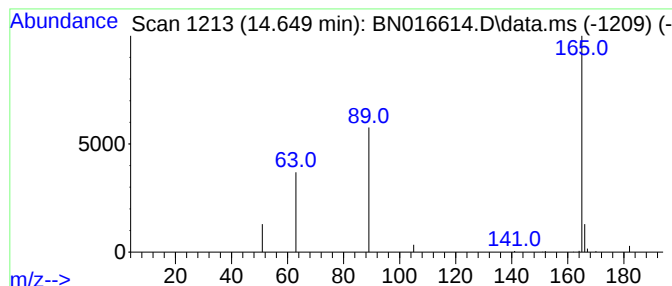
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LabSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
14.649	0.09 ng	40878	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	64
2	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	38
3	2(3H)-Benzoxazolethione, 5-methyl-		165	C8H7NOS	022876-22-8	9
4	4-Methoxyphenyl isothiocyanate		165	C8H7NOS	002284-20-0	9
5	6-Nitro-m-tolunitrile		162	C8H6N2O2	064113-86-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

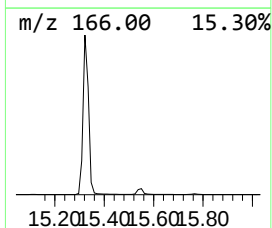
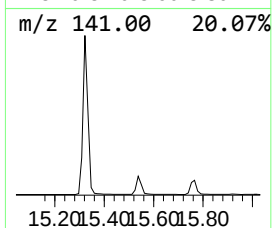
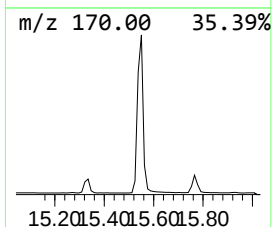
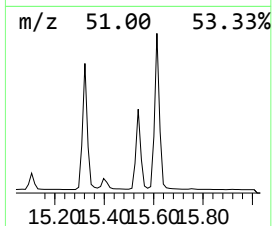
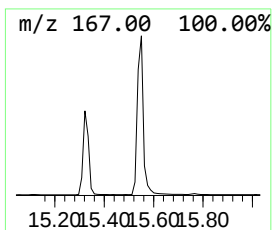
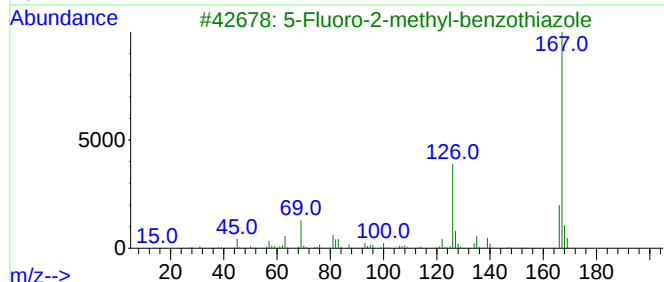
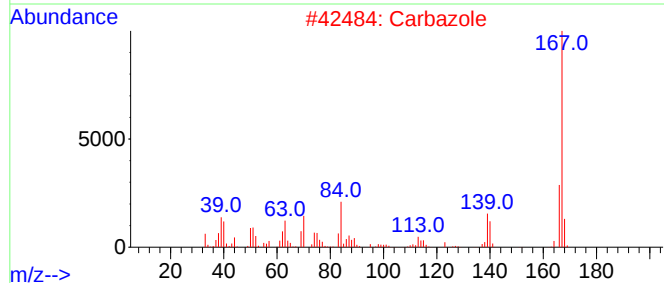
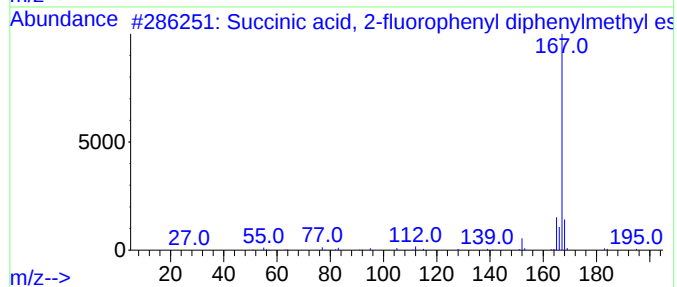
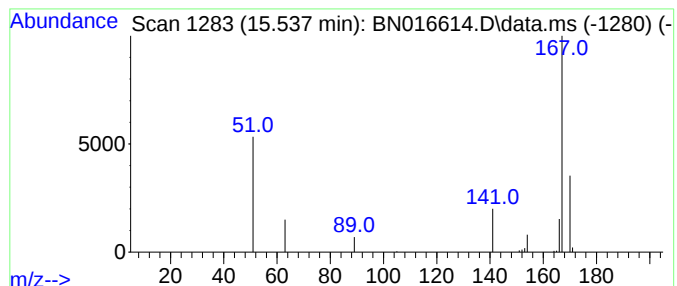
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	58079	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5			Methyl N,N-dimethyl-P-ethylphosp...	167	C5H14NOPS	1416009-05-6	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

