

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016705.D
 Acq On : 03 Oct 2021 13:00
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 73 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: BN016705.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	5555	8215	1.72%	0.103%
2	3.281	20	22	38	rVB	4986	22855	4.79%	0.287%
3	3.595	51	56	81	rVB	6639	30755	6.45%	0.386%
4	5.264	231	237	253	rVB	15533	57554	12.07%	0.722%
5	6.822	401	406	417	rBV	26160	64408	13.51%	0.807%
6	6.979	418	423	429	rVV	17783	40377	8.47%	0.506%
7	7.080	429	434	440	rVV	34440	69215	14.52%	0.868%
8	7.200	440	447	461	rVB	12308	32930	6.91%	0.413%
9	7.523	478	482	489	rVB	6394	14039	2.94%	0.176%
10	7.643	490	495	504	rVB2	46831	110017	23.07%	1.379%
11	7.956	524	529	538	rVB2	44812	99511	20.87%	1.248%
12	8.168	547	552	557	rVB	3131	7278	1.53%	0.091%
13	8.430	572	577	590	rVB3	24232	56479	11.85%	0.708%
14	8.785	601	605	606	rBV	40075	75109	15.75%	0.942%
15	8.823	606	608	616	rVB	32971	60364	12.66%	0.757%
16	9.342	646	649	653	rBV	57557	91707	19.23%	1.150%
17	9.520	660	663	666	rBV	3504	6966	1.46%	0.087%
18	9.596	666	669	678	rVB	9695	17444	3.66%	0.219%
19	9.836	685	688	693	rBV	16563	28161	5.91%	0.353%
20	10.065	703	706	709	rBV	4924	9433	1.98%	0.118%
21	10.407	729	733	735	rBV	102337	182658	38.31%	2.290%
22	10.458	735	737	740	rVV	103554	167451	35.12%	2.099%
23	10.572	743	746	756	rVV	32809	71137	14.92%	0.892%
24	10.749	756	760	763	rVB	31149	53644	11.25%	0.673%
25	11.307	801	804	814	rBV	3177	7943	1.67%	0.100%
26	11.714	855	866	892	rBV	17958	30988	6.50%	0.389%
27	12.003	921	931	940	rBV	56232	91049	19.10%	1.142%
28	12.079	940	948	973	rVB	124934	199601	41.86%	2.502%
29	12.296	988	997	1020	rBV	122951	192678	40.41%	2.416%
30	12.696	1056	1059	1062	rBV	22061	36432	7.64%	0.457%
31	12.772	1062	1065	1071	rVB	18363	32291	6.77%	0.405%
32	12.886	1071	1074	1078	rBV	109755	188520	39.54%	2.364%
33	13.140	1089	1094	1097	rBV	80123	129433	27.15%	1.623%
34	13.343	1107	1110	1116	rVB2	2703	5235	1.10%	0.066%
35	13.736	1138	1141	1143	rBV	13355	18464	3.87%	0.231%
36	13.850	1147	1150	1153	rVB	20664	30523	6.40%	0.383%

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Integrator: RTE

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Sampling : 1

Min Area: 1 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	13.990	1158	1161	1164	rVB	107645	169561	35.56%	2.126%
38	14.269	1180	1183	1186	rBV	142044	200893	42.13%	2.519%
39	14.332	1186	1188	1191	rVB	168332	236625	49.63%	2.967%
40	14.523	1199	1203	1209	rBV2	2002	5339	1.12%	0.067%
41	14.650	1209	1213	1219	rBV2	17157	43689	9.16%	0.548%
42	14.827	1224	1227	1230	rBV	7896	13284	2.79%	0.167%
43	14.903	1230	1233	1236	rBV	10471	15328	3.21%	0.192%
44	15.106	1246	1249	1252	rBV	10224	12895	2.70%	0.162%
45	15.322	1263	1266	1270	rBV2	226367	359662	75.43%	4.509%
46	15.538	1280	1283	1287	rBV	38572	68249	14.31%	0.856%
47	15.614	1287	1289	1293	rVB2	45175	70669	14.82%	0.886%
48	15.766	1298	1301	1305	rBV2	18204	29654	6.22%	0.372%
49	16.227	1335	1338	1341	rBV2	65958	96581	20.26%	1.211%
50	16.324	1343	1346	1350	rVB	44751	71871	15.07%	0.901%
51	16.507	1358	1361	1364	rBV	36028	48728	10.22%	0.611%
52	16.677	1372	1375	1384	rBV	34499	58441	12.26%	0.733%
53	17.018	1400	1403	1405	rBV	93069	163831	34.36%	2.054%
54	17.066	1405	1407	1410	rVV	161731	222377	46.64%	2.788%
55	17.152	1411	1414	1428	rVB	127683	209278	43.89%	2.624%
56	17.431	1434	1437	1452	rBV	112366	169550	35.56%	2.126%
57	18.021	1482	1486	1498	rVB	8679	12477	2.62%	0.156%
58	19.068	1687	1697	1699	rBV	142129	183694	38.53%	2.303%
59	19.098	1699	1703	1720	rVB	212671	287955	60.39%	3.610%
60	19.460	1768	1776	1792	rBV	223712	295981	62.08%	3.711%
61	19.679	1814	1820	1846	rVB	135120	165956	34.81%	2.081%
62	20.378	1918	1921	1924	rBV	116246	157914	33.12%	1.980%
63	20.771	1953	1958	1972	rVB	5613	28990	6.08%	0.363%
64	21.174	1993	1996	1998	rBV	135006	179522	37.65%	2.251%
65	21.217	1998	2000	2003	rVV2	242143	476807	100.00%	5.978%
66	21.270	2003	2005	2008	rVB	220587	275068	57.69%	3.449%
67	22.056	2076	2079	2082	rBV	193277	234102	49.10%	2.935%
68	22.321	2101	2104	2108	rVB	3109	4960	1.04%	0.062%
69	22.810	2219	2230	2237	rBV	123403	202982	42.57%	2.545%
70	22.855	2237	2243	2266	rVB	119041	200156	41.98%	2.509%
71	23.389	2388	2399	2417	rBV	79216	162535	34.09%	2.038%
72	23.488	2418	2428	2470	rVB	76877	147670	30.97%	1.851%
73	24.090	2596	2604	2621	rVB	7381	13756	2.89%	0.172%
74	24.861	2822	2829	2850	rVB	6729	14449	3.03%	0.181%
75	25.781	3075	3098	3147	rBV5	65003	235658	49.42%	2.954%
76	26.466	3279	3298	3335	rVB	28249	88254	18.51%	1.106%

