

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016627.D
 Acq On : 01 Oct 2021 08:58
 Operator : CG/JU
 Sample : M3833-01
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE123D1-20210918

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: BN016627.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	6	8	11	rVB	24491	29572	12.76%	0.946%
2	3.253	16	19	43	rVB	37706	156682	67.59%	5.012%
3	3.502	43	46	68	rVB	8793	37986	16.39%	1.215%
4	3.816	76	80	96	rVB	11250	47347	20.43%	1.515%
5	4.821	185	189	202	rVB	41111	92592	39.94%	2.962%
6	5.263	234	237	245	rVB	7475	19328	8.34%	0.618%
7	6.232	339	342	349	rVB	2384	5137	2.22%	0.164%
8	6.646	383	387	397	rBV	5548	13234	5.71%	0.423%
9	6.849	403	409	415	rBV2	9170	26133	11.27%	0.836%
10	7.264	449	454	460	rVB3	7806	20508	8.85%	0.656%
11	7.633	490	494	499	rBV	46341	97802	42.19%	3.129%
12	7.707	499	502	506	rVB	3947	6718	2.90%	0.215%
13	7.864	515	519	525	rBV	6758	13844	5.97%	0.443%
14	8.168	549	552	554	rBV	3417	6032	2.60%	0.193%
15	8.306	564	567	569	rVB	7977	9963	4.30%	0.319%
16	8.784	601	605	610	rBV	25660	50141	21.63%	1.604%
17	8.949	616	618	621	rVB	4551	7147	3.08%	0.229%
18	10.191	713	716	719	rBV	139362	231807	100.00%	7.416%
19	10.407	729	733	736	rBV	100550	173832	74.99%	5.561%
20	11.205	793	796	802	rBV2	3197	6531	2.82%	0.209%
21	12.003	920	931	942	rBV	45143	73488	31.70%	2.351%
22	12.886	1071	1074	1078	rBV2	92049	162984	70.31%	5.214%
23	13.114	1089	1092	1094	rBV	5097	7532	3.25%	0.241%
24	13.178	1094	1097	1104	rVB2	9167	17792	7.68%	0.569%
25	14.269	1180	1183	1187	rBV	130741	194250	83.80%	6.214%
26	14.434	1193	1196	1198	rBV	8598	12616	5.44%	0.404%
27	14.890	1229	1232	1234	rBV2	3569	7134	3.08%	0.228%
28	14.941	1234	1236	1239	rVB2	3403	6109	2.64%	0.195%
29	15.017	1239	1242	1245	rBV2	9647	18279	7.89%	0.585%
30	15.449	1272	1276	1278	rBV4	3171	6700	2.89%	0.214%
31	15.550	1281	1284	1286	rBV3	2665	6828	2.95%	0.218%
32	15.639	1286	1291	1294	rVB3	6995	19336	8.34%	0.619%
33	15.715	1294	1297	1299	rBV	12148	21749	9.38%	0.696%
34	15.766	1299	1301	1305	rVB	17218	31372	13.53%	1.004%
35	15.842	1305	1307	1311	rBV2	3356	7944	3.43%	0.254%
36	15.956	1312	1316	1318	rVV3	3804	11564	4.99%	0.370%

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Integrator: RTE

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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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.007	1318	1320	1321	rVB2	6267	7770	3.35%	0.249%
38	16.324	1343	1346	1348	rBV	6059	13670	5.90%	0.437%
39	16.385	1348	1351	1353	rVV	13672	26264	11.33%	0.840%
40	16.470	1356	1358	1361	rVB3	2830	6883	2.97%	0.220%
41	16.592	1365	1368	1373	rVB2	5497	15205	6.56%	0.486%
42	16.835	1386	1388	1397	rVB2	8778	24198	10.44%	0.774%
43	17.017	1400	1403	1405	rBV	104273	160727	69.34%	5.142%
44	17.066	1405	1407	1409	rVV	30966	43525	18.78%	1.392%
45	17.127	1409	1412	1415	rVB3	5688	12987	5.60%	0.415%
46	17.224	1416	1420	1422	rBV	14336	29416	12.69%	0.941%
47	17.273	1422	1424	1425	rBV	4046	6761	2.92%	0.216%
48	17.431	1435	1437	1446	rVB3	6665	25480	10.99%	0.815%
49	17.577	1446	1449	1453	rBV2	5462	16337	7.05%	0.523%
50	17.760	1459	1464	1468	rBV4	1871	8111	3.50%	0.259%
51	17.906	1473	1476	1477	rVV	10418	22639	9.77%	0.724%
52	17.942	1477	1479	1497	rVB	20418	45521	19.64%	1.456%
53	18.135	1504	1509	1517	rVB3	1602	2926	1.26%	0.094%
54	18.249	1525	1532	1537	rBV3	2287	4586	1.98%	0.147%
55	18.308	1538	1544	1550	rVB	6784	9869	4.26%	0.316%
56	18.408	1559	1564	1568	rBV2	5543	7909	3.41%	0.253%
57	18.447	1568	1572	1573	rBV	4273	4369	1.88%	0.140%
58	18.586	1594	1600	1605	rBV	3645	6357	2.74%	0.203%
59	18.631	1605	1609	1612	rBV	2755	3694	1.59%	0.118%
60	18.710	1620	1625	1629	rBV	4983	7389	3.19%	0.236%
61	18.835	1643	1650	1655	rBV3	7992	12708	5.48%	0.407%
62	18.889	1655	1661	1663	rBV3	2927	4953	2.14%	0.158%
63	18.969	1673	1677	1687	rBV3	2378	5026	2.17%	0.161%
64	19.063	1689	1696	1712	rVB	147240	203702	87.88%	6.516%
65	19.242	1728	1732	1737	rBV	6299	8416	3.63%	0.269%
66	19.386	1757	1761	1765	rBV2	1858	2500	1.08%	0.080%
67	19.430	1765	1770	1773	rVV	5634	8144	3.51%	0.261%
68	19.460	1773	1776	1779	rVV	6723	8722	3.76%	0.279%
69	19.490	1779	1782	1788	rVV	3872	5222	2.25%	0.167%
70	19.544	1788	1793	1800	rVB	4162	6036	2.60%	0.193%
71	19.678	1813	1820	1837	rVB	144956	186973	80.66%	5.981%
72	20.006	1885	1886	1888	rBV	4466	6467	2.79%	0.207%
73	20.972	1975	1977	1980	rBV	8172	12401	5.35%	0.397%
74	21.026	1980	1982	1988	rVB	3905	5945	2.56%	0.190%
75	21.164	1993	1995	1998	rBV	41772	60360	26.04%	1.931%
76	21.227	1998	2001	2011	rVB	122227	192689	83.12%	6.164%

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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	22.109	2081	2084	2089	rBV2	16157	22167	9.56%	0.709%
78	22.321	2101	2104	2108	rBV2	2873	5593	2.41%	0.179%
79	23.484	2415	2427	2469	rVB	97961	197333	85.13%	6.313%