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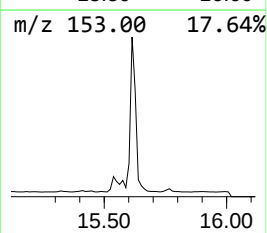
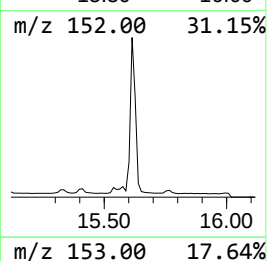
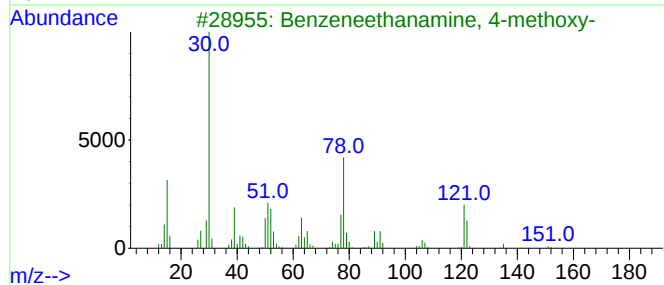
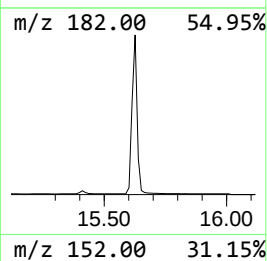
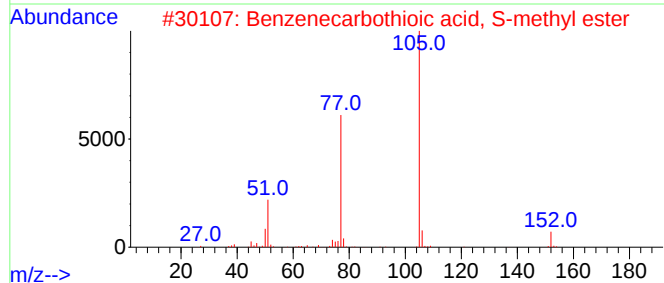
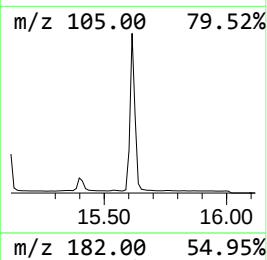
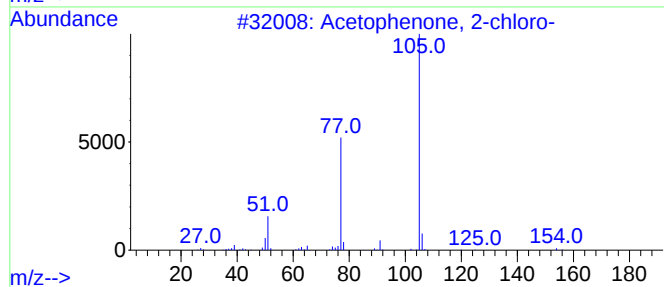
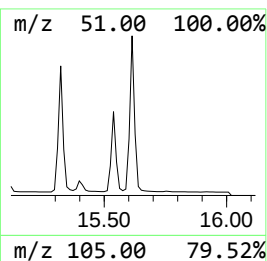
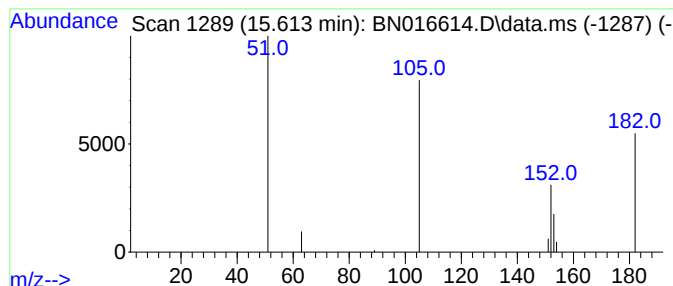
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	61676	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



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Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