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

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

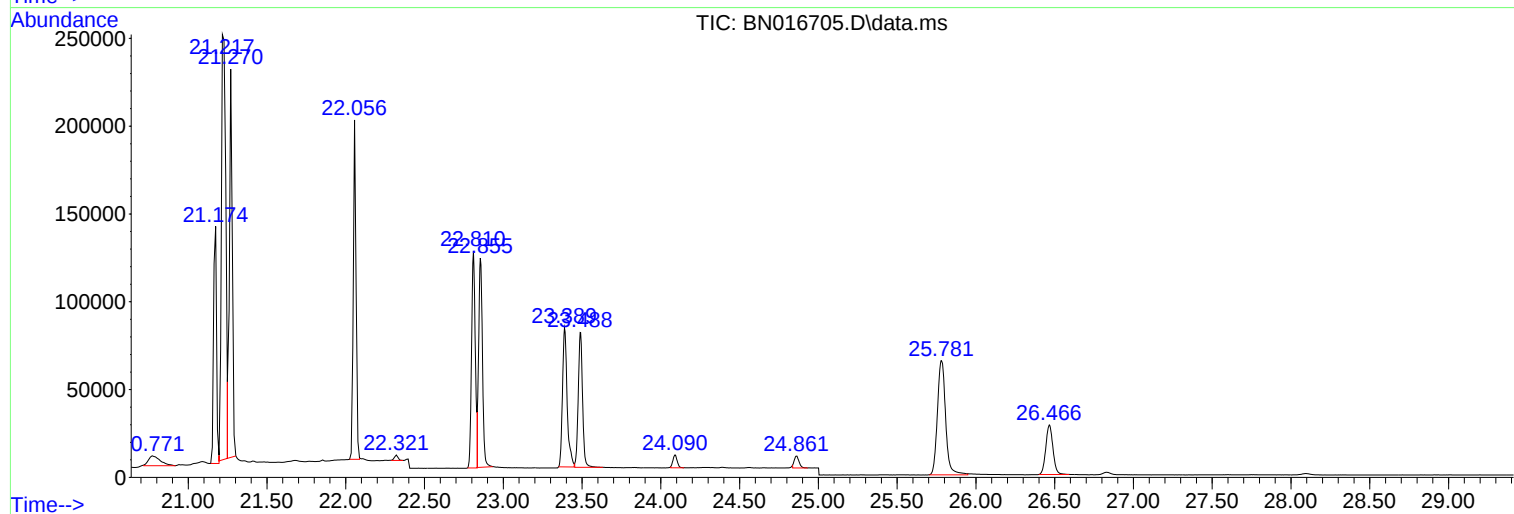
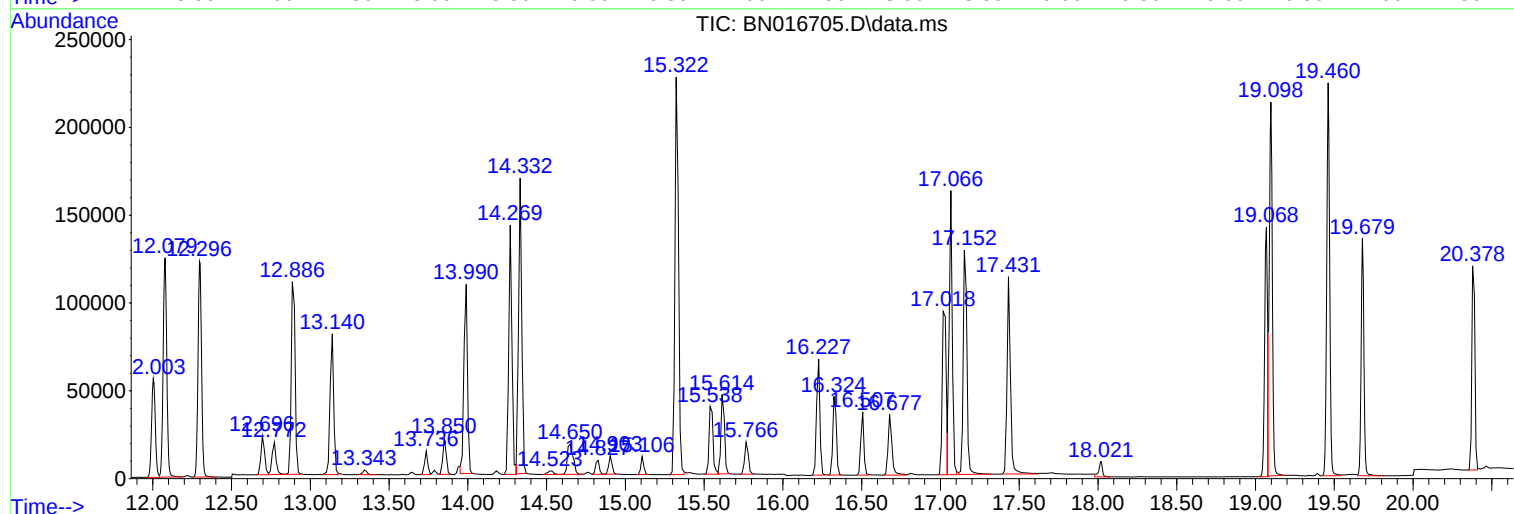
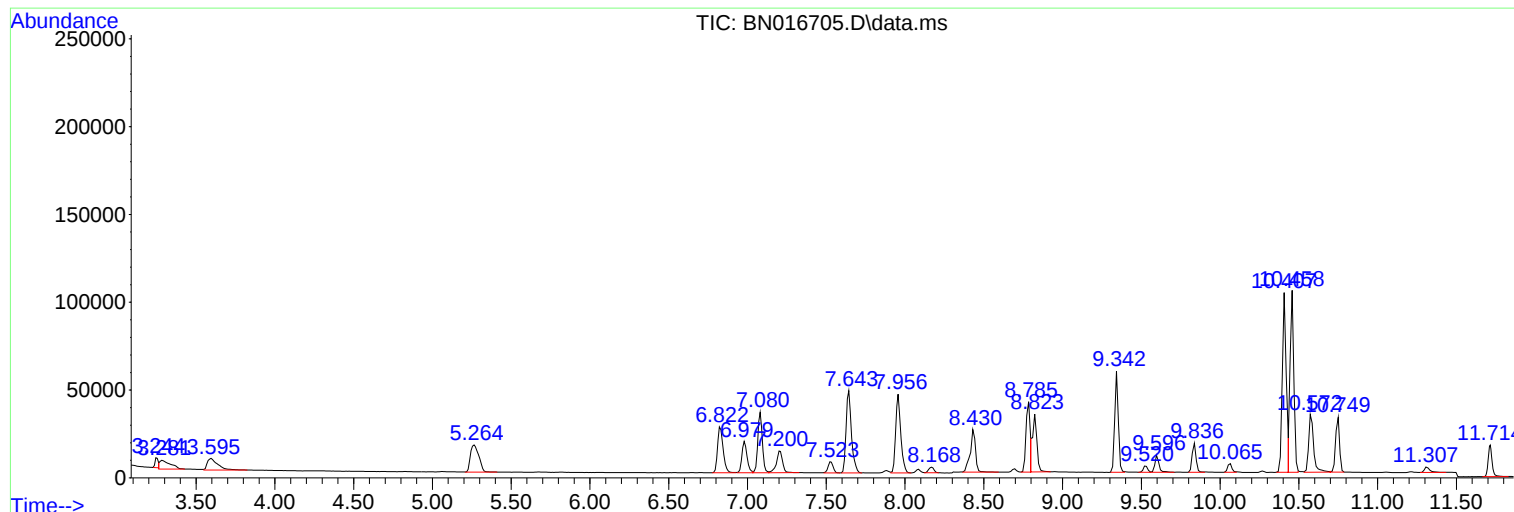
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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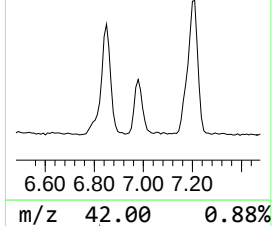
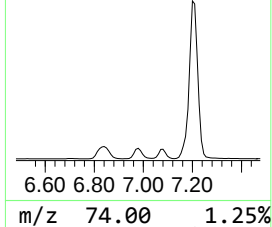
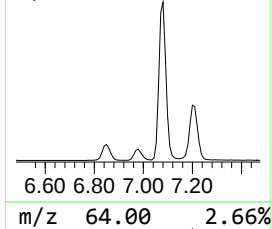
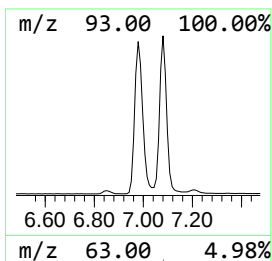
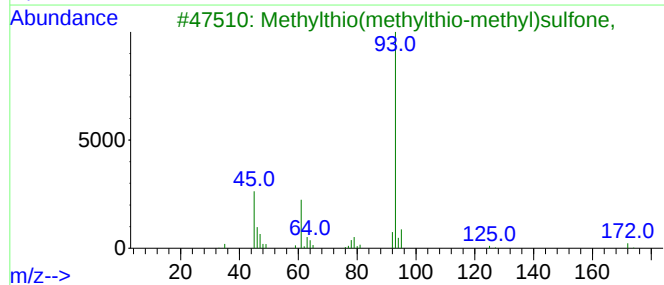
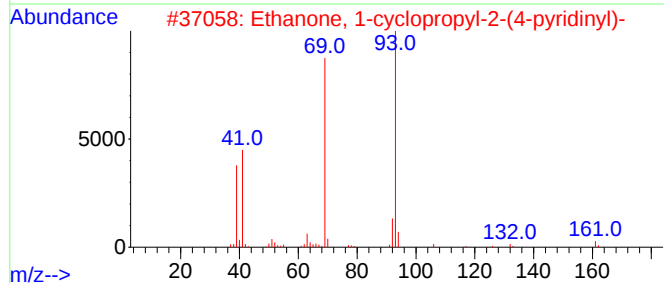
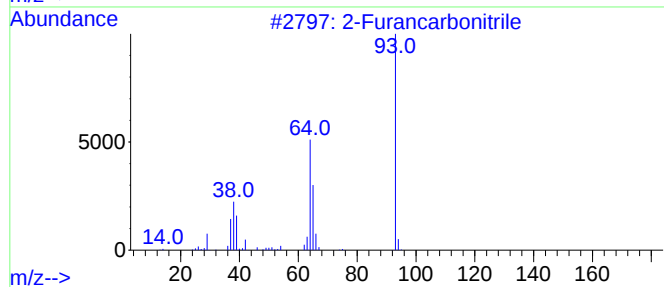
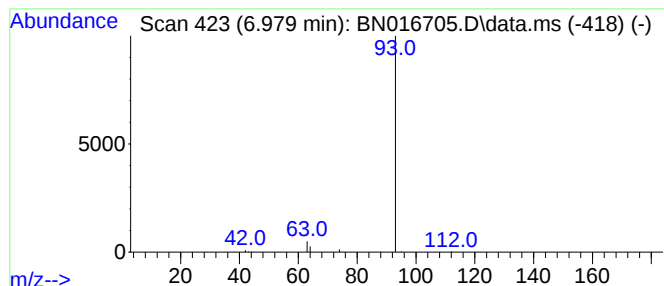
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Furancarbonitrile Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.15 ng	40377	1,4-Dichlorobenzene-d4	7.643

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furancarbonitrile	93	C5H3NO	000617-90-3	3
2			Ethanone, 1-cyclopropyl-2-(4-pyr...	161	C10H11NO	006580-95-6	2
3			Methylthio(methylthio-methyl)sul...	172	C3H8O2S3	058000-45-6	1
4			Nortricyclyl bromide	172	C7H9Br	1000342-32-2	1
5			Bis(2-chloroethyl) ether	142	C4H8Cl2O	000111-44-4	1



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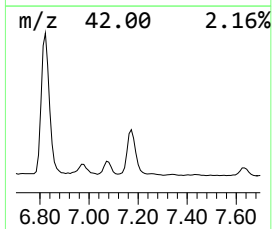
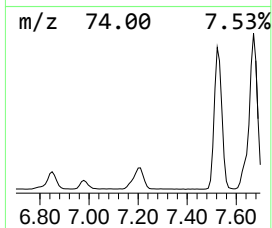
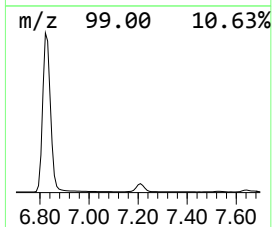
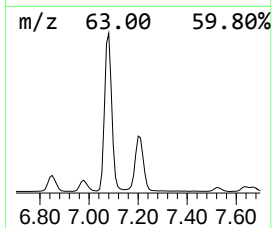
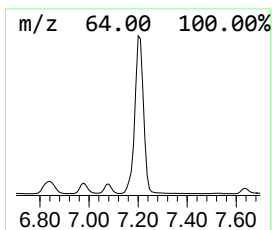
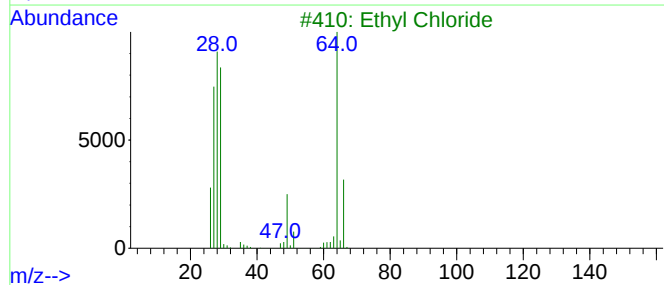
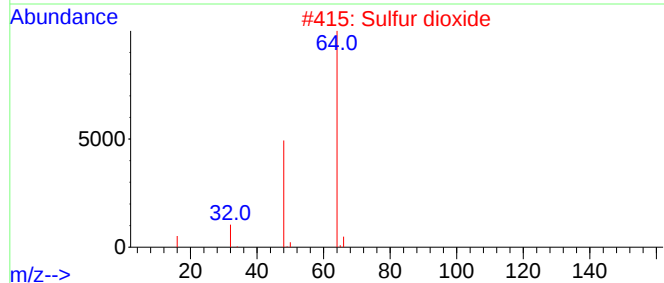
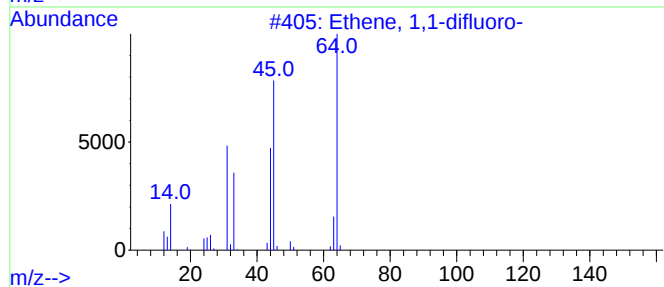
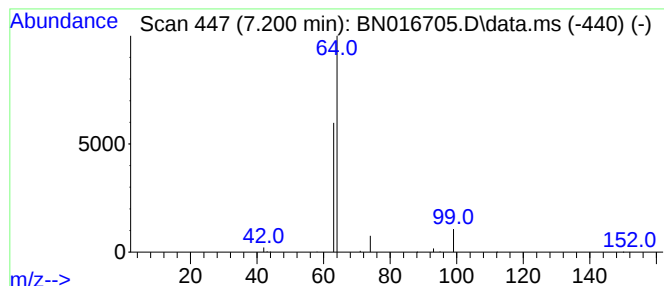
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.12 ng	32930	1,4-Dichlorobenzene-d4	7.643