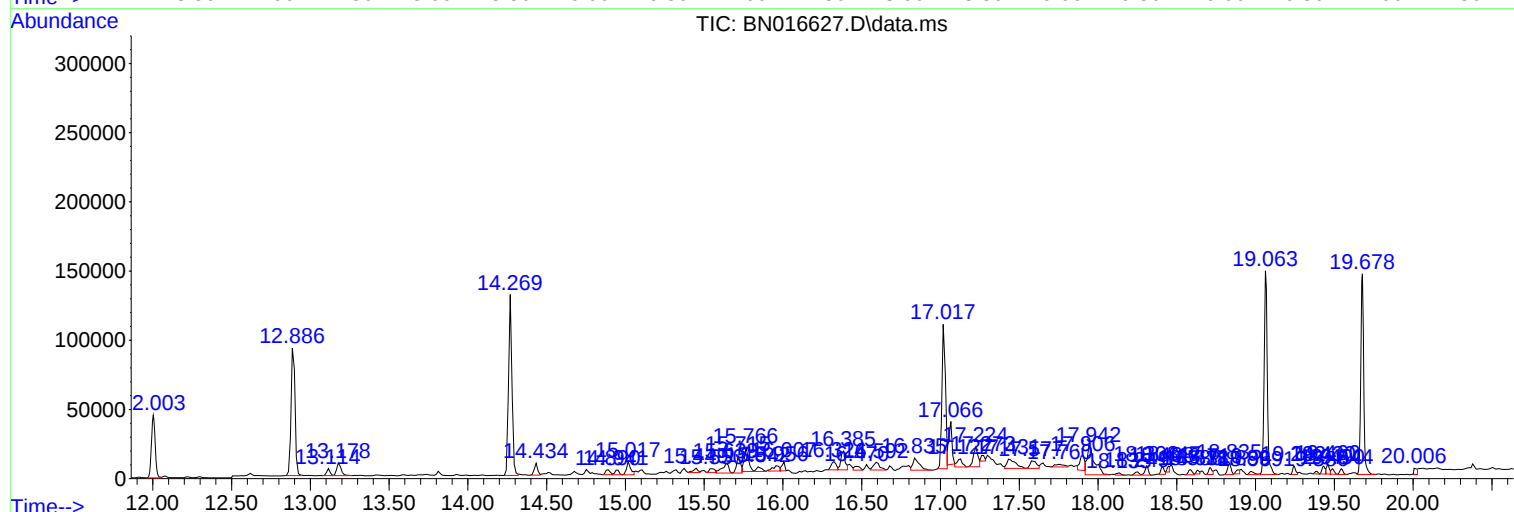
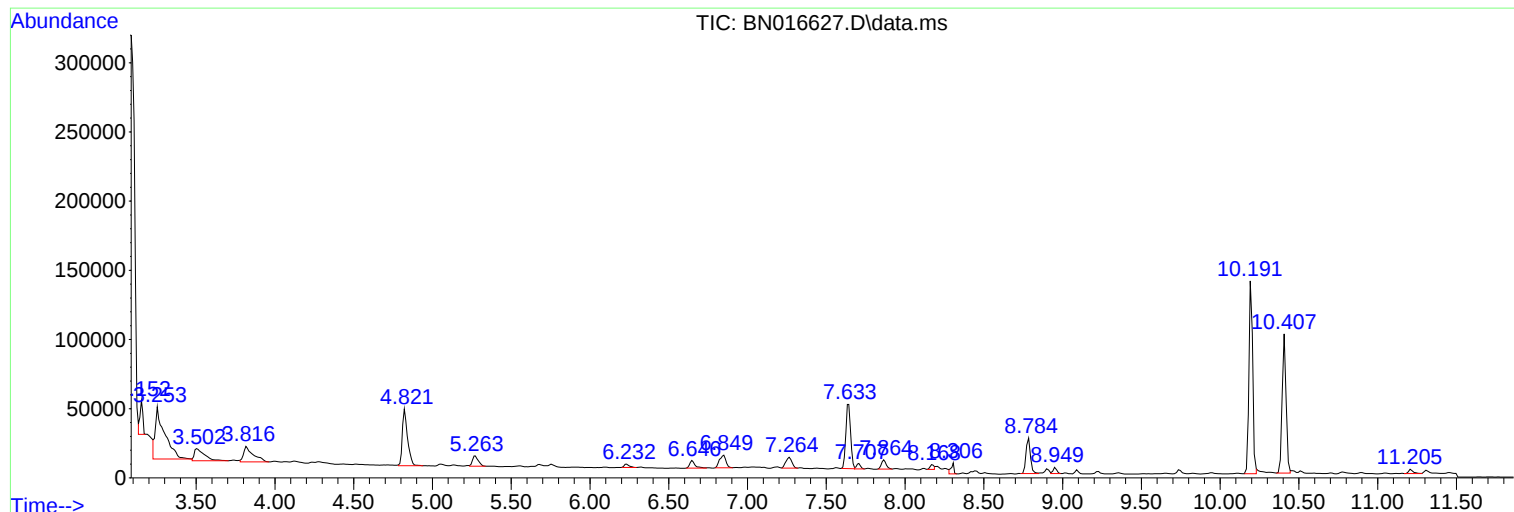
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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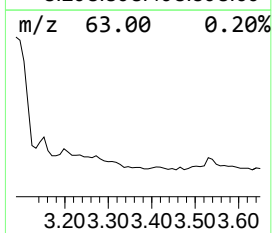
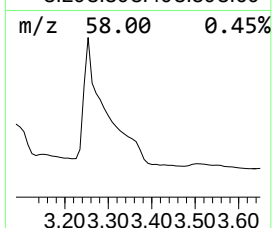
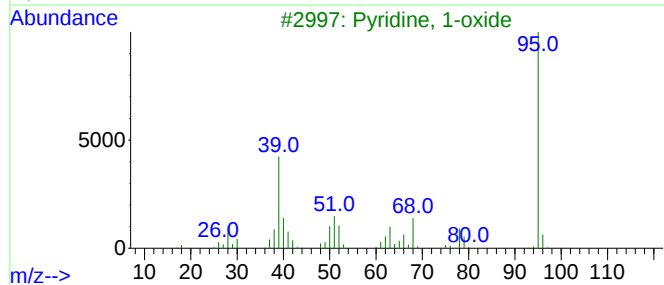
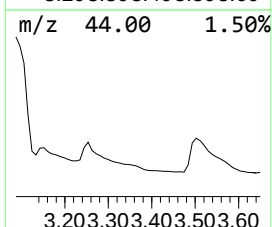
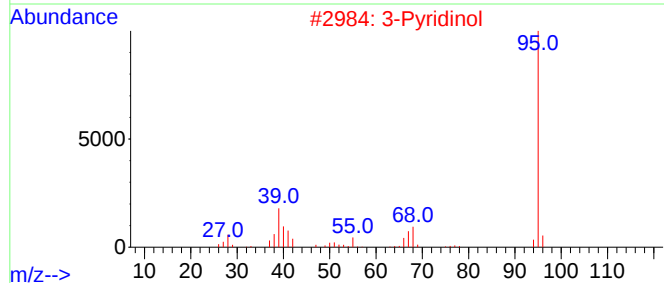
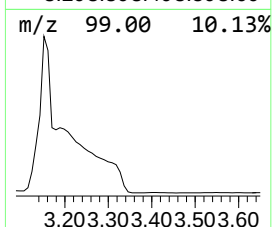
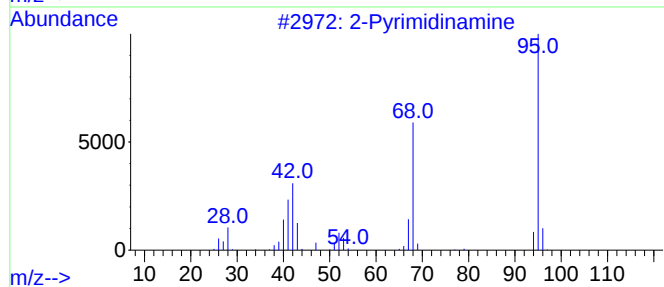
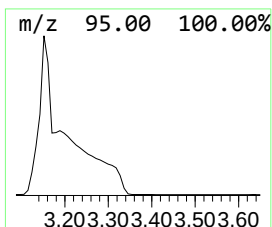
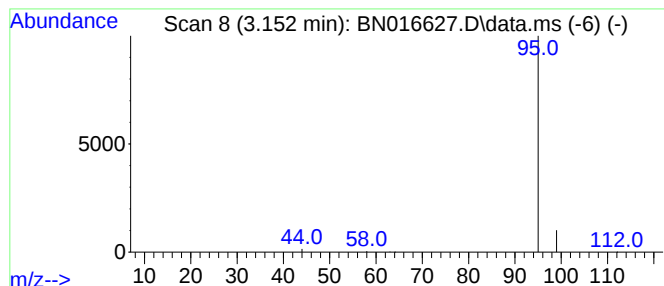
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pyrimidinamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.12 ng	29572	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
2		3-Pyridinol	95	C5H5NO	000109-00-2	2
3		Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
4		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
5		4-Pyridinone	95	C5H5NO	1000433-50-4	2



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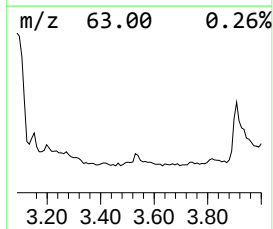
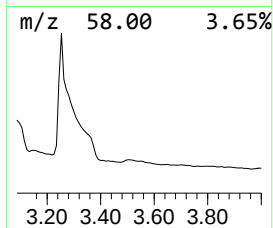
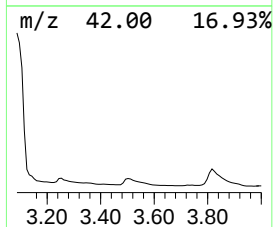
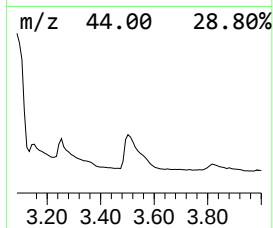
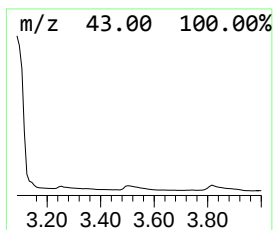
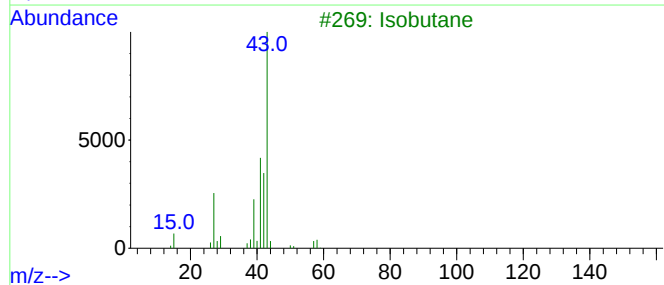
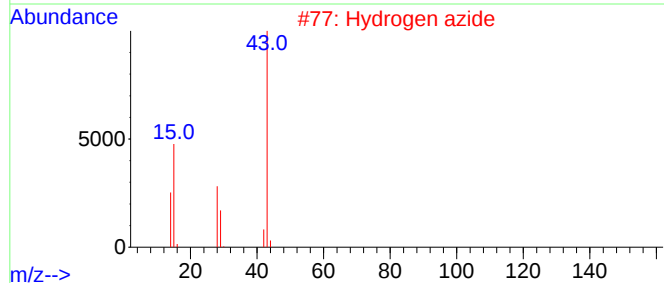
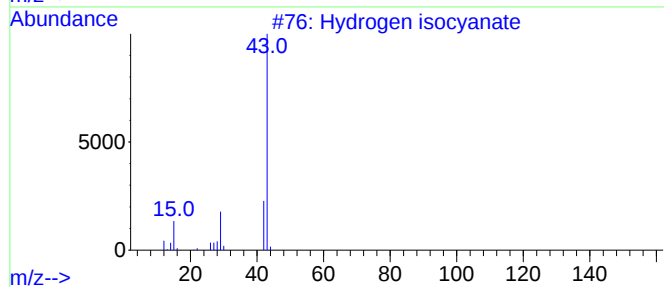
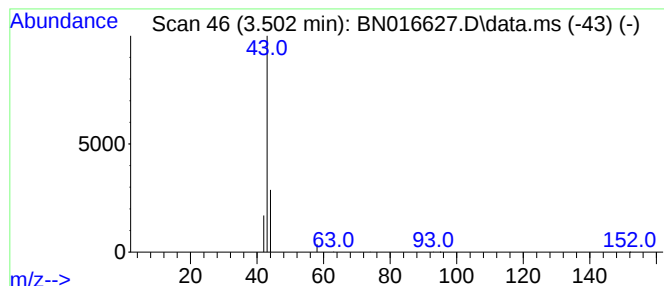
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hydrogen isocyanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.502	0.16 ng	37986	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrogen isocyanate	43	CHNO	000075-13-8	3
2			Hydrogen azide	43	HN3	007782-79-8	3
3			Isobutane	58	C4H10	000075-28-5	3
4			Ethylene oxide	44	C2H4O	000075-21-8	2
5			Acetaldehyde	44	C2H4O	000075-07-0	2



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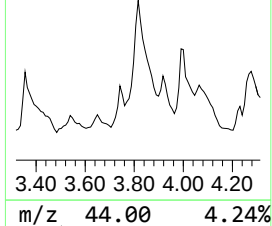
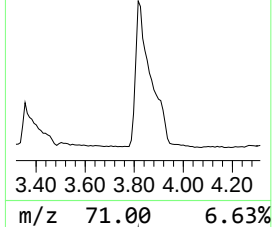
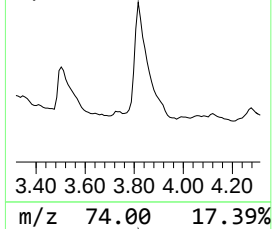
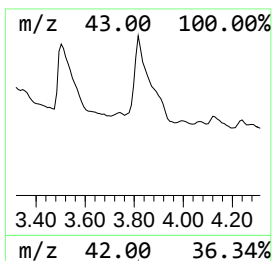
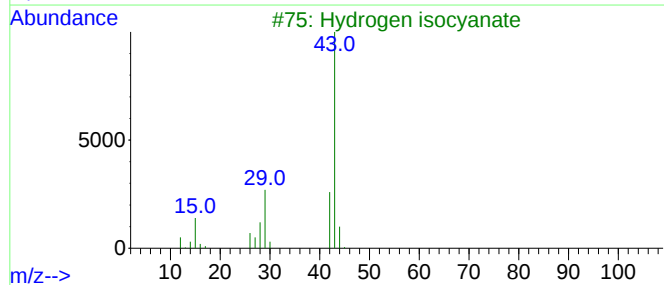
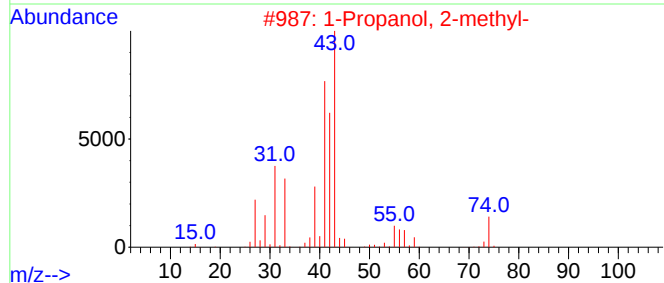
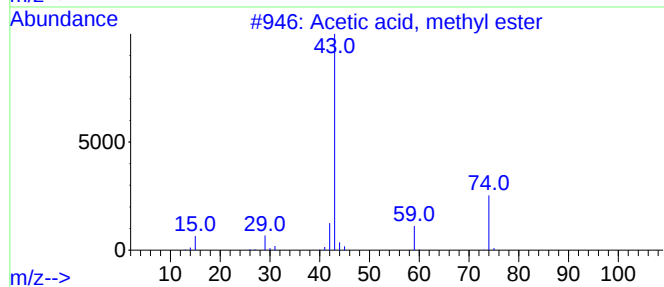
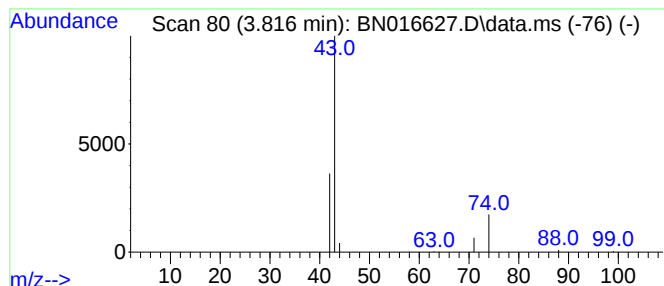
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.19 ng	47347	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	5
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
3			Hydrogen isocyanate	43	CHNO	000075-13-8	3
4			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
5			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3