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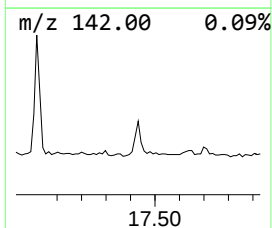
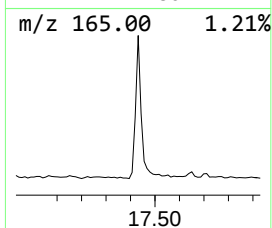
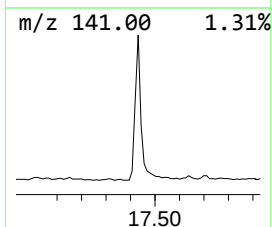
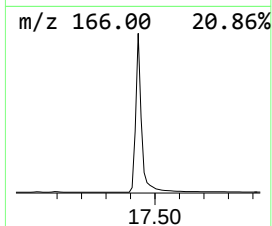
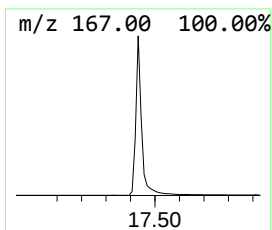
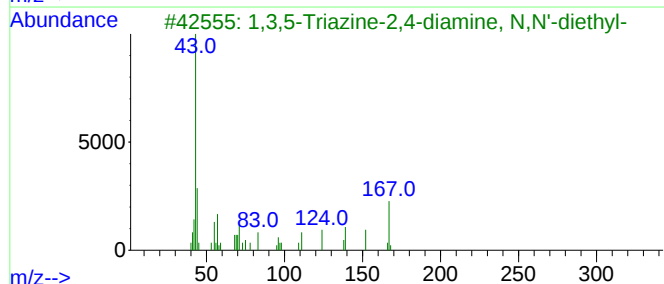
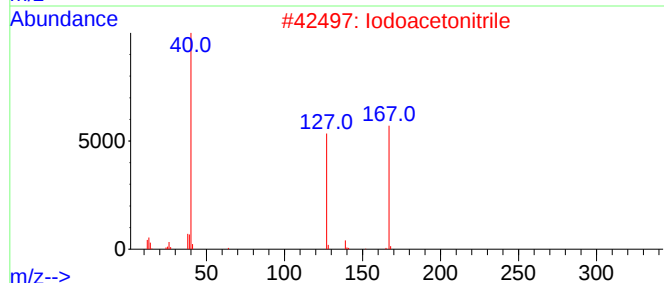
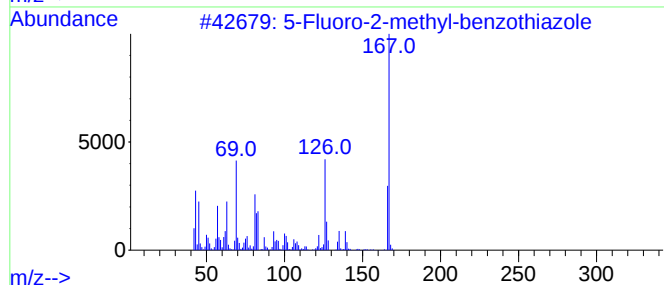
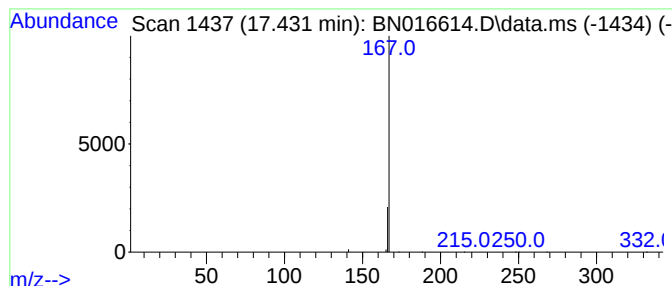
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.35 ng	125832	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			1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
4			1-Cyclopropanecarbonylpiperidin...	167	C9H13NO2	063463-43-4	4
5			2(1H)-Pyrimidinone, 4-[(2-methyl...	167	C8H13N3O	119608-70-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016614.D
Acq On : 30 Sep 2021 23:58
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