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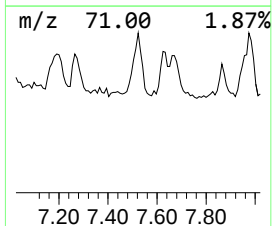
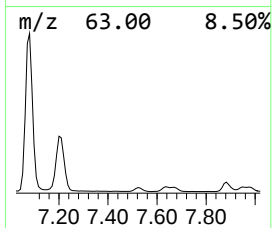
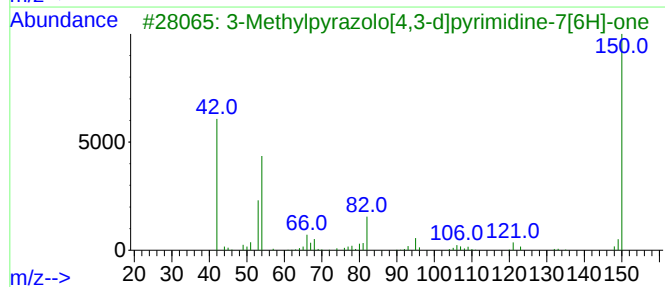
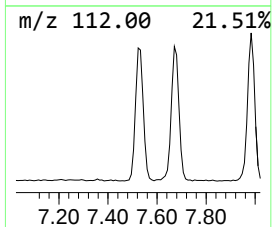
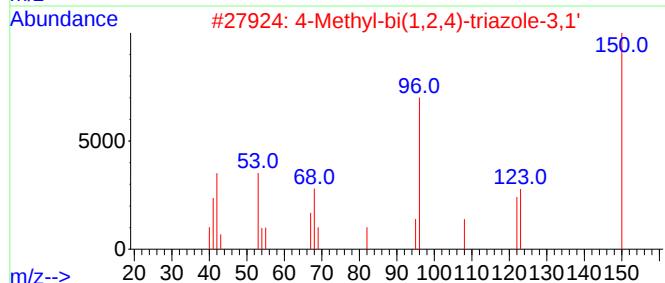
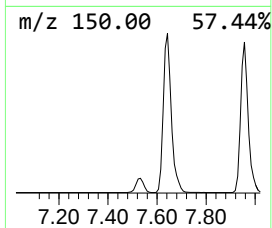
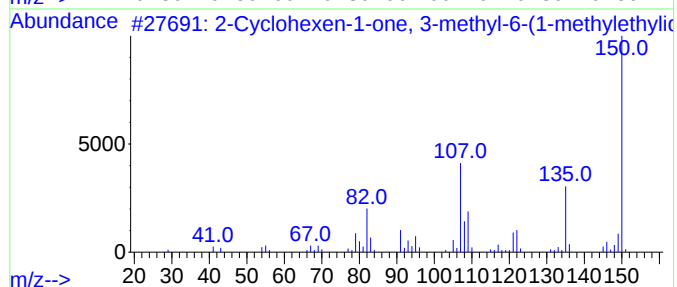
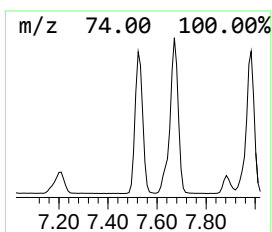
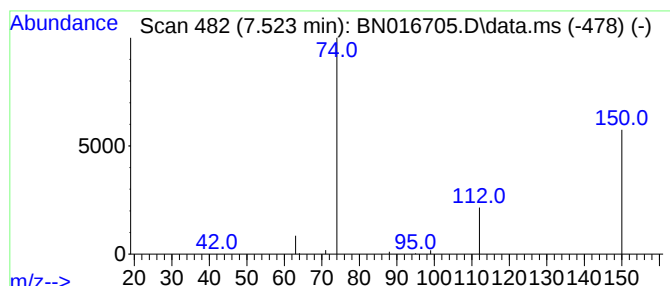
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Cyclohexen-1-one, 3-methy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	14039	1,4-Dichlorobenzene-d4	7.643

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



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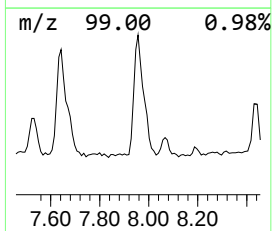
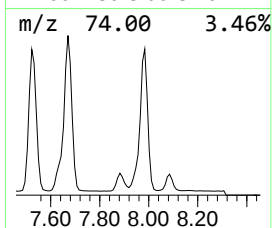
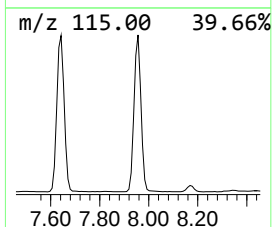
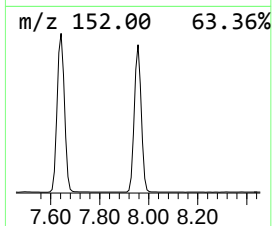
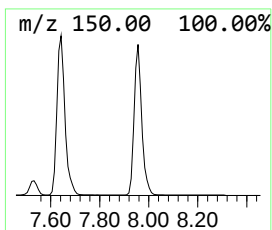
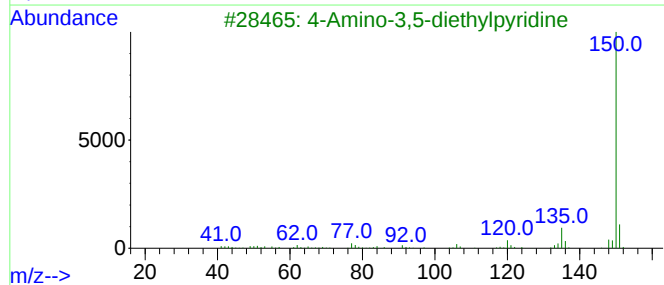
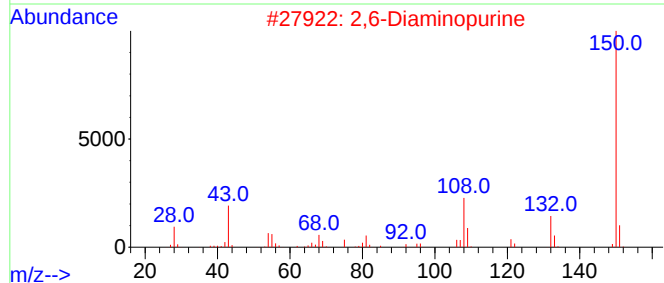
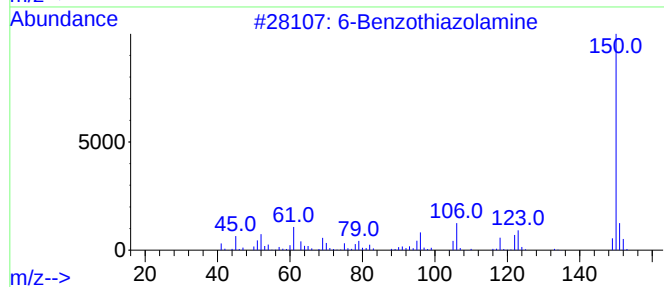
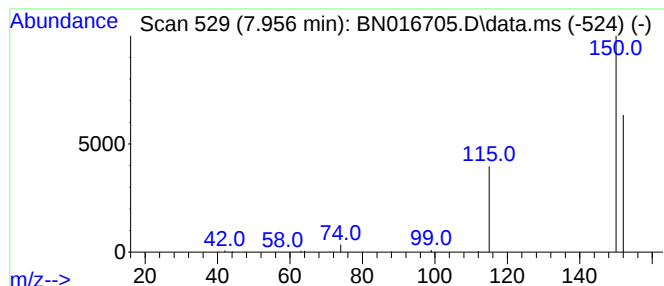
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6-Benzothiazolamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	99511	1,4-Dichlorobenzene-d4	7.643

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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

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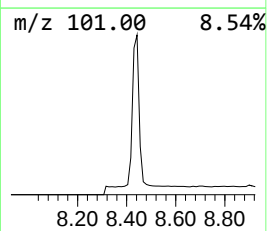
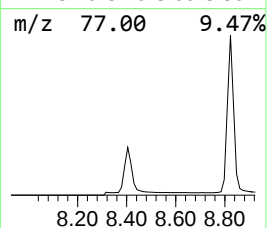
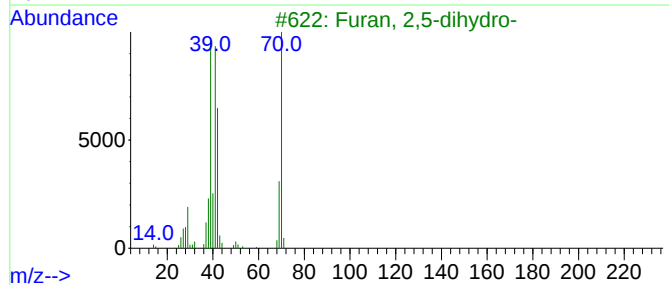
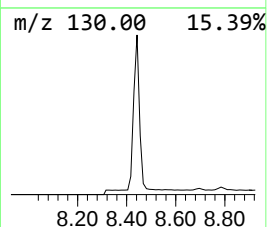
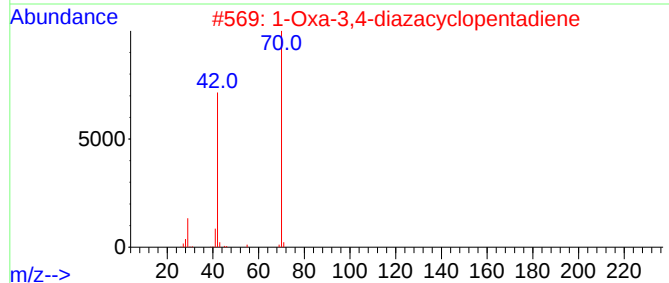
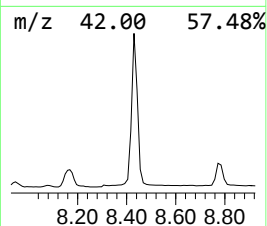
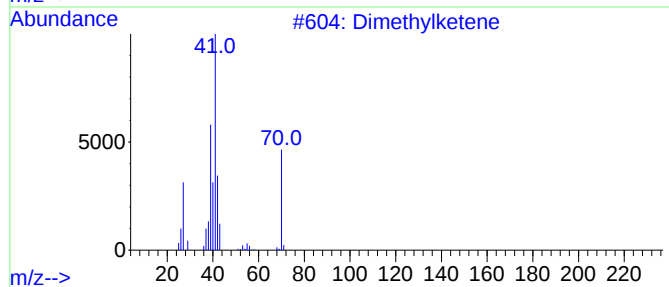
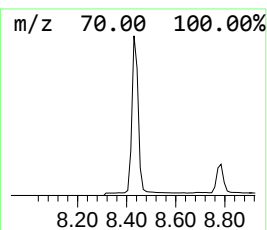
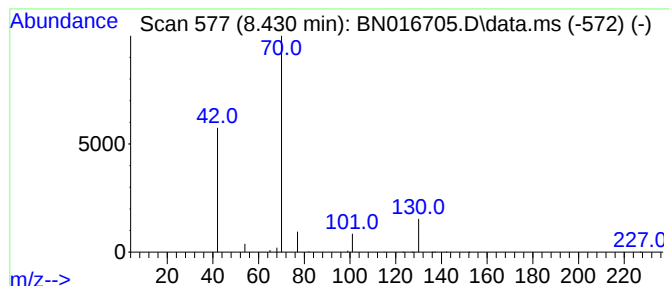
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dimethylketene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.21 ng	56479	1,4-Dichlorobenzene-d4	7.643