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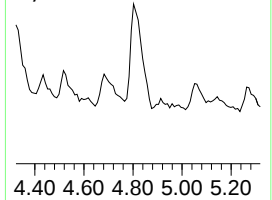
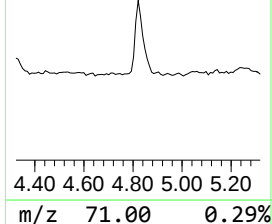
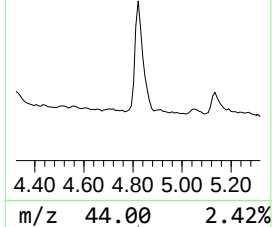
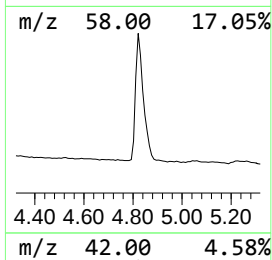
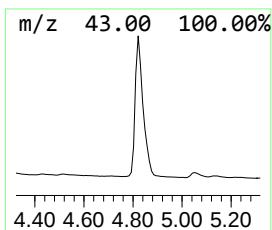
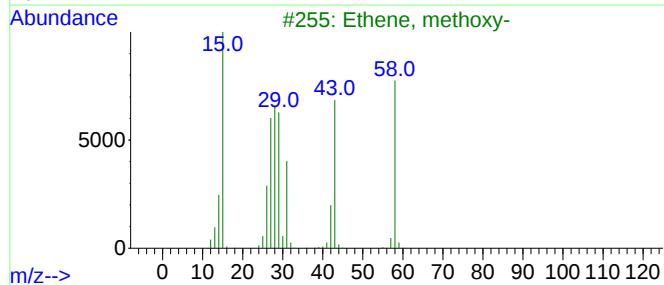
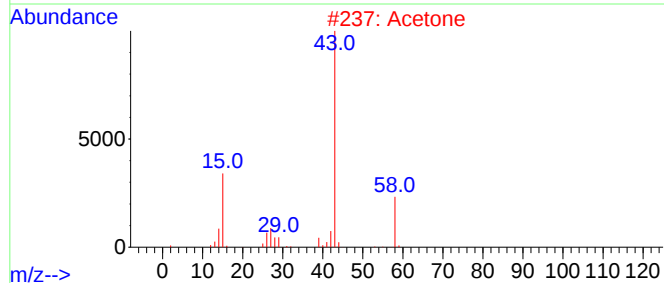
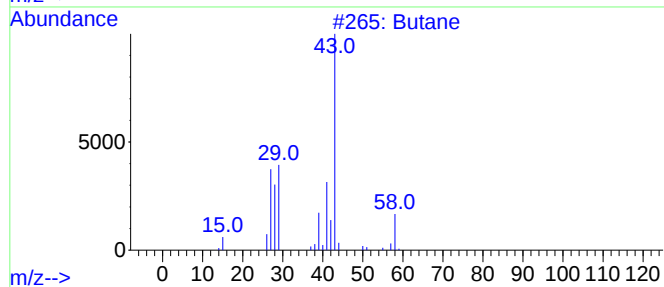
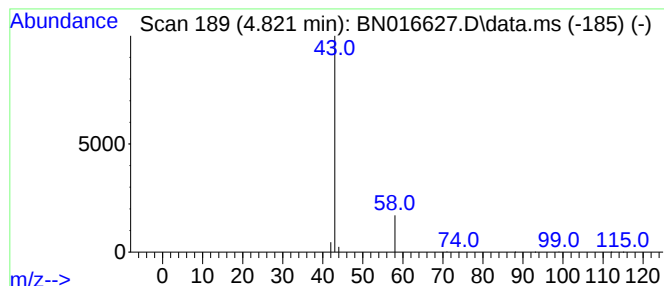
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.38 ng	92592	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE123D1-20210918

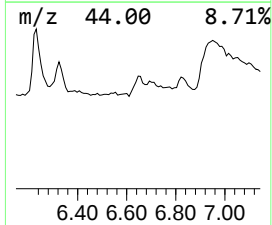
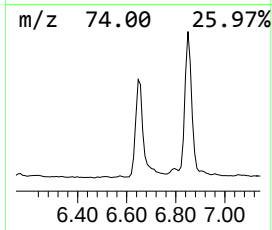
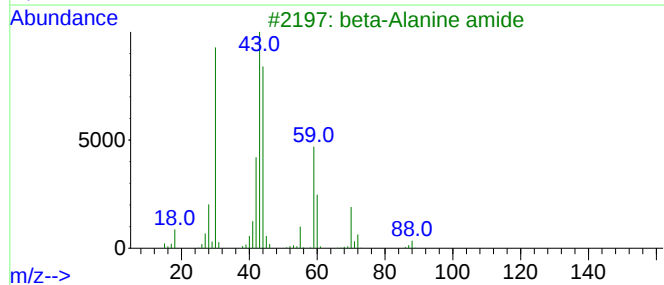
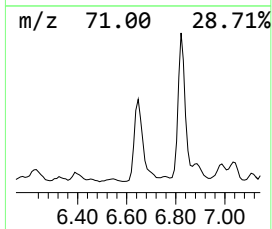
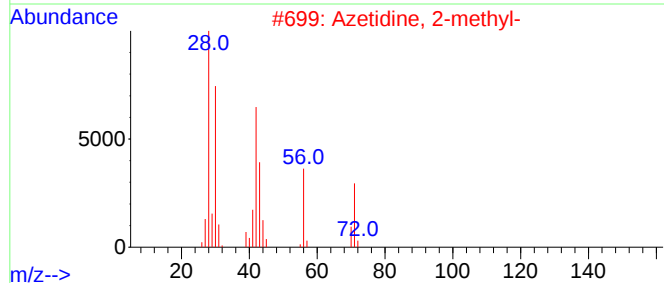
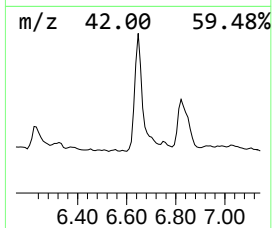
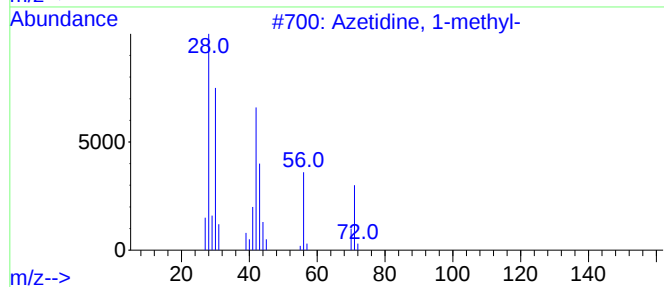
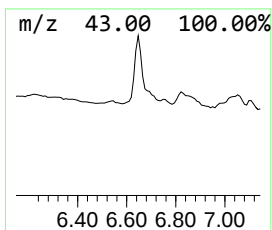
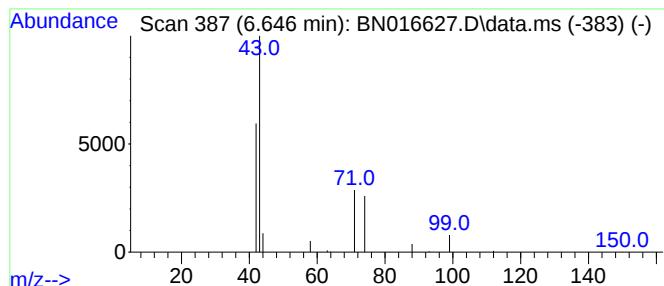
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Azetidine, 1-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.05 ng	13234	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	7
2			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	7
3			beta-Alanine amide	88	C3H8N2O	004726-85-6	5
4			Methoxyacetonitrile	71	C3H5NO	001738-36-9	5
5			Urea, methyl-	74	C2H6N2O	000598-50-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