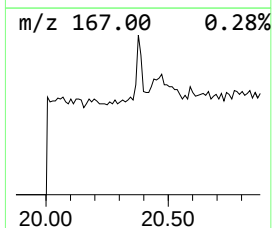
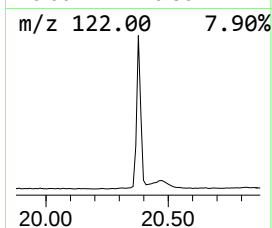
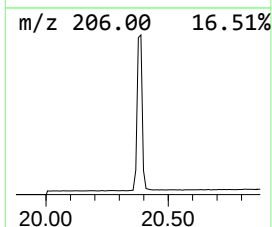
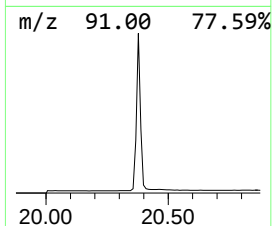
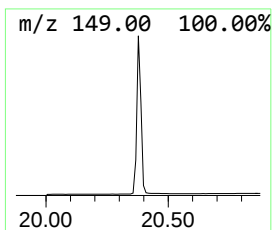
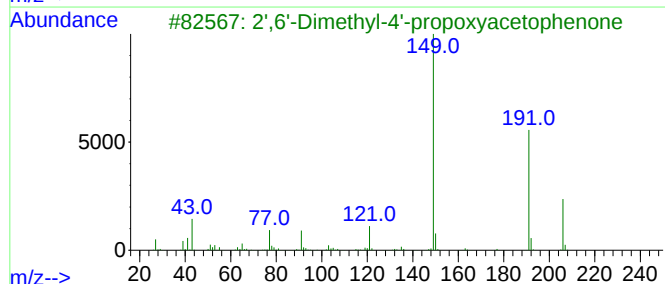
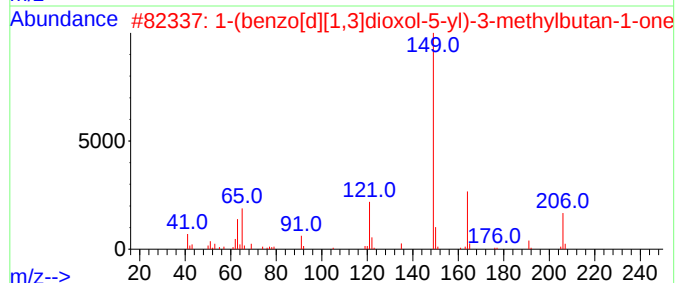
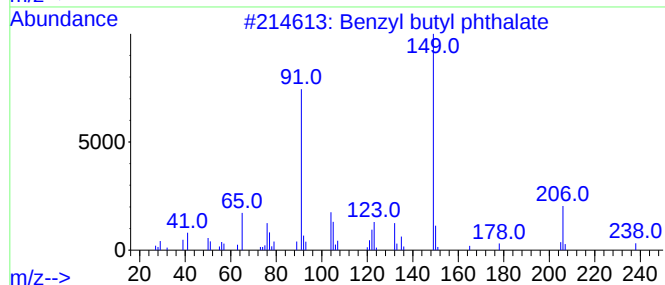
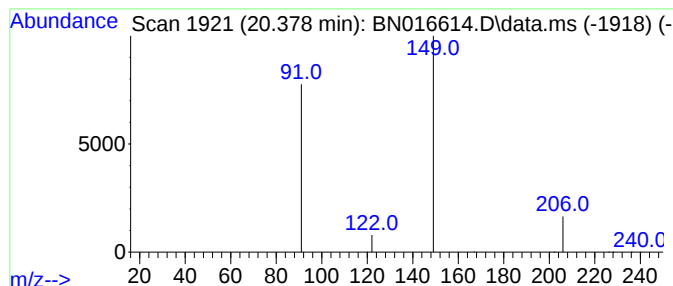
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	55246	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



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Misc :
ALS Vial : 19 Sample Multiplier: 1