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethylketene	70	C4H6O	000598-26-5	5
2			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4
3			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	4
4			1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4
5			(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
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LabSampleId :
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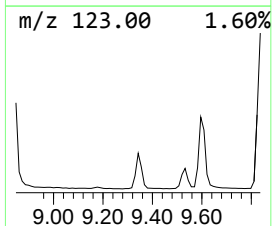
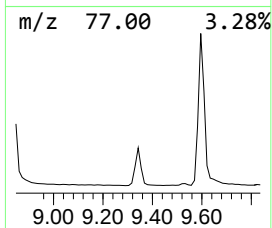
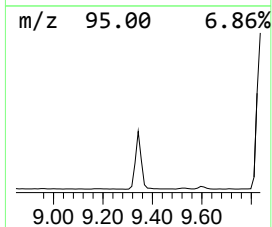
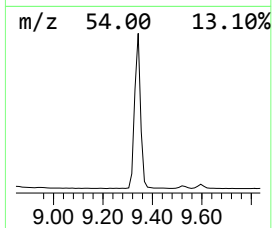
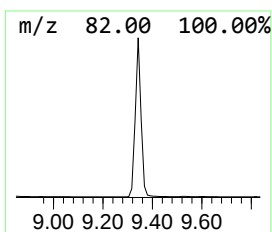
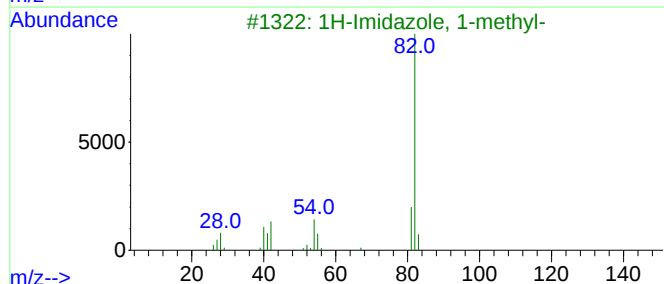
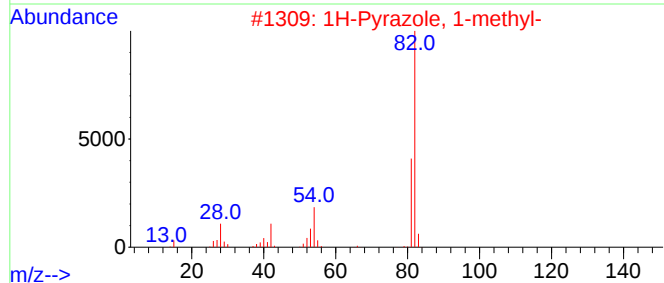
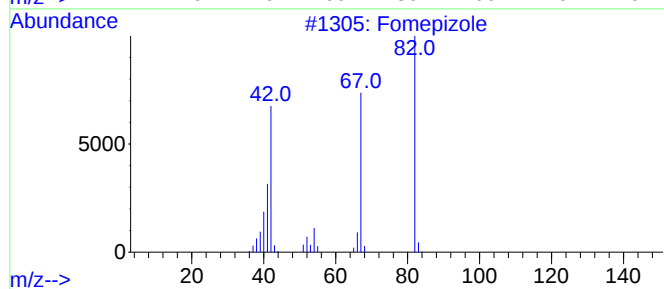
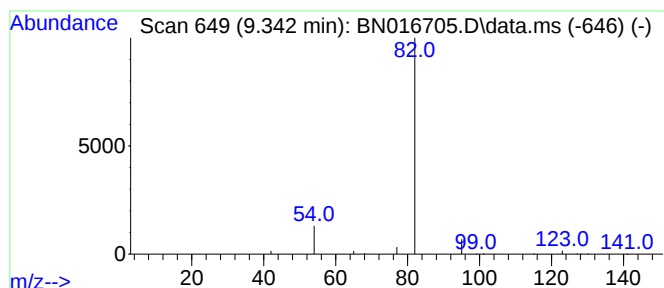
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.20 ng	91707	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
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Instrument :
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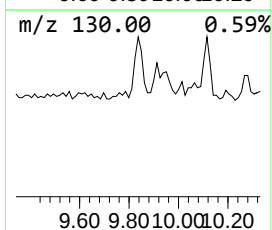
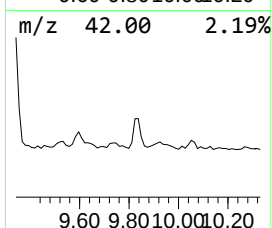
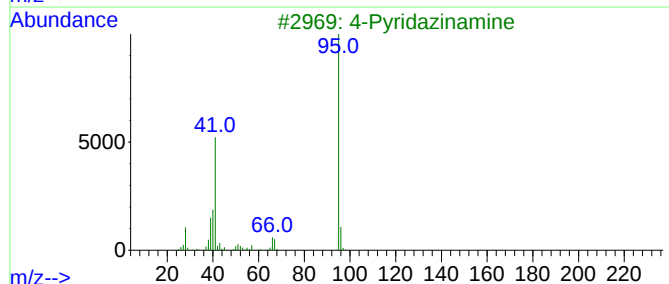
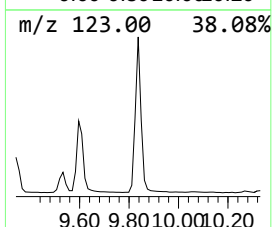
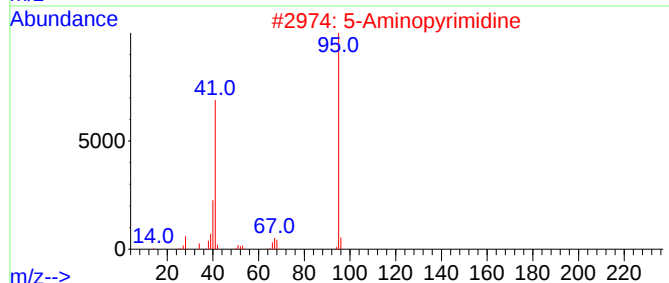
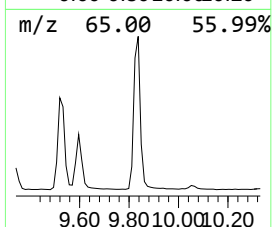
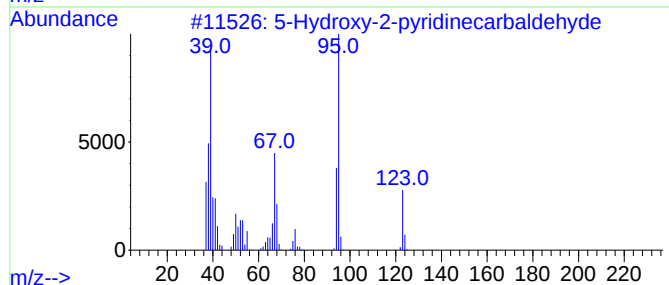
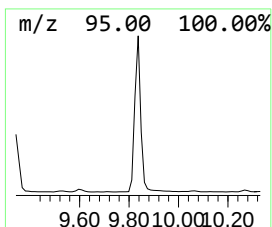
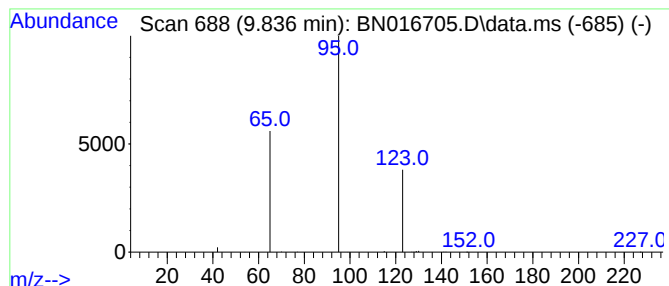
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Hydroxy-2-pyridinecarbal... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	28161	Naphthalene-d8	10.407

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2		5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
3		4-Pyridazinamine	95	C4H5N3	020744-39-2	2
4		Aminopyrazine	95	C4H5N3	005049-61-6	2
5		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
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Misc :
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Instrument :
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LabSampleId :
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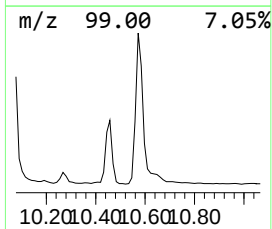
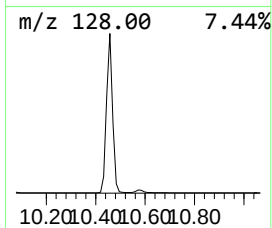
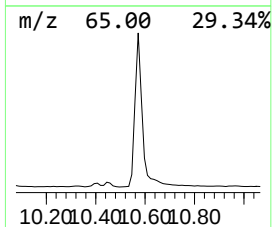
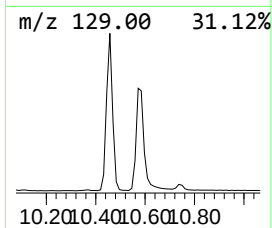
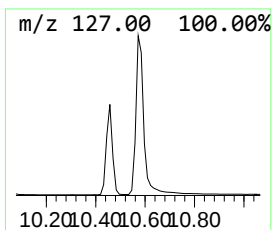
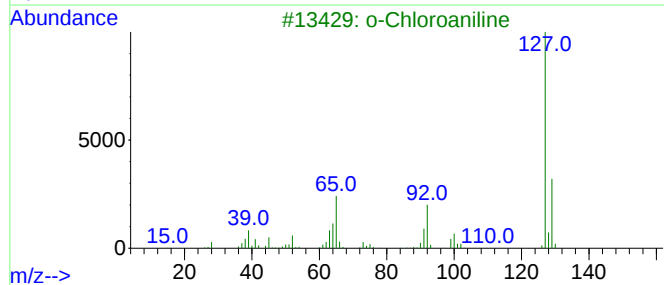
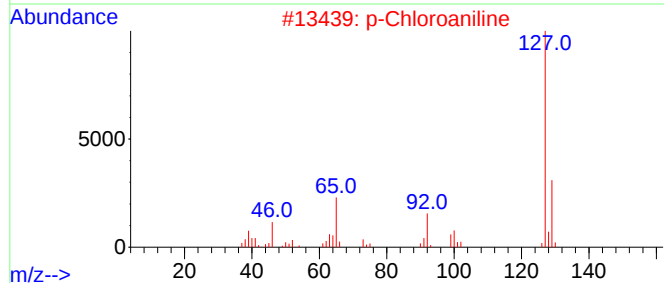
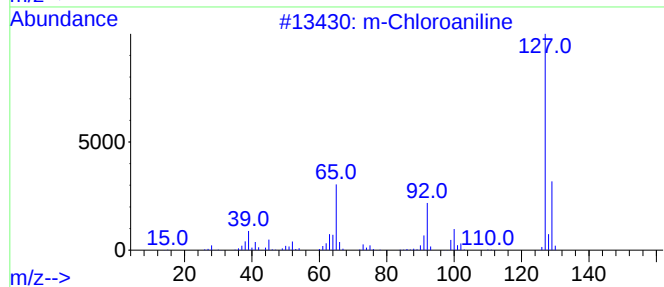
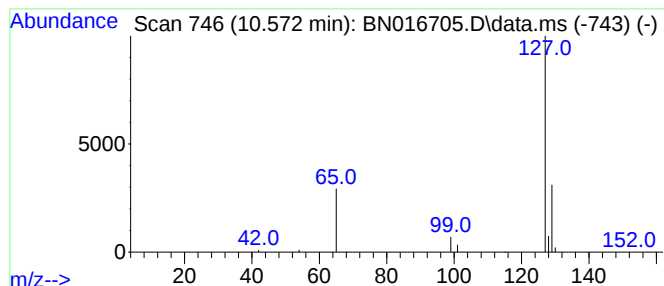
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 m-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.16 ng	71137	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
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Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