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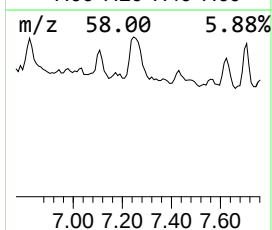
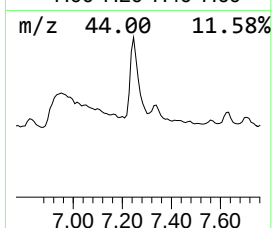
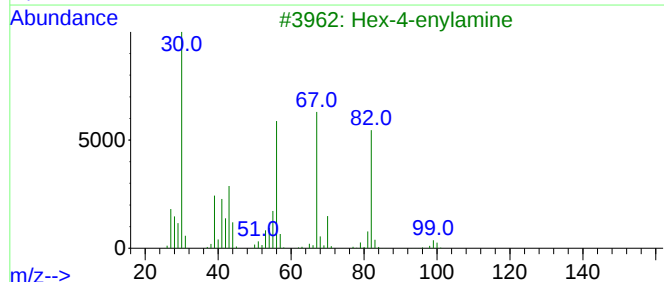
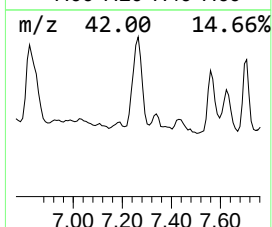
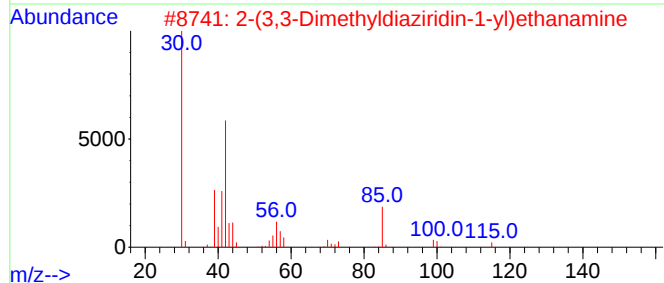
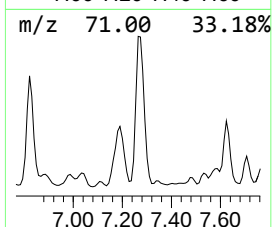
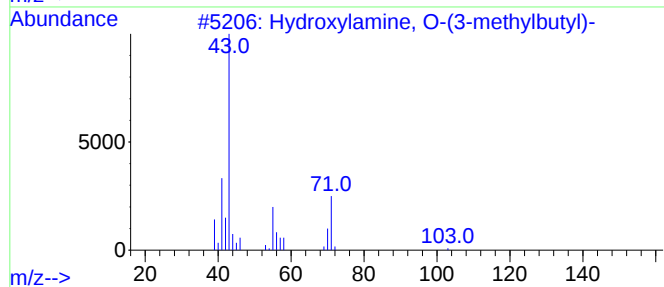
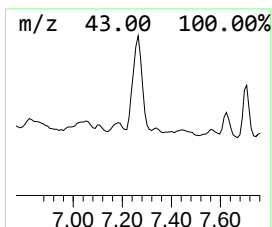
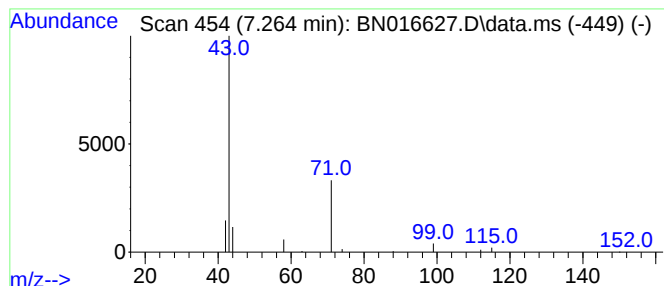
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hydroxylamine, O-(3-methylb... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.08 ng	20508	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
2		2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	5
3		Hex-4-enylamine	99	C6H13N	055108-01-5	5
4		1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5		Pentanoic acid, 3-hydroxy-4-meth...	146	C7H14O3	065596-31-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
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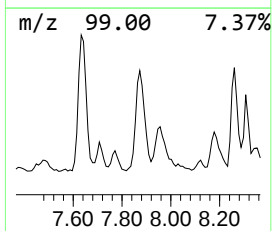
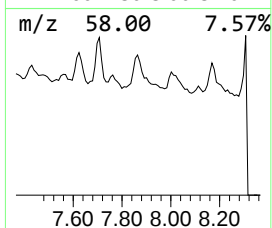
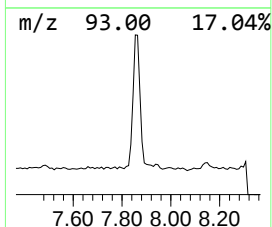
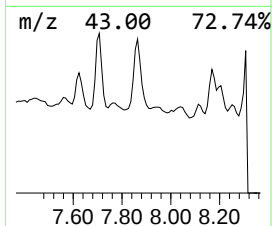
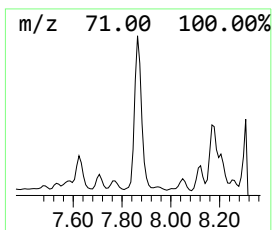
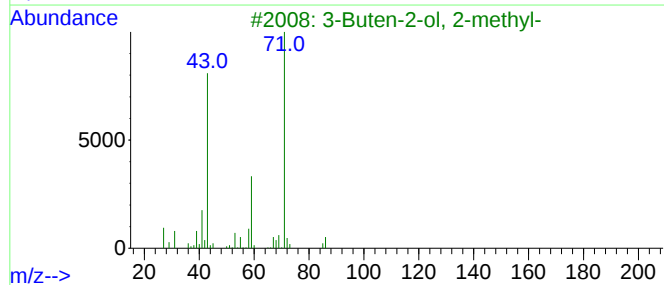
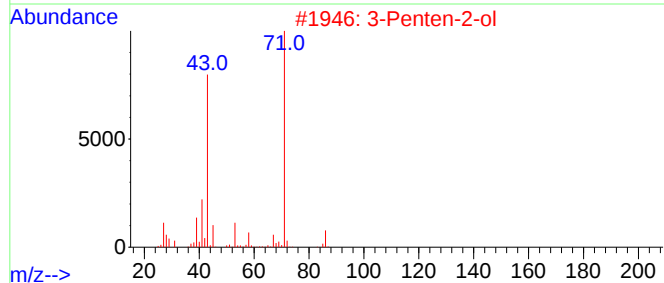
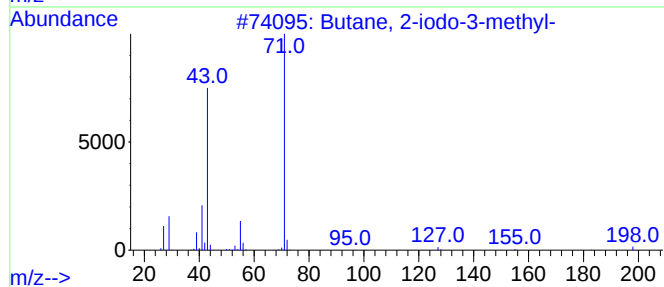
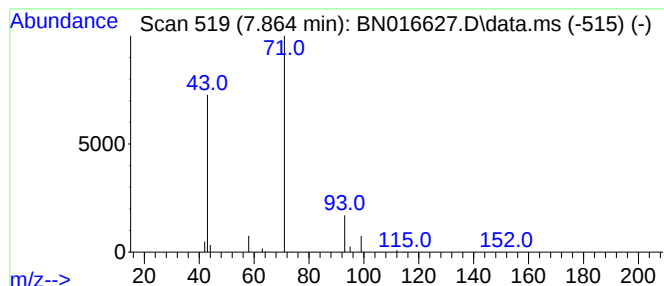
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butane, 2-iodo-3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.06 ng	13844	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
2			3-Penten-2-ol	86	C5H10O	001569-50-2	4
3			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
4			Methallyl butyrate	142	C8H14O2	1000428-83-8	4
5			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
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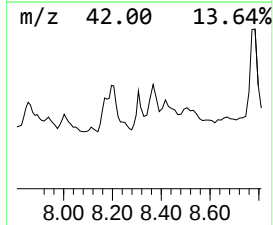
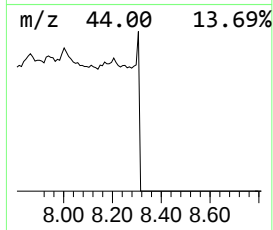
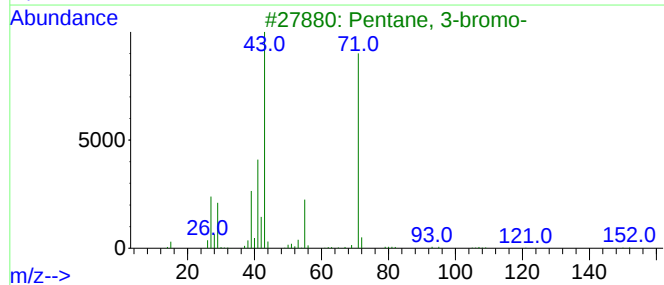
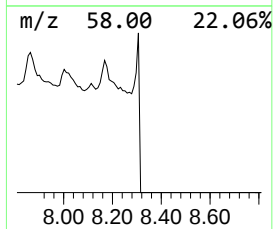
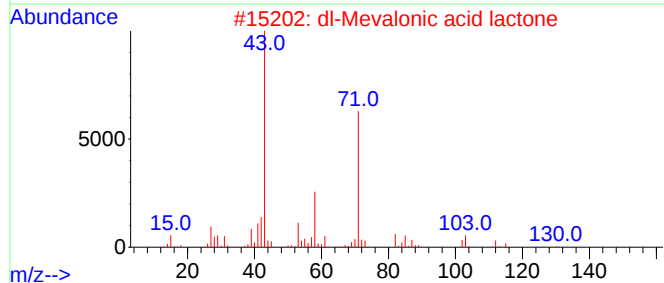
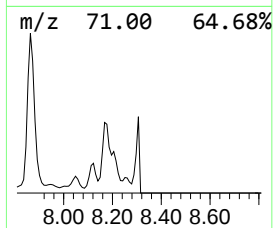
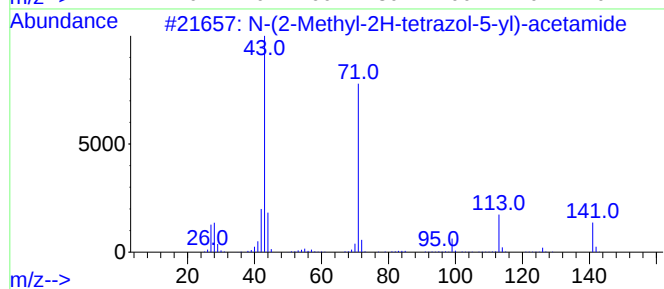
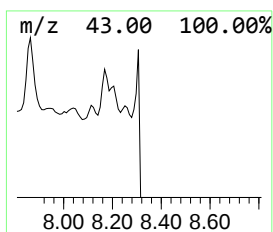
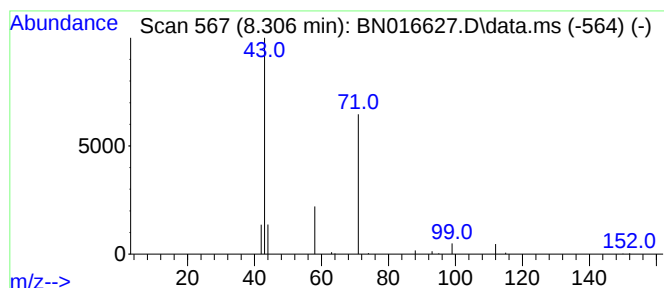
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 N-(2-Methyl-2H-tetrazol-5-yl) Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.04 ng	9963	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2-Methyl-2H-tetrazol-5-yl)-ac...	141	C4H7N5O	006154-06-9	42
2			dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	39
3			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	9
4			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	9
5			4-Nonanone	142	C9H18O	004485-09-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
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Misc :
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ClientSampleId :
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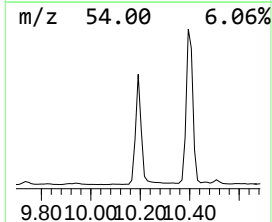
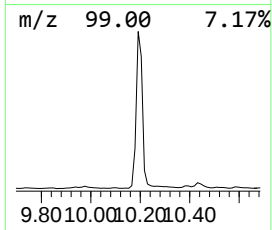
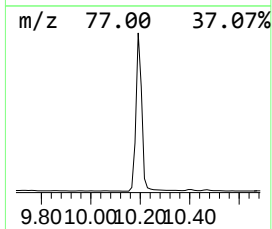
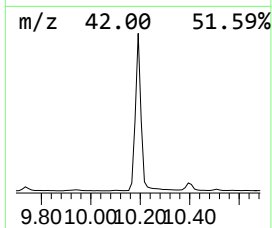
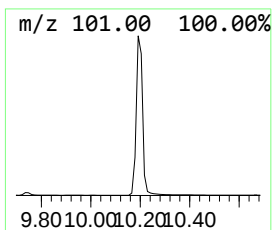
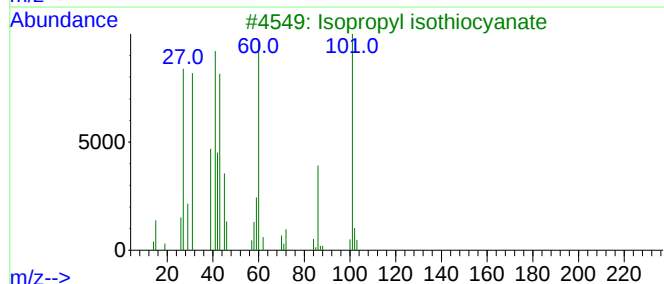
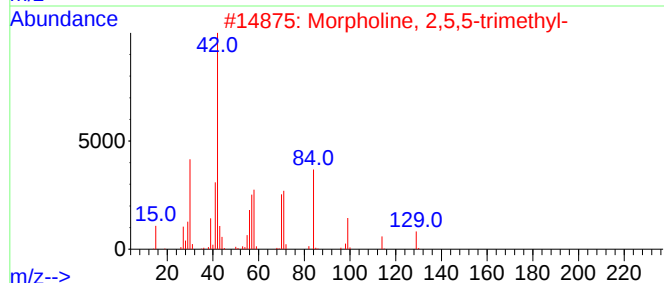
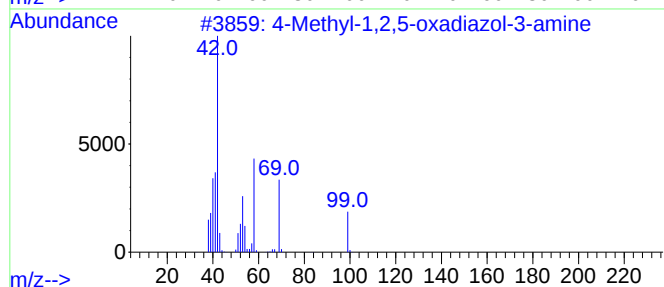
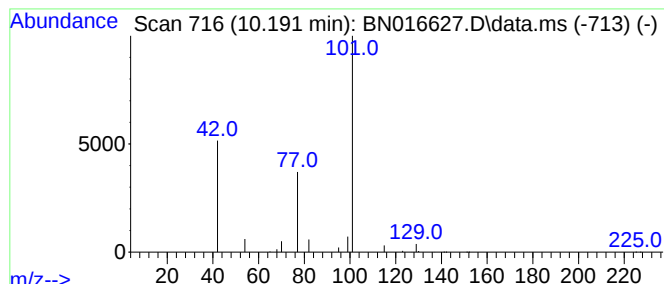
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4-Methyl-1,2,5-oxadiazol-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.53 ng	231807	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
2			Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
3			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5