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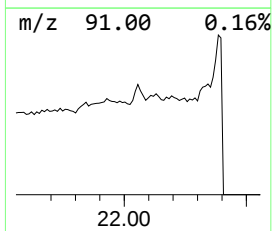
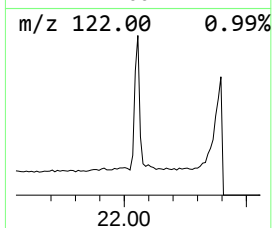
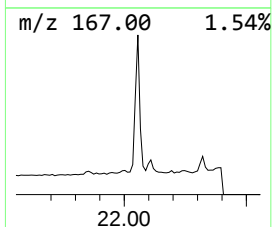
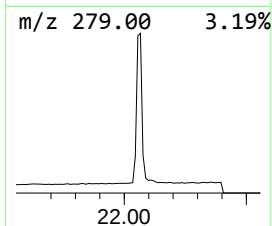
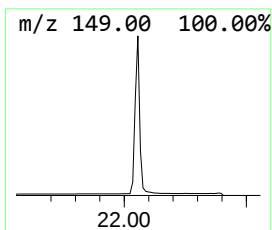
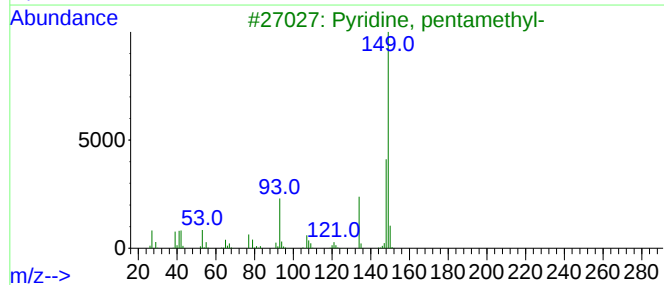
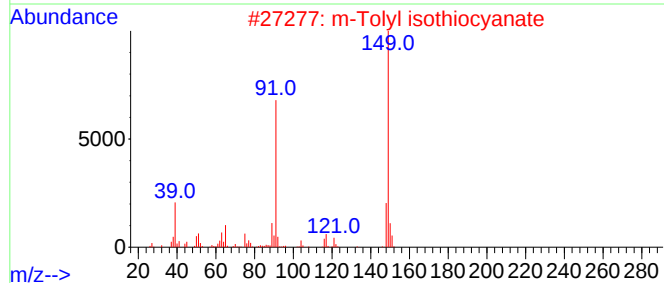
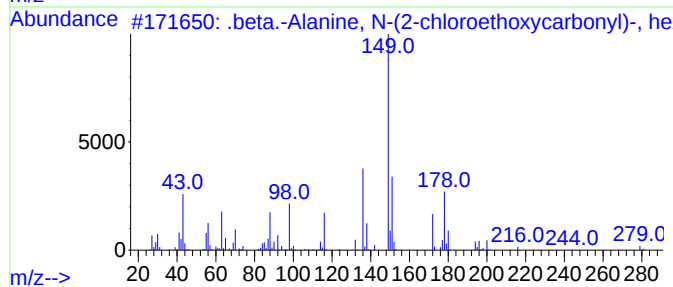
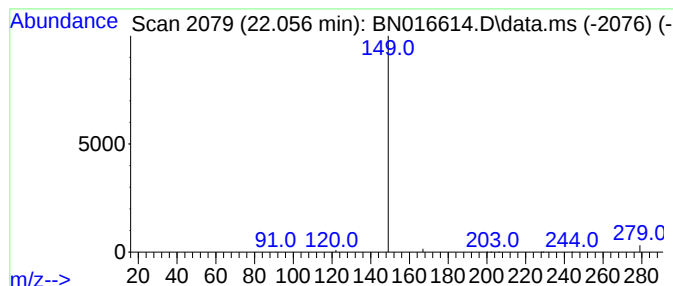
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	75304	Chrysene-d12	21.227

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



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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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	35610	1	7.642	120789	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32314	1	7.642	120789	0.4
Thietane	7.522	0.0	ng	14579	1	7.642	120789	0.4
6-Benzothiazola...	7.956	0.4	ng	107706	1	7.642	120789	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	50706	1	7.642	120789	0.4
Fomepizole	9.342	0.2	ng	78834	2	10.406	189198	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	26781	2	10.406	189198	0.4
o-Chloroaniline	10.584	0.1	ng	58197	2	10.406	189198	0.4
Methane, iodo-	11.709	0.1	ng	24947	2	10.406	189198	0.4
2-Propyl-4-meth...	12.301	0.4	ng	196359	2	10.406	189198	0.4
Z-2-Propenoic a...	12.695	0.1	ng	28202	3	14.269	192199	0.4
E-2-Propenoic a...	12.772	0.1	ng	24258	3	14.269	192199	0.4
Naphthalene, 2-...	13.139	0.3	ng	123136	3	14.269	192199	0.4
Benzene, 2-meth...	13.850	0.1	ng	26079	3	14.269	192199	0.4
Benzene, 1-meth...	14.649	0.1	ng	40878	3	14.269	192199	0.4
Succinic acid, ...	15.537	0.1	ng	58079	3	14.269	192199	0.4
Acetophenone, 2...	15.614	0.1	ng	61676	3	14.269	192199	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	125832	4	17.017	144091	0.4
Benzyl butyl ph...	20.378	0.1	ng	55246	5	21.227	377408	0.4
.beta.-Alanine,...	22.056	0.1	ng	75304	5	21.227	377408	0.4