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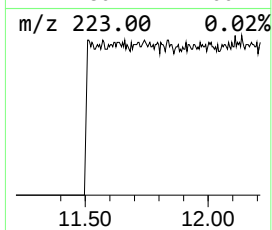
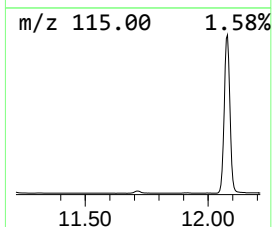
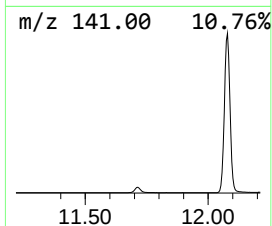
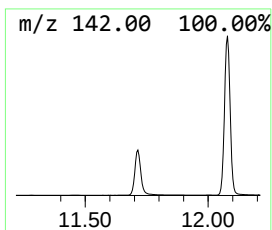
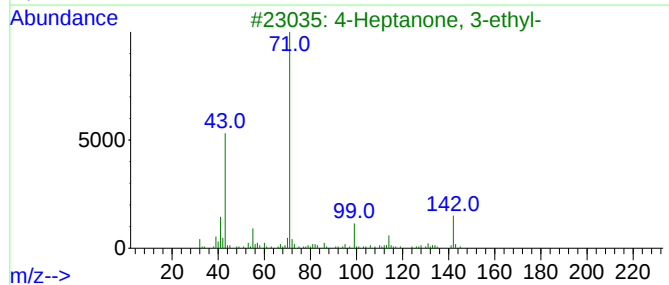
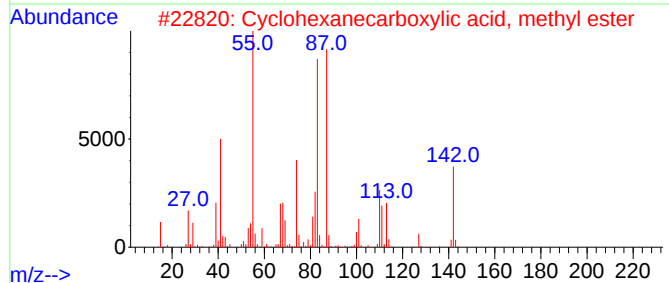
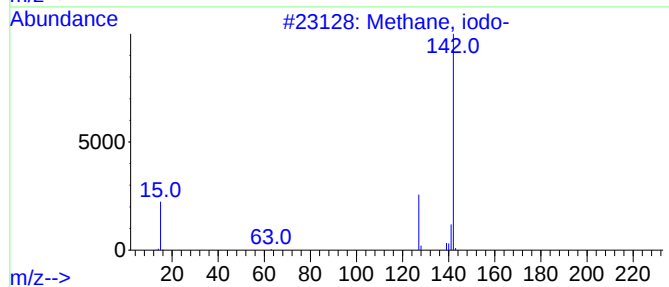
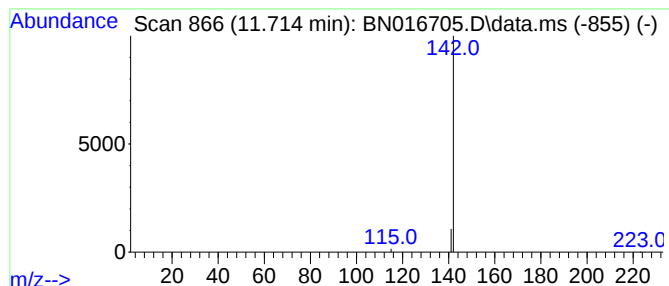
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methane, iodo- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.714	0.07 ng	30988	Naphthalene-d8	10.407

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



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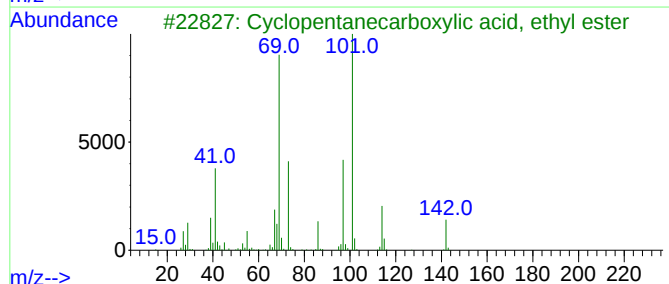
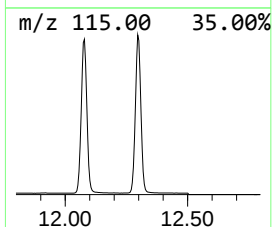
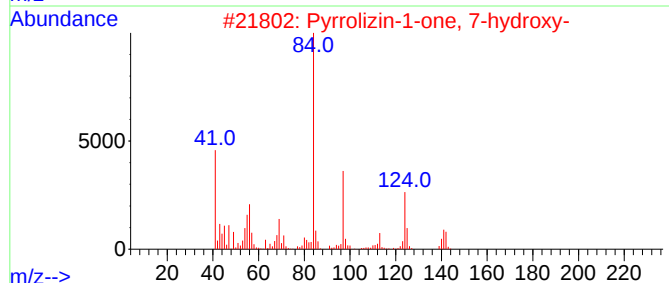
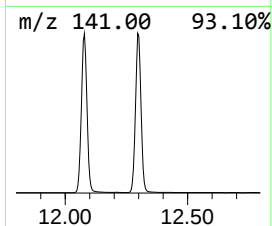
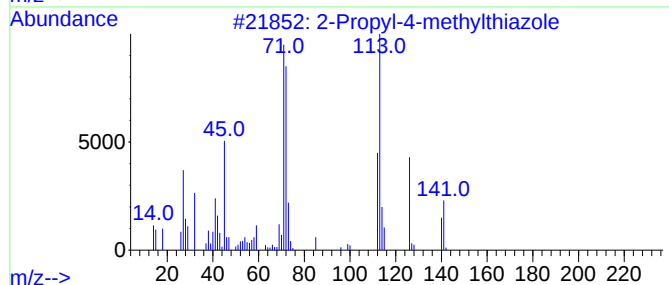
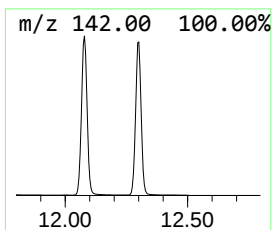
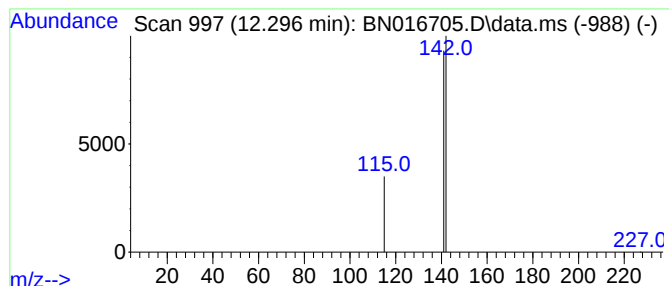
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.42 ng	192678	Naphthalene-d8	10.407

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 03 Oct 2021 13:00
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Misc :
ALS Vial : 73 Sample Multiplier: 1

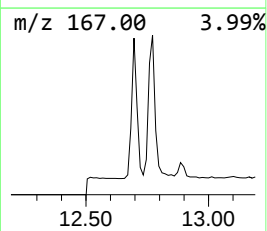
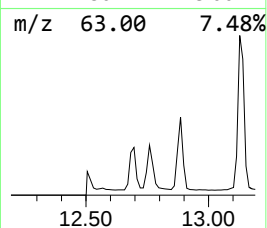
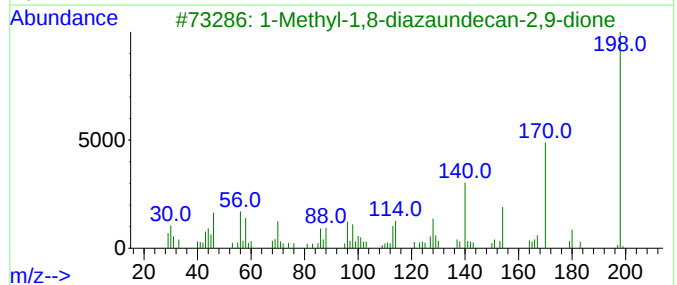
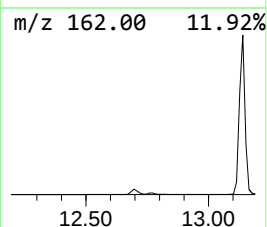
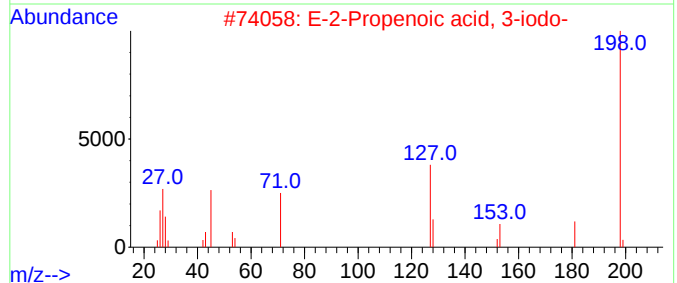
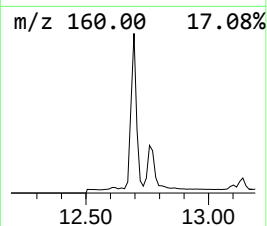
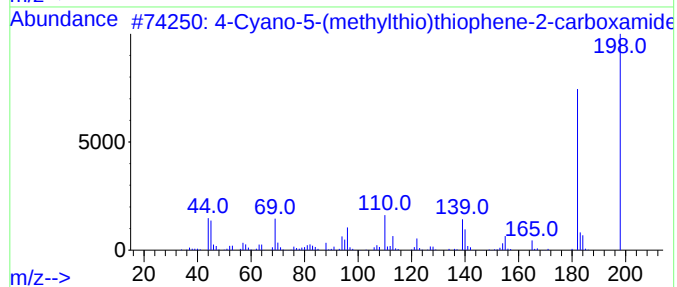
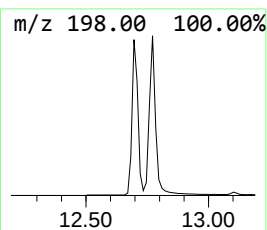
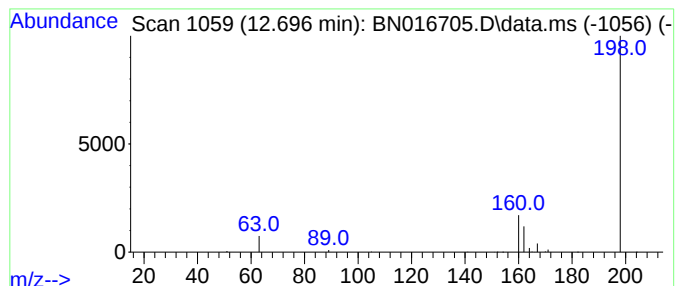
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BNA_N
LabSampleId :
SSTDCCC0.4

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.696	0.07 ng	36432	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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

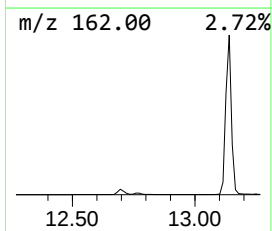
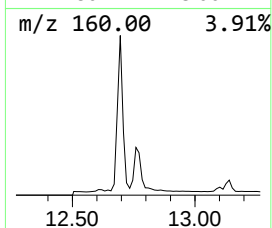
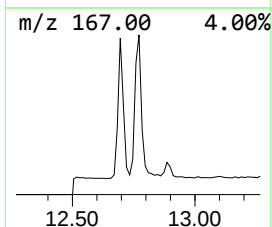
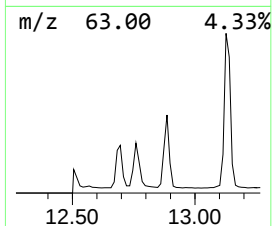
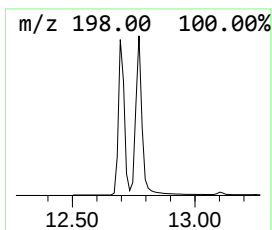
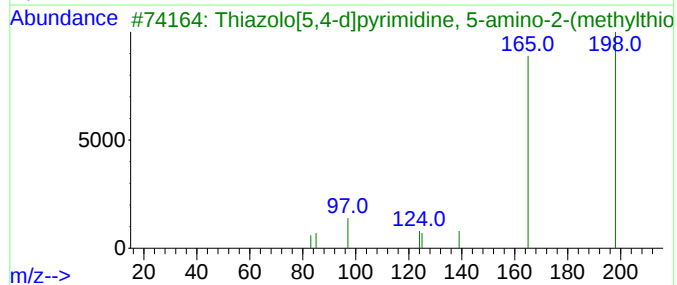
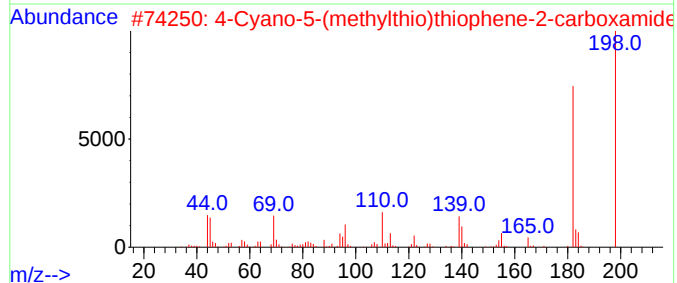
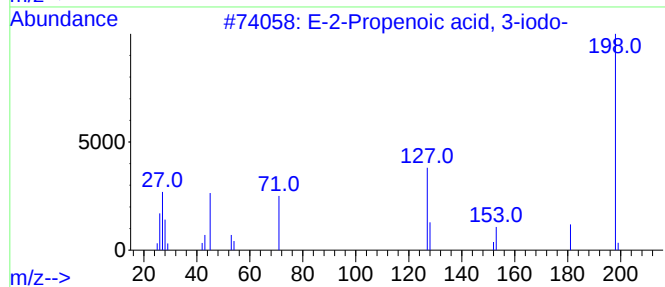
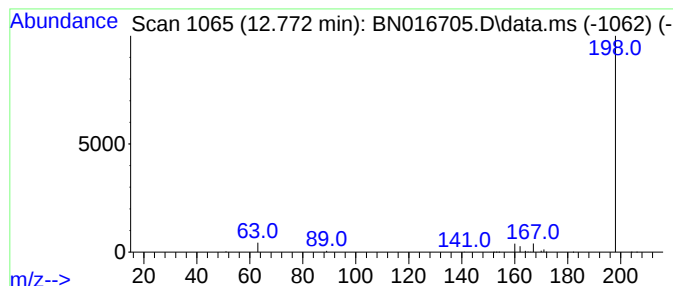
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.06 ng	32291	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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