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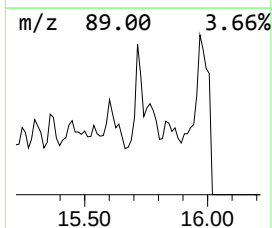
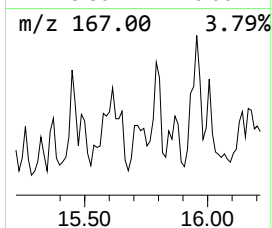
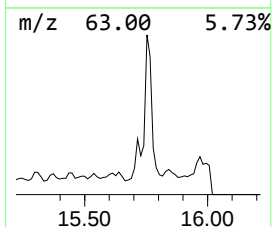
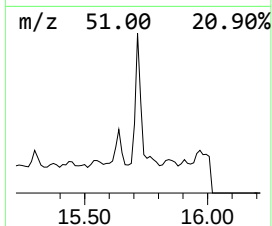
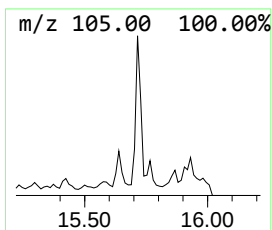
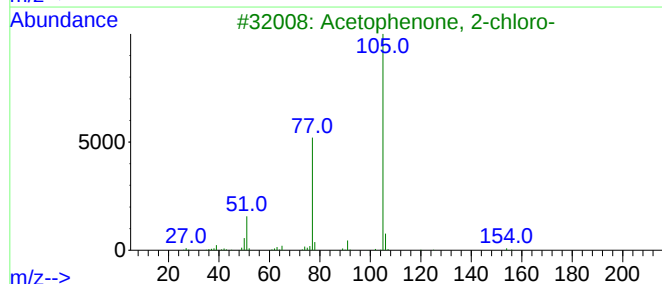
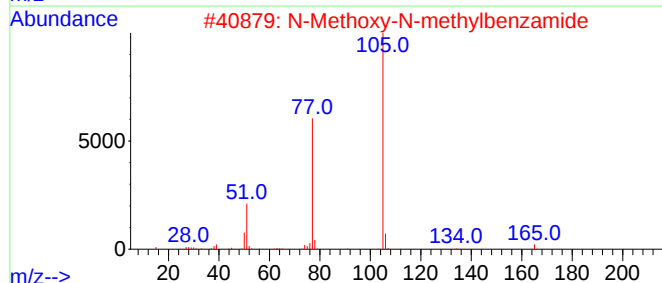
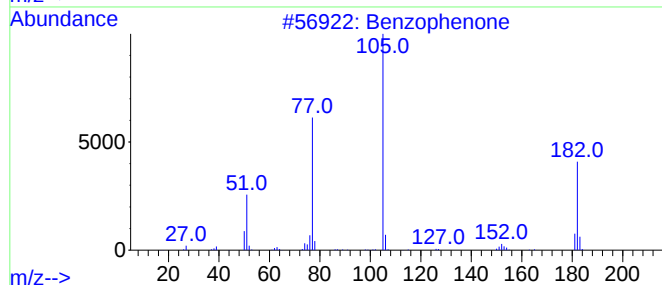
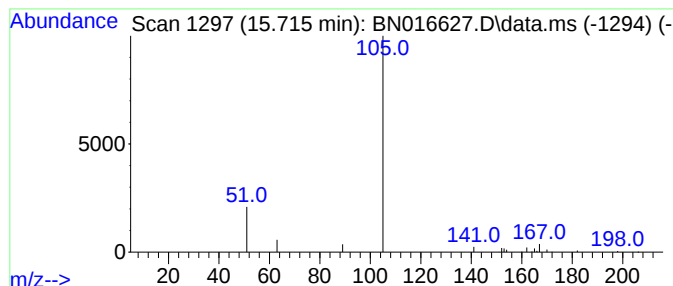
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzophenone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	0.05 ng	21749	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	9
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	5
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	4
4			2-Propenoic acid, 2-bromo-, meth...	164	C4H5BrO2	004519-46-4	4
5			1,1-Diphenyl-2-phenylthiobut-3-e...	332	C22H20OS	097370-20-2	4



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ALS Vial : 30 Sample Multiplier: 1

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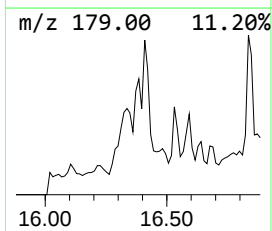
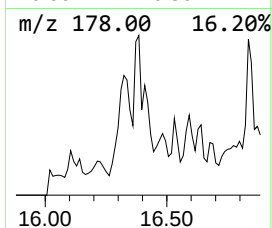
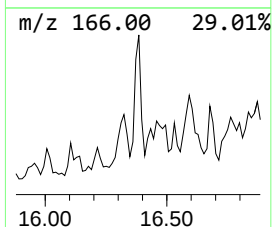
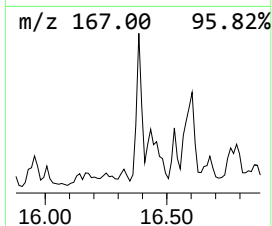
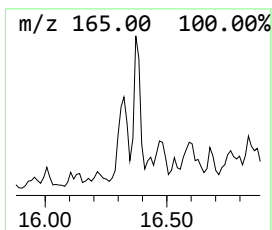
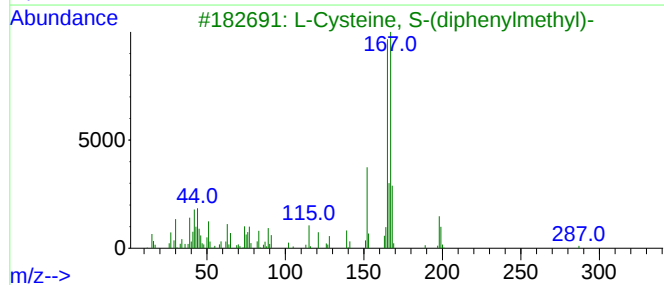
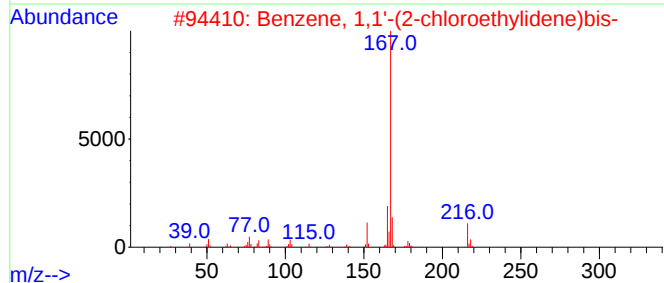
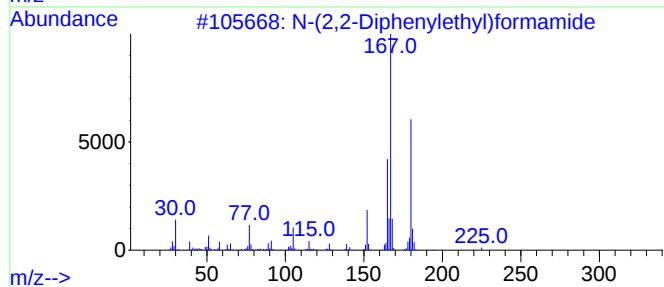
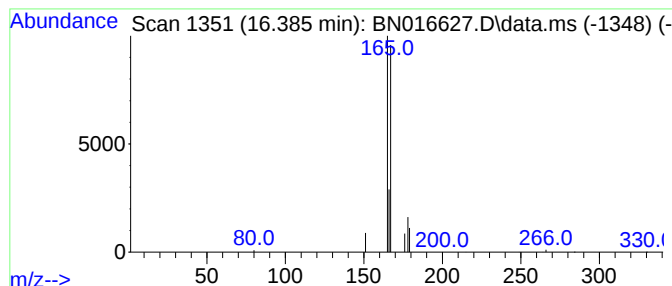
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 N-(2,2-Diphenylethyl)formamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.385	0.07 ng	26264	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2,2-Diphenylethyl)formamide	225	C15H15NO	019501-33-8	25
2			Benzene, 1,1'-(2-chloroethyliden...	216	C14H13Cl	005216-46-6	9
3			L-Cysteine, S-(diphenylmethyl)-	287	C16H17NO2S	005191-80-0	9
4			1,1'-Biphenyl, 4-pentyl-	224	C17H20	007116-96-3	9
5			6-[1-(1-Azepanyl)ethyl]-N2,N2-di...	264	C13H24N6	923208-22-4	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

