**Series 31- for Prof. Todd**

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| **Compound** | **Mol. Mass (g/mol)** | **Amount weighed (mg)** | **SMILES** |
| DA-RS-01-032 | 306.81 | 1.9 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC=C(Cl)C=C3 |
| DA-RS-01-037 | 317.36 | 2.0 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC=C([N+]([O-])=O)C=C3 |
| DA-RS-01-038A | 219.26 | 2.0 | O=C1N=C(S)S/C1=C\C2=CC=C(OC)C=C2 |
| DA-RS-01-038B | 302.39 | 2.0 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC=C(OC)C=C3 |
| DA-RS-01-042 | 362.44 | 1.9 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC(OC)=C(OC)C(OC)=C3 |
| DA-RS-01-052 | 272.37 | 2.0 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC=CC=C3 |
| DA-RS-01-053 | 258.34 | 1.9 | O=C1N=C(N2CCCC2)S/C1=C\C3=CC=CC=C3 |
| DA-RS-01-055 | 292.78 | 1.8 | O=C1N=C(N2CCCC2)S/C1=C\C3=CC=C(Cl)C=C3 |
| DA-RS-01-056 | 274.37 | 1.8 | O=C1N=C(N2CCOCC2)S/C1=C\C3=CC=CC=C3 |
| DA-RS-01-058 | 332.42 | 1.9 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC(OC)=C(OC)C=C3 |
| DA-RS-01-060 | 318.39 | 1.6 | O=C1N=C(N2CCCC2)S/C1=C\C3=CC(OC)=C(OC)C=C3 |
| DA-RS-01-061 | 288.37 | 2.0 | O=C1N=C(N2CCCC2)S/C1=C\C3=CC=C(OC)C=C3 |
| DA-RS-01-062 | 308.78 | 2.0 | O=C1N=C(N2CCOCC2)S/C1=C\C3=CC=C([N+]([O-])=O)C=C3 |
| DA-RS-01-064 | 304.36 | 2.0 | O=C1N=C(N2CCOCC2)S/C1=C\C3=CC=C(OC)C=C3 |
| DA-RS-01-065 | 334.65 | 1.5 | O=C1N=C(N2CCOCC2)S/C1=C\C3=CC(OC)=C(OC)C=C3 |
| DA-RS-01-066 | 364.42 | 1.9 | O=C1N=C(N2CCOCC2)S/C1=C\C3=CC(OC)=C(OC)C(OC)=C3 |
| DA-RS-01-067 | 348.42 | 2.0 | O=C1N=C(N2CCCC2)S/C1=C\C3=CC(OC)=C(OC)C(OC)=C3 |
| DA-RS-01-070 | 308.4 | 2.0 | O=C1N=C(N(CC2=CC=CC=C2)C)S/C1=C\C3=CC=CC=C3 |
| DA-RS-01-071 | 288.37 | 1.9 | O=C1N=C(N2CCCCC2)S/C1=C\C3=CC(O)=CC=C3 |
| DA-RS-01-073 | 327.40 | 1.8 | O=C1N=C(N2CCCCC2)S/C1=C\C3C(C=CC=C4)=C4NC3=O |
| DA-RS-01-075 | 398.4 | 1.7 | O=C1N=C(N(CC2=CC=CC=C2)C)S/C1=C\C3=CC(OC)=C(OC)C(OC)=C3 |
| DA-RS-01-076 | 342.8 | 2.0 | O=C1N=C(N(CC2=CC=CC=C2)C)S/C1=C\C3=CC(Cl)=CC=C3 |
| DA-RS-01-077 | 353.4 | 2.0 | O=C1N=C(N(CC2=CC=CC=C2)C)S/C1=C\C3=CC([N+]([O-])=O)=CC=C3 |