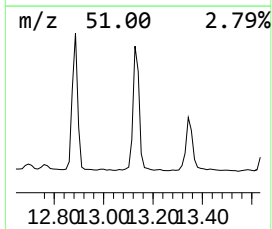
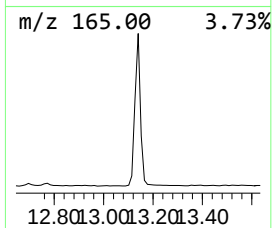
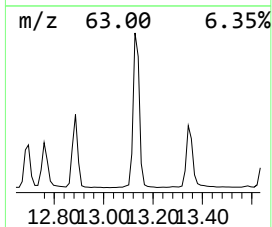
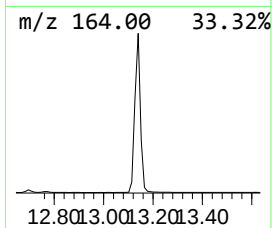
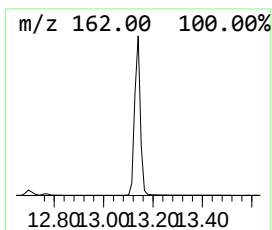
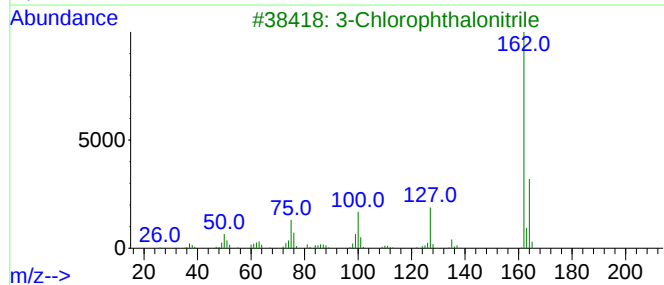
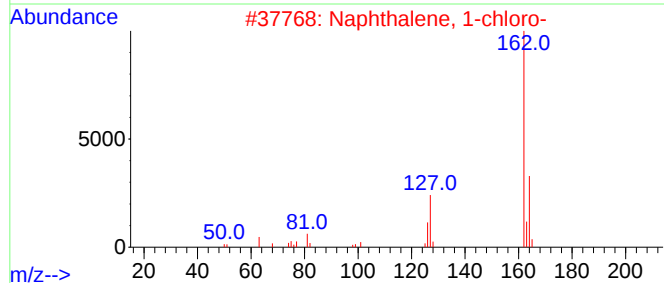
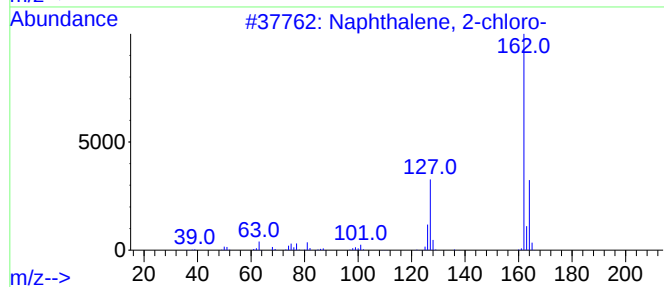
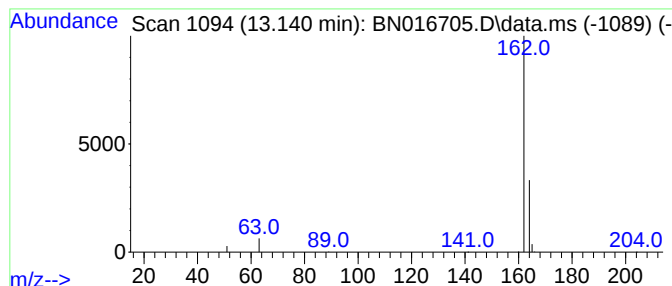
Instrument :
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LabSampleId :
SSTDCCC0.4

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.	
13.140	0.26 ng	129433	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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

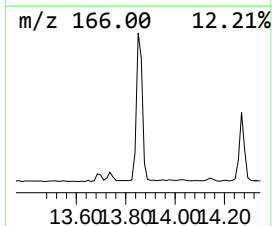
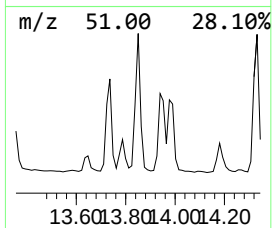
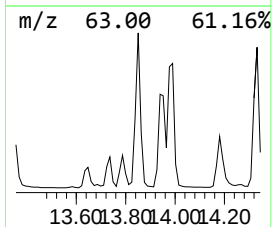
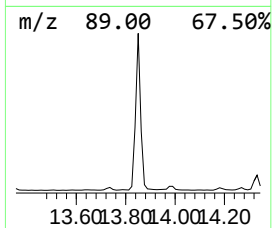
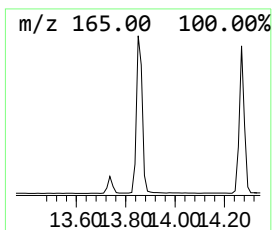
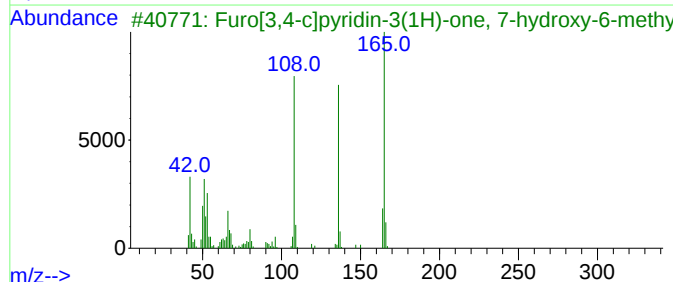
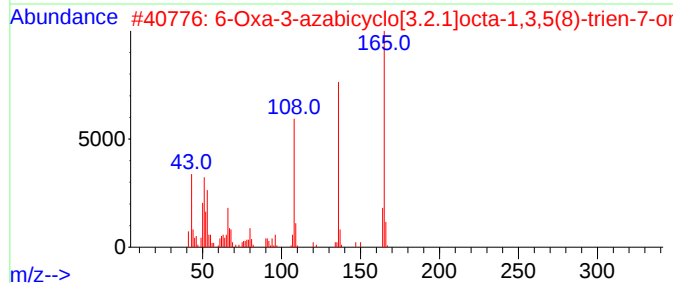
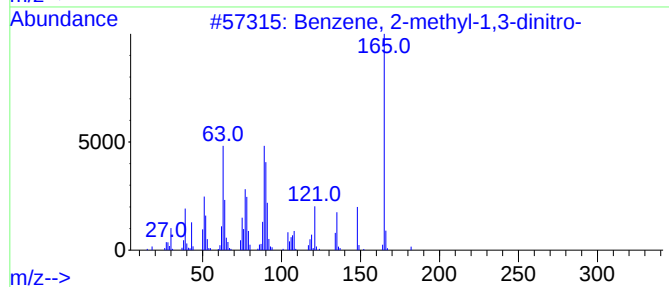
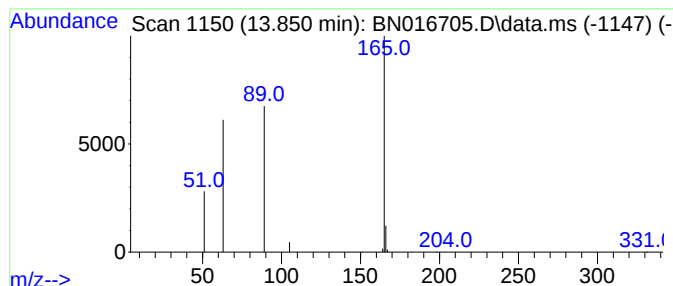
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LabSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.850	0.06 ng	30523	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	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
4	7-Hydroxy-2,4-dihydro-1,4-benzox...		165	C8H7NO3	067193-97-9	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

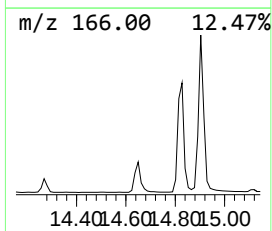
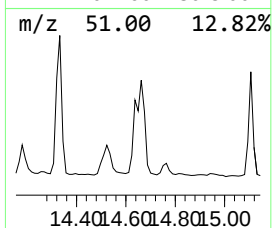
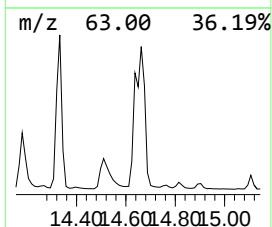
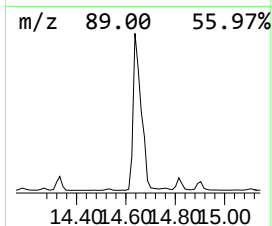
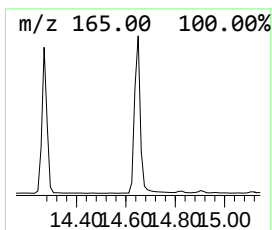
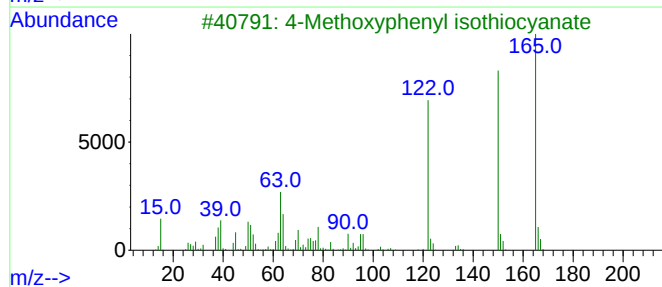
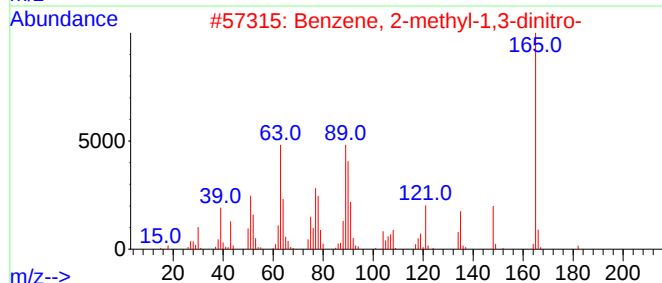
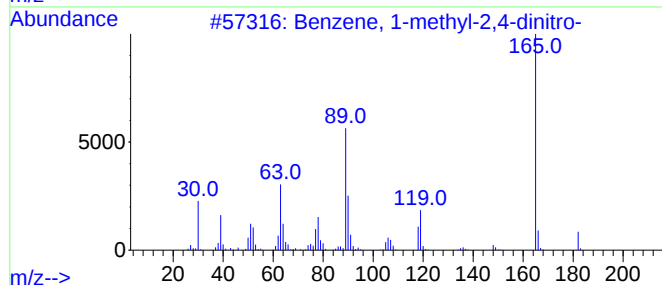
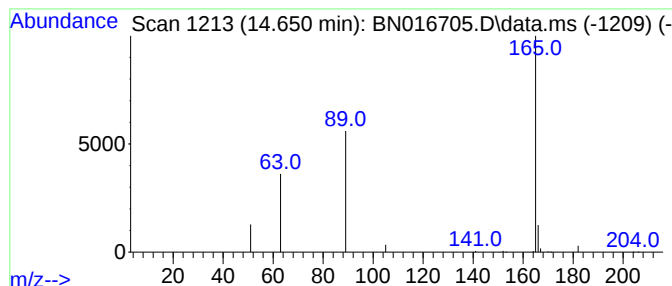
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.650	0.09 ng	43689	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	43
2			Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3			4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	9
4			2(3H)-Benzoxazothione, 5-methyl-	165	C8H7NOS	022876-22-8	9
5			Benzamide, 3,4-dimethoxy-N-(2-ph...	439	C28H41NO3	1000491-47-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