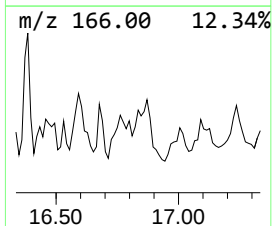
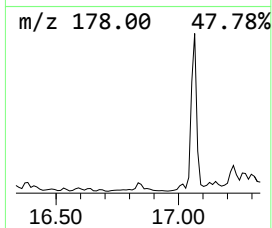
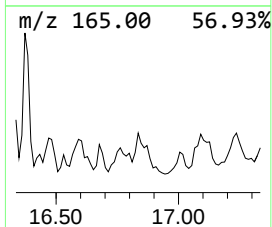
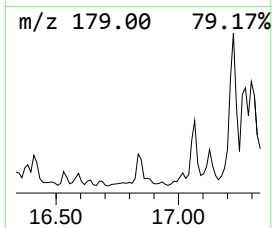
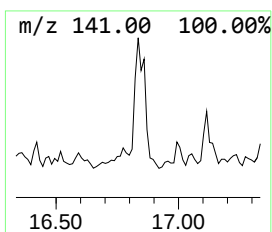
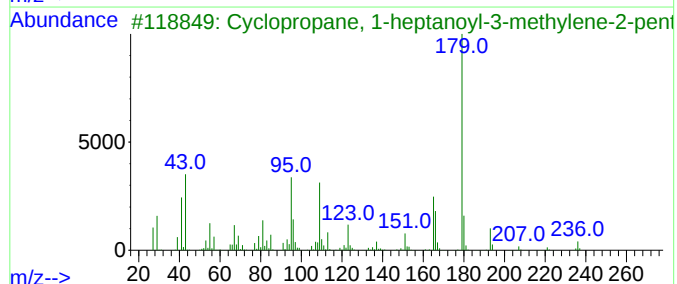
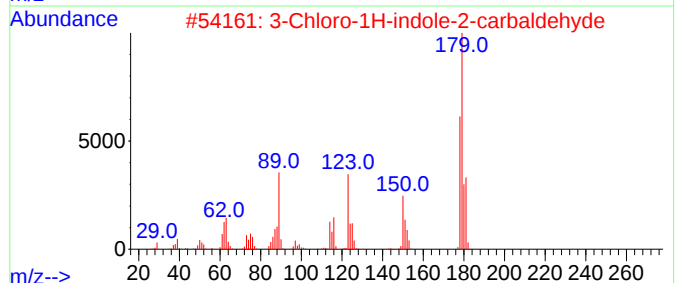
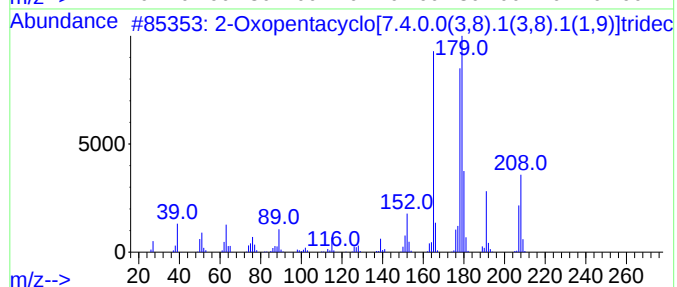
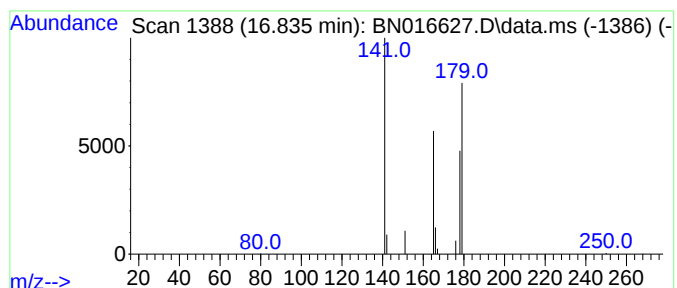
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-Oxopentacyclo[7.4.0.0(3,8... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.835	0.06 ng	24198	Phenanthrene-d10	17.017	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxopentacyclo[7.4.0.0(3,8).1(3...	208	C15H12O	113775-08-9	47
2	3-Chloro-1H-indole-2-carbaldehyde	179	C9H6ClNO	110912-15-7	9
3	Cyclopropane, 1-heptanoyl-3-meth...	236	C16H28O	1000157-26-0	9
4	Benzoyloxy(butyl)dimethylsilane	222	C13H22OSi	1000282-45-8	9
5	5,7-Dihydro-dibenzo(c,E)thiepin ...	228	C14H12OS	069945-00-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE123D1-20210918

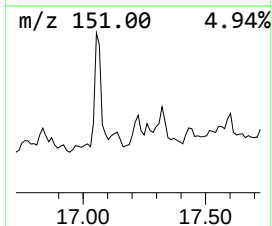
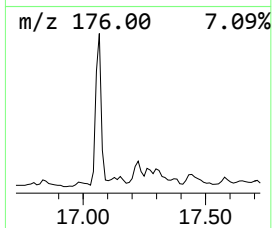
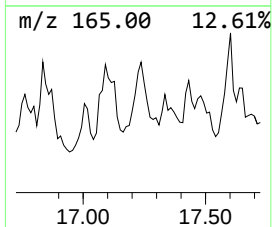
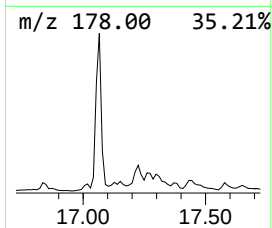
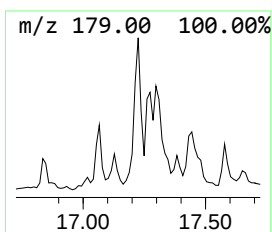
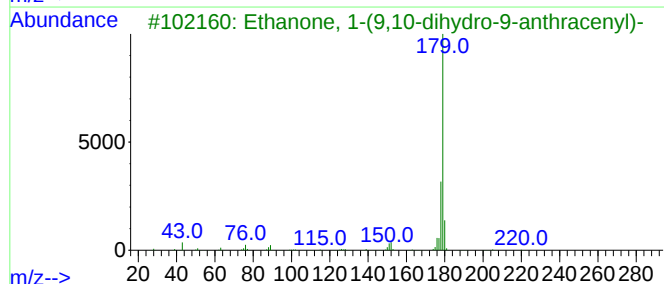
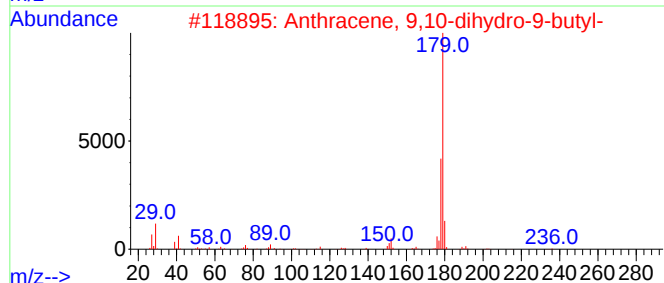
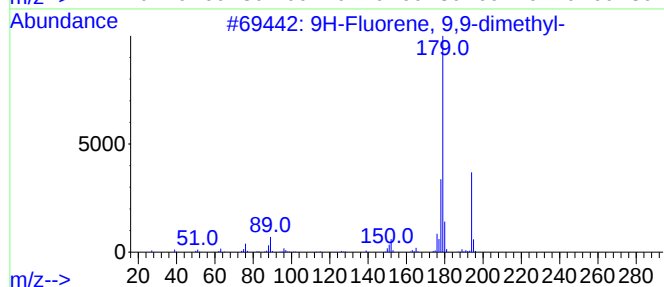
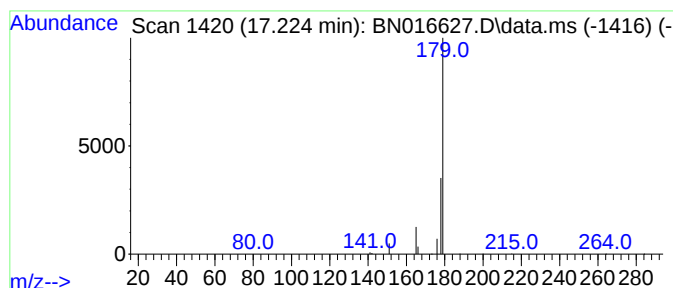
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 9H-Fluorene, 9,9-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.224	0.07 ng	29416	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	9	
2	Anthracene, 9,10-dihydro-9-butyl-	236	C18H20	010394-60-2	9	
3	Ethanone, 1-(9,10-dihydro-9-anth...	222	C16H14O	054585-45-4	9	
4	Anthracene, 9-ethyl-9,10-dihydro-	208	C16H16	000605-82-3	9	
5	Benzo[g]quinoline	179	C13H9N	000260-36-6	5	



