CMB114 CW4 Tutorial and Testing Documentation

Throughout the development I have ran countless tests to see if little pieces of code run well here and there, however, this document houses the tests I have run on the final application, showcasing its abilities as a well set-out, visual forefront for running ORCA calculations on any compound.

**Pre-programmed Molecules:**

A screenshot of a computer

Description automatically generatedThe user can select a molecule from the pre-programmed list in the upper-most dropdown menu as pictured below:

These molecules will then be displayed in the right-hand frame of the GUI, whilst their properties will be outputted to a label in the ‘Molecule Properties:’ section of the left-hand frame:

A screenshot of a computer

Description automatically generated