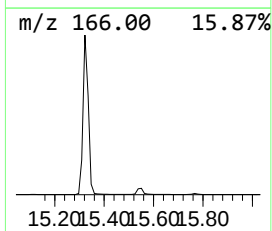
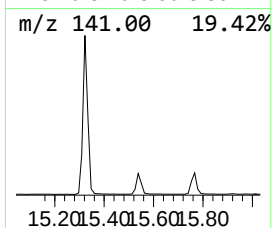
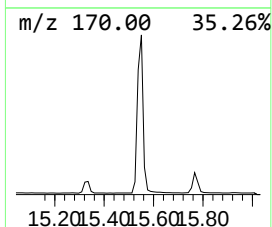
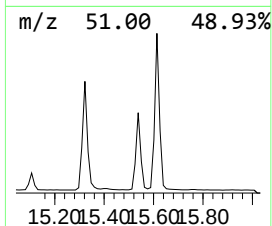
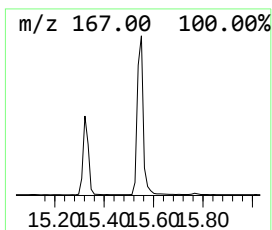
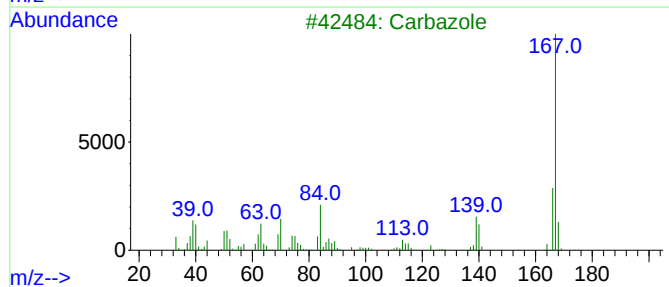
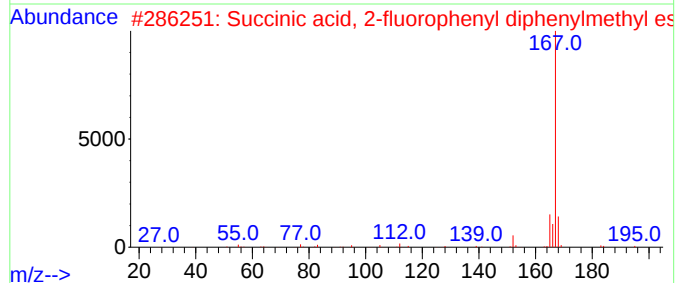
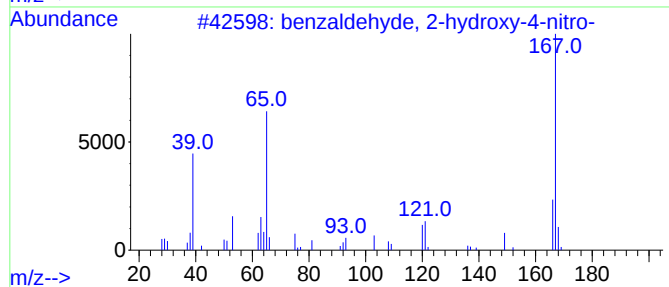
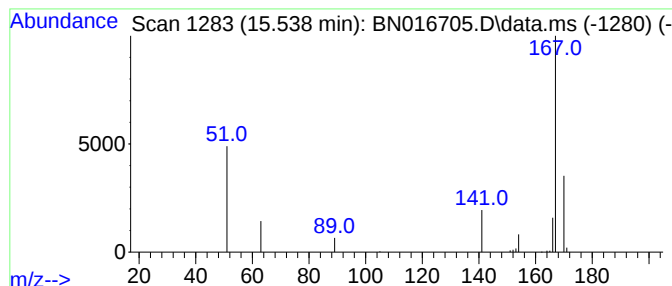
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 benzaldehyde, 2-hydroxy-4-n... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.538	0.14 ng	68249	Acenaphthene-d10	14.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5NO4	1000404-52-2	9
2	Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
3	Carbazole	167	C12H9N	000086-74-8	7
4	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	5
5	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

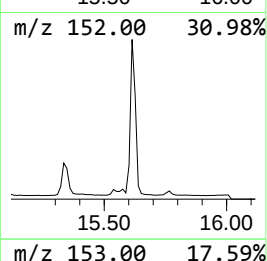
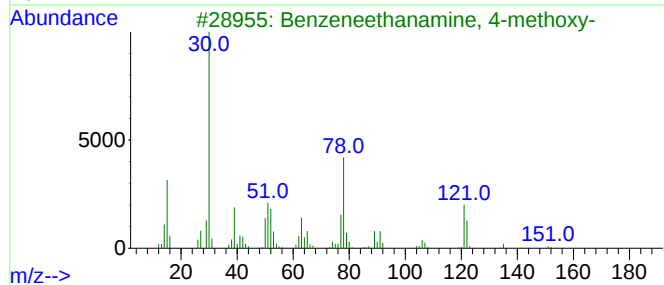
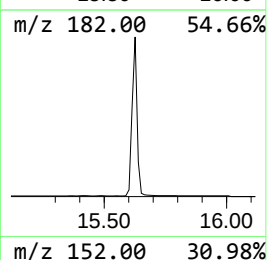
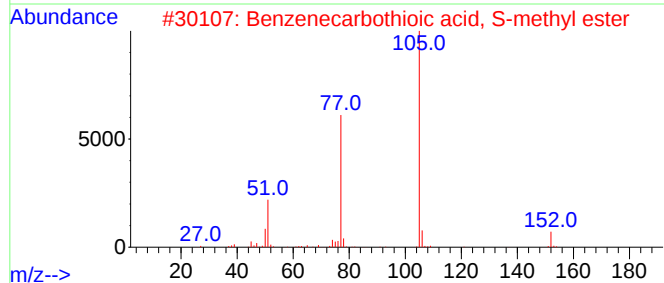
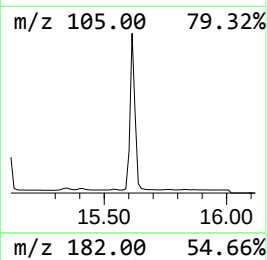
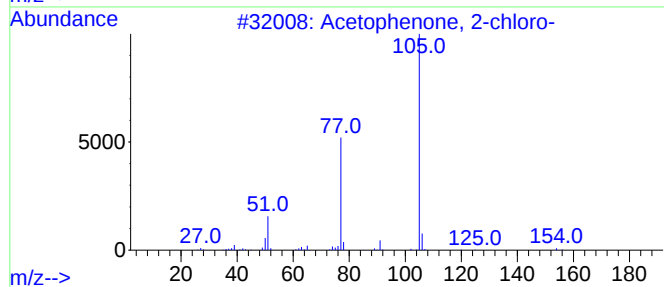
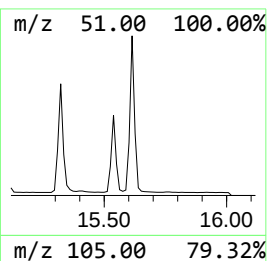
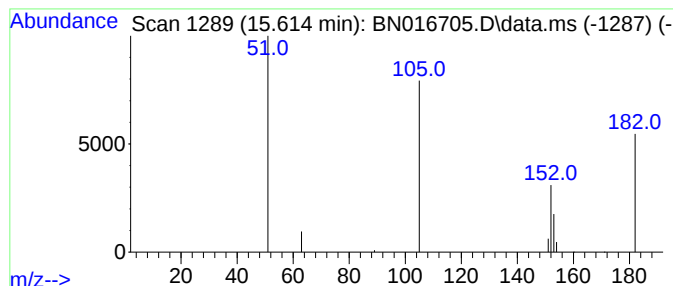
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LabSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Acetophenone, 2-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.614	0.14 ng	70669	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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

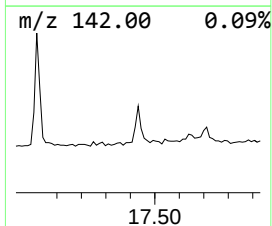
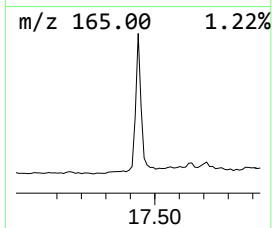
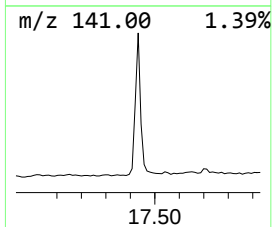
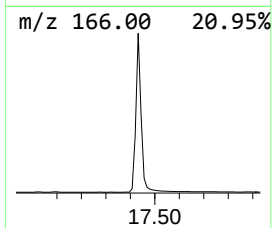
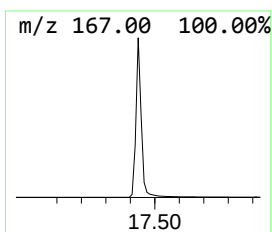
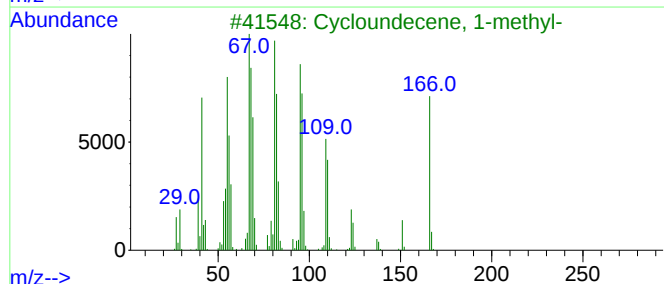
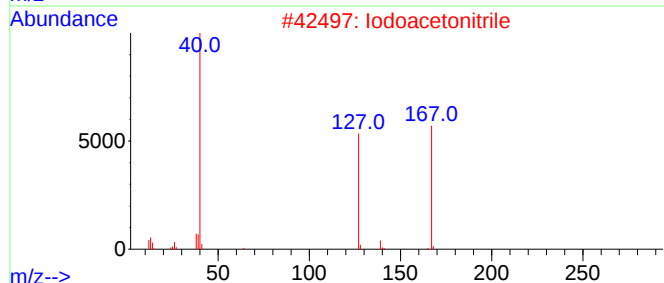
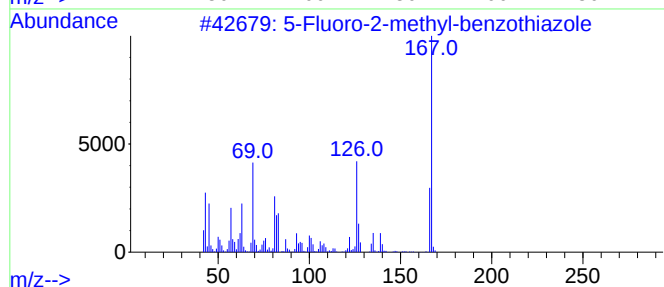
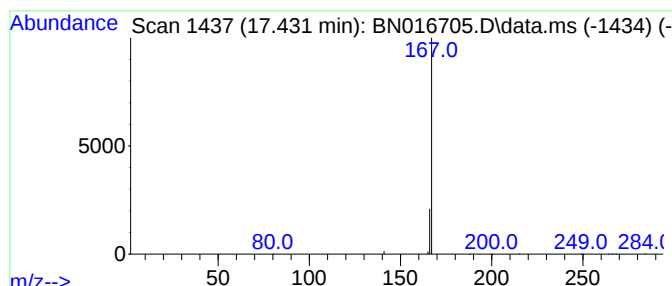
Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.432	0.41 ng	169550	Phenanthrene-d10		17.030	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole		167	C8H6FN5	000399-75-7	5
2	Iodoacetoneitrile		167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-		166	C12H22	088828-82-4	4
4	1,3,5-Triazine-2,4-diamine, N,N'...		167	C7H13N5	004150-59-8	4
5	1-Cyclopropanecarbonylpiperidin-...		167	C9H13NO2	063463-43-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