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

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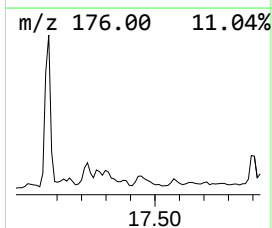
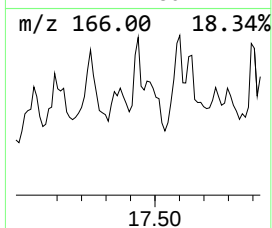
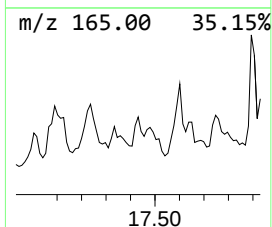
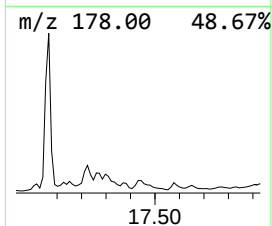
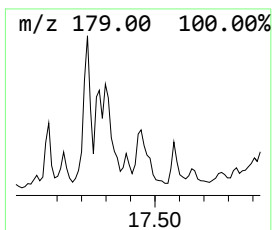
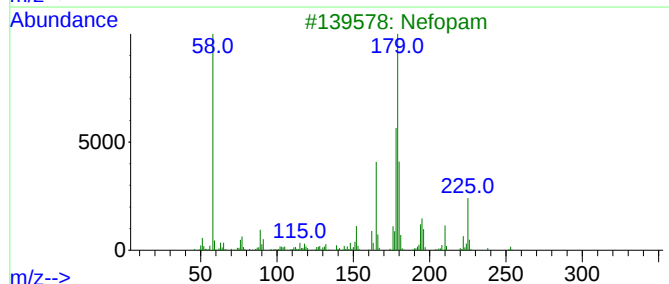
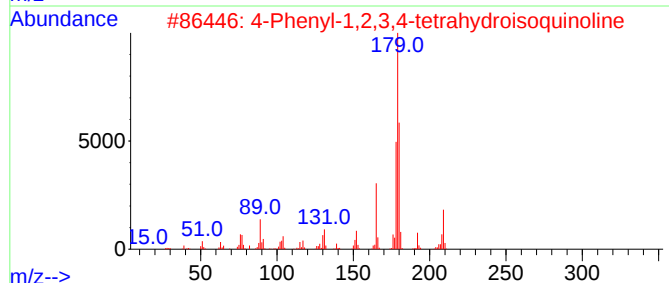
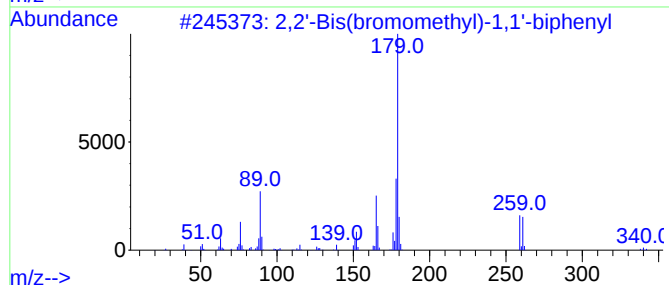
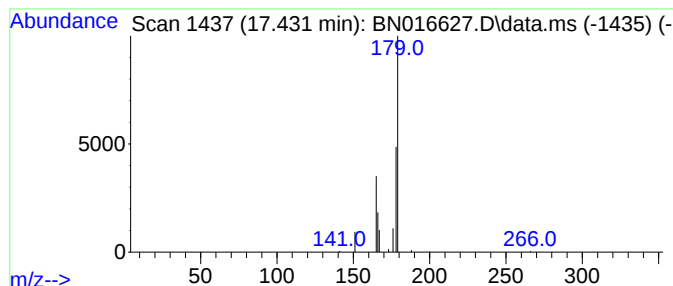
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,2'-Bis(bromomethyl)-1,1'-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.06 ng	25480	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2'-Bis(bromomethyl)-1,1'-biphenyl	338	C14H12Br2	038274-14-5	74
2			4-Phenyl-1,2,3,4-tetrahydroisoqu...	209	C15H15N	075626-12-9	64
3			Nefopam	253	C17H19NO	013669-70-0	39
4			3-Chloro-1H-indole-2-carbaldehyde	179	C9H6ClNO	110912-15-7	9
5			2-(2-Methyl-acryloyl)-cyclohexanone	166	C10H14O2	1000185-67-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

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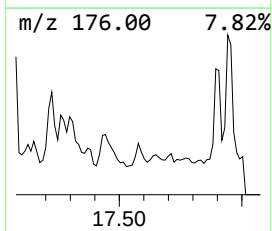
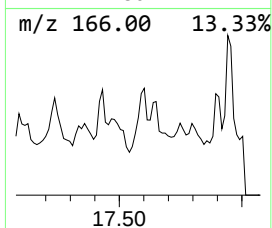
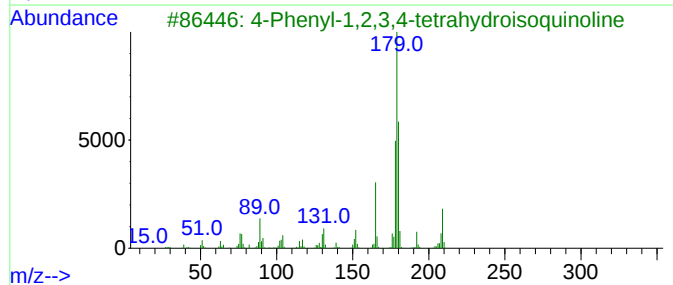
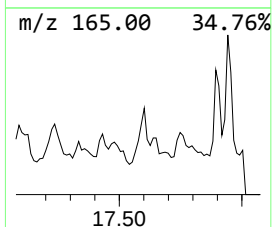
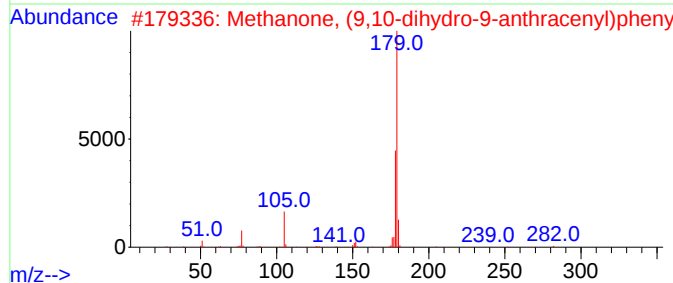
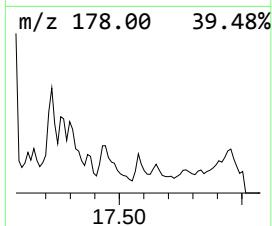
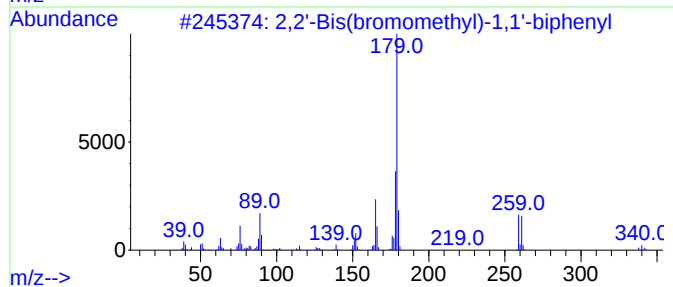
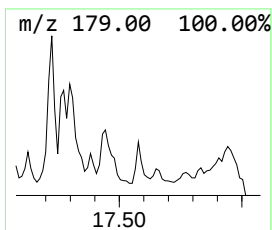
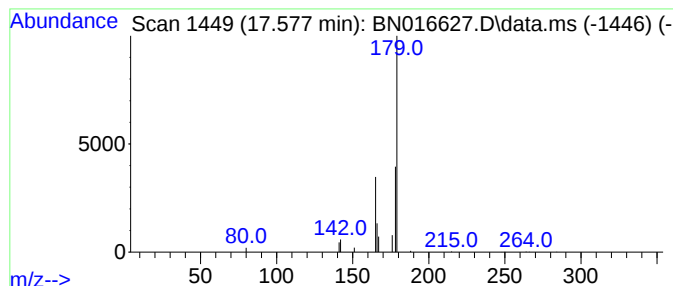
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2,2'-Bis(bromomethyl)-1,1'-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.577	0.04 ng	16337	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2'-Bis(bromomethyl)-1,1'-biphenyl	338	C14H12Br2	038274-14-5	43
2			Methanone, (9,10-dihydro-9-anthr...	284	C21H16O	050688-77-2	42
3			4-Phenyl-1,2,3,4-tetrahydroisoqu...	209	C15H15N	075626-12-9	40
4			Nefopam	253	C17H19NO	013669-70-0	39
5			1,1'-biphenyl, 2,2'-bis(chlorome...	250	C14H12Cl2	1000401-37-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

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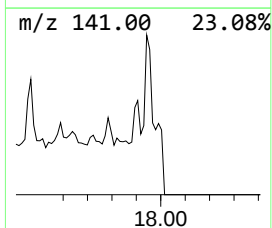
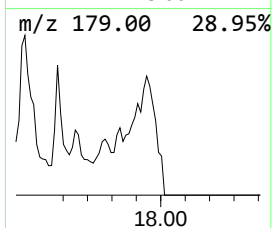
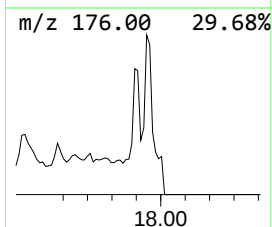
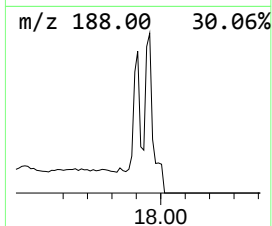
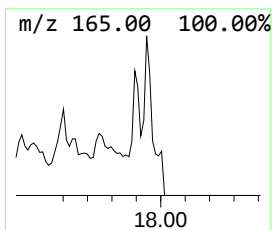
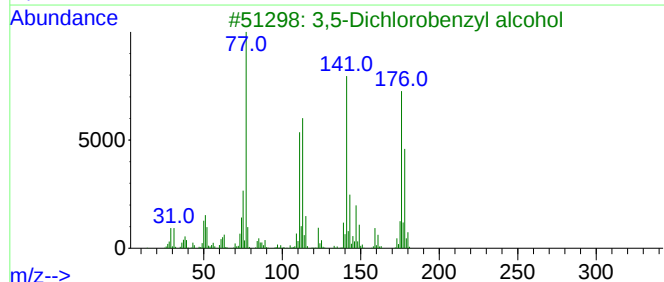
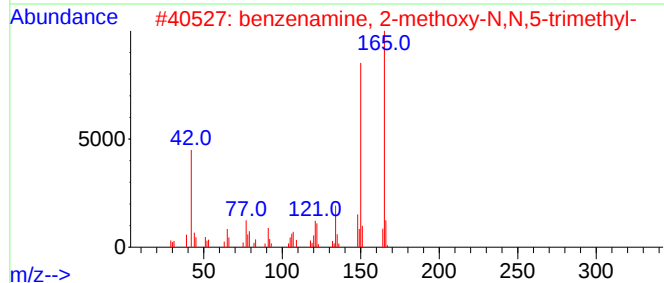
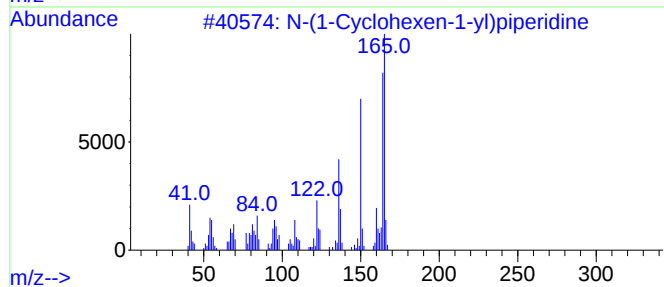
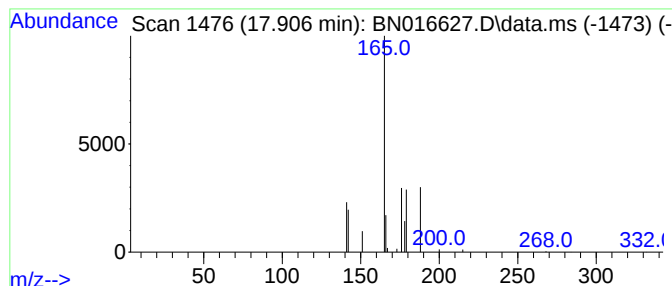
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 N-(1-Cyclohexen-1-yl)piperi... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.906	0.06 ng	22639	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(1-Cyclohexen-1-yl)piperidine	165	C11H19N	002981-10-4	9
2			benzenamine, 2-methoxy-N,N,5-tri...	165	C10H15NO	1000404-49-9	9
3			3,5-Dichlorobenzyl alcohol	176	C7H6Cl2O	060211-57-6	9
4			2-(3,4-Dihydronaphthalen-1-yl)ac...	188	C12H12O2	004709-55-1	9
5			(3H)Benzo[c]pyrrole, 3-methyl-3-...	208	C14H12N2	059341-20-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
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Misc :
ALS Vial : 30 Sample Multiplier: 1

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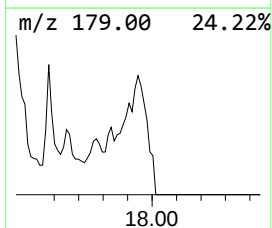
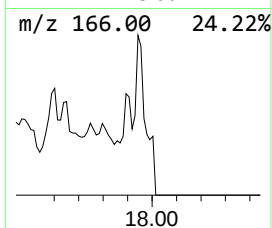
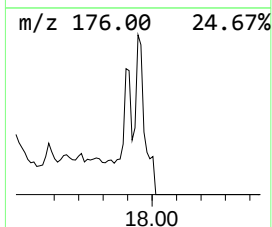
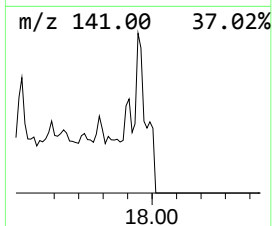
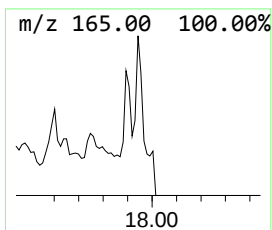
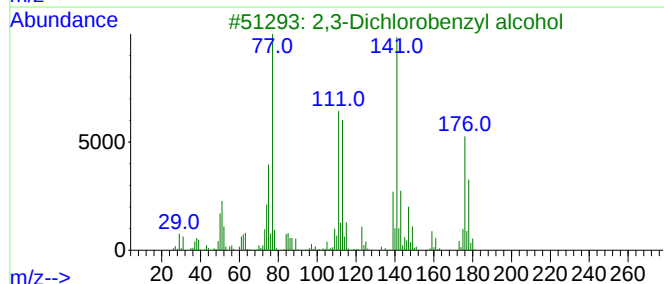
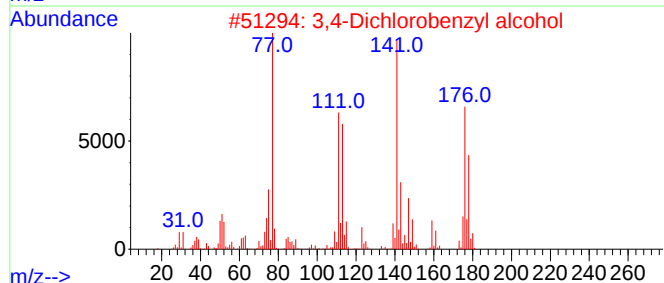
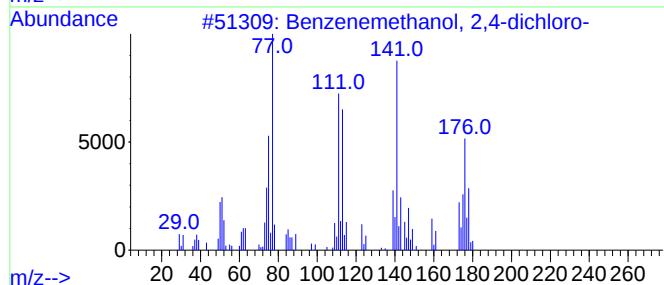
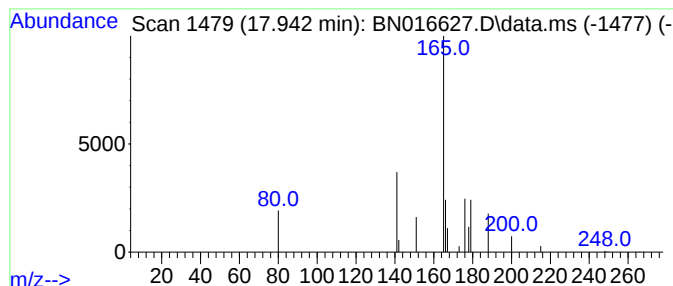
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzenemethanol, 2,4-dichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.942	0.11 ng	45521	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanol, 2,4-dichloro-	176	C7H6Cl2O	001777-82-8	9
2			3,4-Dichlorobenzyl alcohol	176	C7H6Cl2O	001805-32-9	9
3			2,3-Dichlorobenzyl alcohol	176	C7H6Cl2O	038594-42-2	9
4			2,6-Dichlorobenzyl alcohol	176	C7H6Cl2O	015258-73-8	9
5			4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016627.D
Acq On : 01 Oct 2021 08:58
Operator : CG/JU
Sample : M3833-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE123D1-20210918

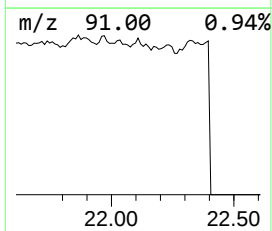
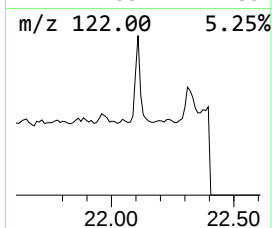
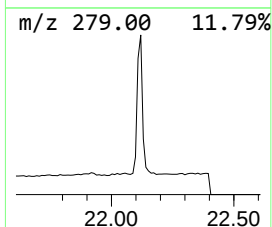
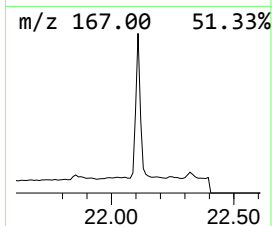
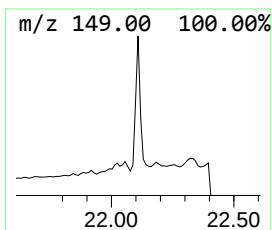
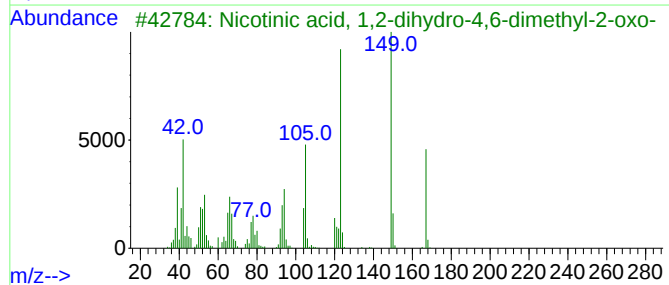
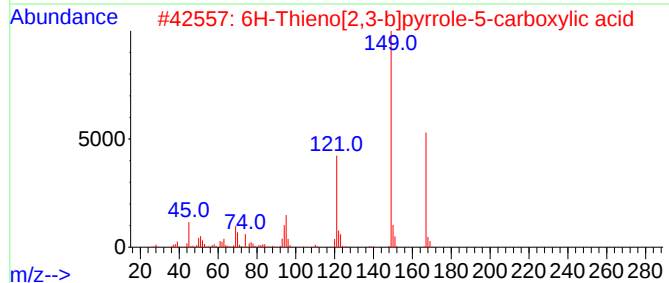
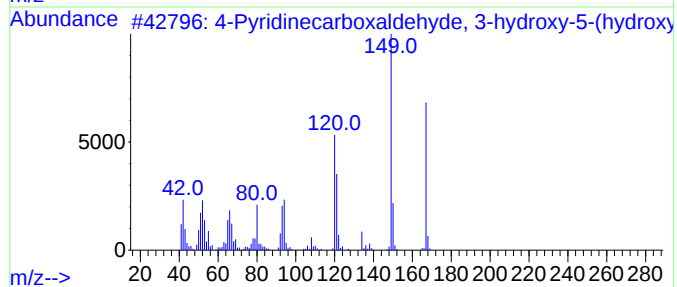
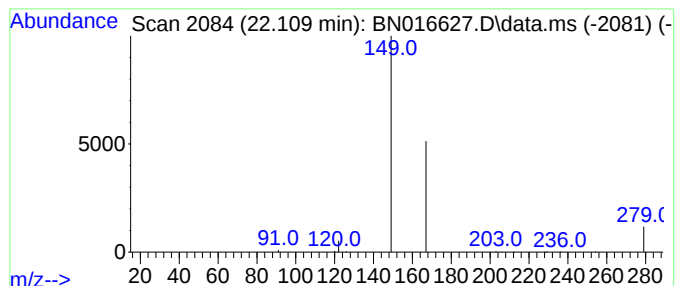
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 4-Pyridinecarboxaldehyde, 3... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.109	0.05 ng	22167	Chrysene-d12	21.238

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	9
2		6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5NO2S	051856-25-8	9
3		Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5
4		4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	5
5		2-Amino-6-methoxybenzoic acid	167	C8H9NO3	1000496-75-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016627.D
 Acq On : 01 Oct 2021 08:58
 Operator : CG/JU
 Sample : M3833-01
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE123D1-20210918

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-Pyrimidinamine	3.152	0.1	ng	29572	1	7.642	97802	0.4
Hydrogen isocya...	3.502	0.2	ng	37986	1	7.642	97802	0.4
Acetic acid, me...	3.816	0.2	ng	47347	1	7.642	97802	0.4
Butane	4.821	0.4	ng	92592	1	7.642	97802	0.4
Azetidine, 1-me...	6.646	0.1	ng	13234	1	7.642	97802	0.4
Hydroxylamine, ...	7.264	0.1	ng	20508	1	7.642	97802	0.4
Butane, 2-iodo-...	7.864	0.1	ng	13844	1	7.642	97802	0.4
N-(2-Methyl-2H-...	8.306	0.0	ng	9963	1	7.642	97802	0.4
4-Methyl-1,2,5-...	10.191	0.5	ng	231807	2	10.407	173832	0.4
Benzophenone	15.715	0.1	ng	21749	4	17.017	160727	0.4
N-(2,2-Diphenyl...	16.385	0.1	ng	26264	4	17.017	160727	0.4
2-Oxopentacyclo...	16.835	0.1	ng	24198	4	17.017	160727	0.4
9H-Fluorene, 9...	17.224	0.1	ng	29416	4	17.017	160727	0.4
2,2'-Bis(bromom...	17.431	0.1	ng	25480	4	17.017	160727	0.4
2,2'-Bis(bromom...	17.577	0.0	ng	16337	4	17.017	160727	0.4
N-(1-Cyclohexen...	17.906	0.1	ng	22639	4	17.017	160727	0.4
Benzenemethanol...	17.942	0.1	ng	45521	4	17.017	160727	0.4
4-Pyridinecarbo...	22.109	0.0	ng	22167	5	21.238	192689	0.4