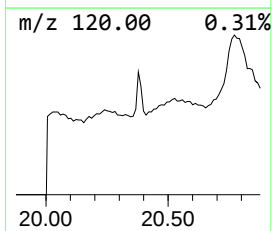
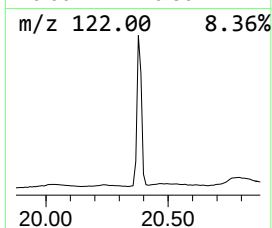
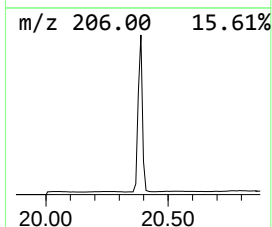
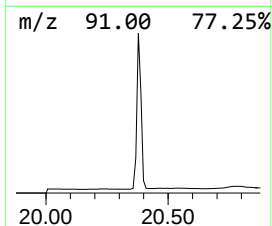
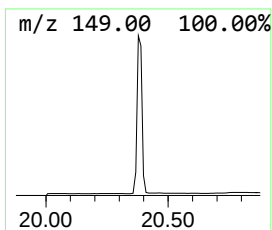
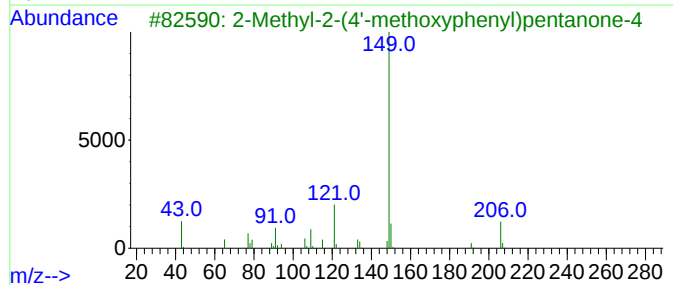
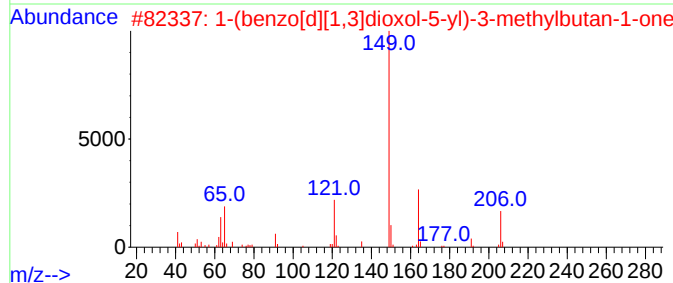
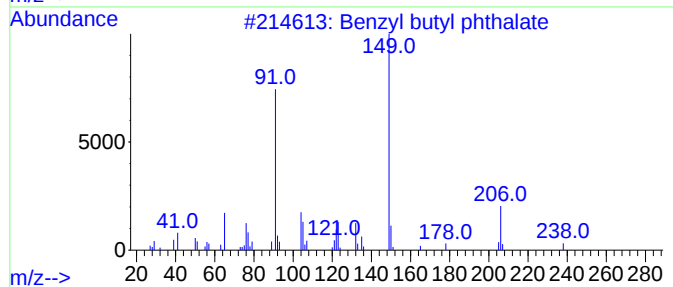
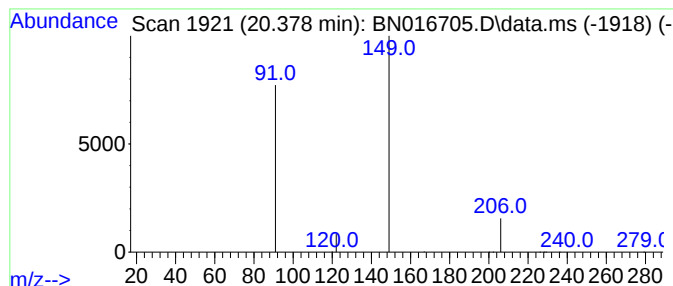
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzyl butyl phthalate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.13 ng	157914	Chrysene-d12	21.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl butyl phthalate	312	C19H20O4	000085-68-7	43
2			1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3			2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	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 : BN016705.D
Acq On : 03 Oct 2021 13:00
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 73 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

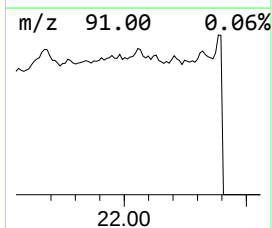
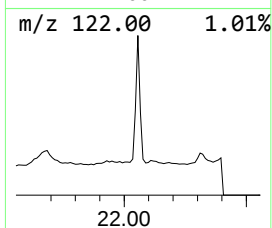
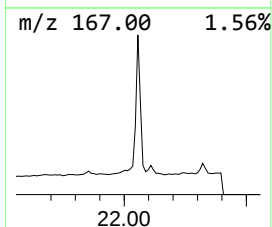
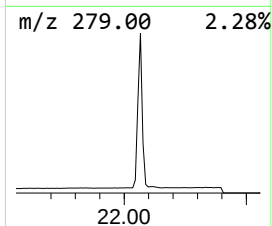
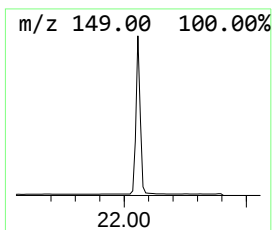
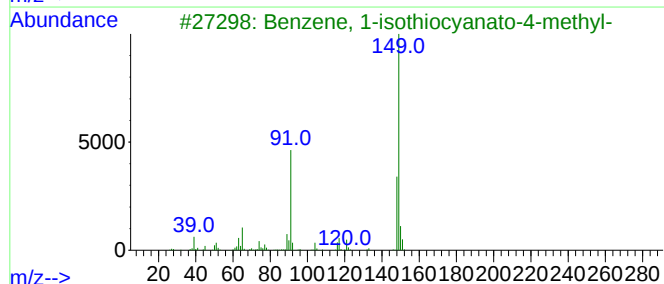
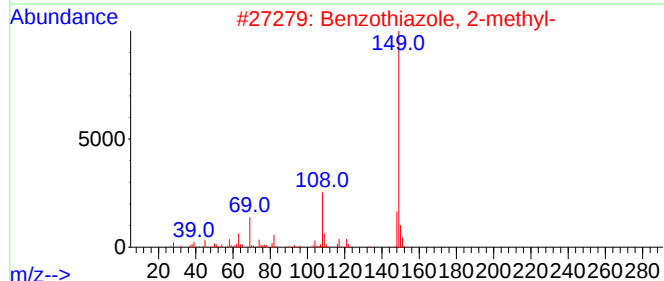
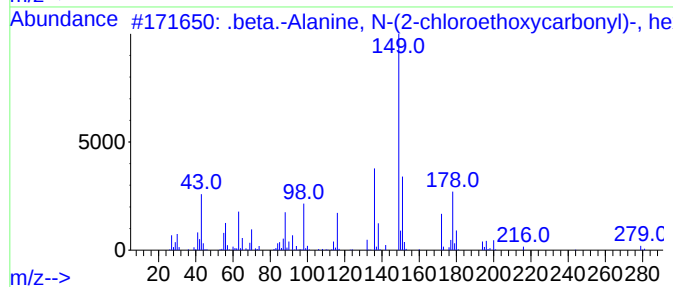
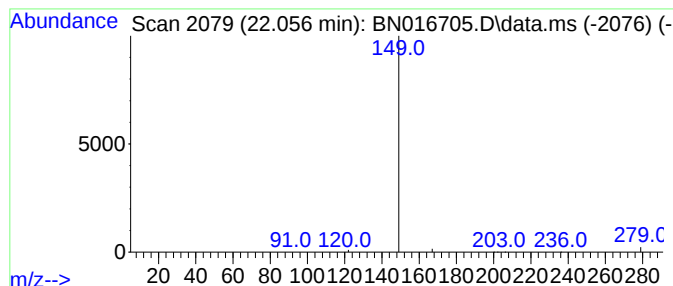
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.20 ng	234102	Chrysene-d12	21.238

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2		Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3		Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4		Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016705.D
 Acq On : 03 Oct 2021 13:00
 Operator : CG/JU
 Sample : SSTDCCC0.4
 Misc :
 ALS Vial : 73 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
2-Furancarboxit...	6.979	0.1	ng	40377	1	7.643	110017	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32930	1	7.643	110017	0.4
2-Cyclohexen-1-...	7.523	0.1	ng	14039	1	7.643	110017	0.4
6-Benzothiazola...	7.956	0.4	ng	99511	1	7.643	110017	0.4
Dimethylketene	8.430	0.2	ng	56479	1	7.643	110017	0.4
Fomepizole	9.342	0.2	ng	91707	2	10.407	182658	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	28161	2	10.407	182658	0.4
m-Chloroaniline	10.572	0.2	ng	71137	2	10.407	182658	0.4
Methane, iodo-	11.714	0.1	ng	30988	2	10.407	182658	0.4
2-Propyl-4-meth...	12.296	0.4	ng	192678	2	10.407	182658	0.4
4-Cyano-5-(meth...	12.696	0.1	ng	36432	3	14.269	200893	0.4
E-2-Propenoic a...	12.772	0.1	ng	32291	3	14.269	200893	0.4
Naphthalene, 2-...	13.140	0.3	ng	129433	3	14.269	200893	0.4
Benzene, 2-meth...	13.850	0.1	ng	30523	3	14.269	200893	0.4
Benzene, 1-meth...	14.650	0.1	ng	43689	3	14.269	200893	0.4
benzaldehyde, 2...	15.538	0.1	ng	68249	3	14.269	200893	0.4
Acetophenone, 2...	15.614	0.1	ng	70669	3	14.269	200893	0.4
5-Fluoro-2-meth...	17.432	0.4	ng	169550	4	17.030	163831	0.4
Benzyl butyl ph...	20.378	0.1	ng	157914	5	21.238	476807	0.4
.beta.-Alanine,...	22.056	0.2	ng	234102	5	21.238	476807	0.4