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 functionality of the software, showcasing its abilities as a well set-out, visual forefront for running Orca calculations on any compound.

**Pre-programmed Molecules:**

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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:

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**Custom Molecules from SMILES:**

SMILES is a universally recognised, short-hand way of writing molecular formulae, usually for usage in computing.

The RDKit python library can interpret any SMILES string, giving the user the ability to write in any molecule they wish, to display it on the screen.

The user must input the SMILES string into the entry box, press ‘Draw’ and the molecule will be displayed on the right-hand frame. A few examples:

Caffeine:

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Insulin B:

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Description automatically generatedBenzo(a)pyrene:

**ORCA Functionality:**

From the ‘Custom SMILES code’ entry, the user can also write an input file for the Orca command-line application, to run calculations and find orbital energies, single point energies, optimise geometry, and much more.

To do this, the user simply must input the SMILES code of the compound they would like to create the input file for, select the required arguments from the drop-down menus and click the ‘Generate Orca Input’ button.

The Orca input will then be written to a .txt file within the ORCA\_input directory, in the main project directory.

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**Testing:**

Below are tests of a few molecules to compare the Orca input files produced by both my software and Avogadro to showcase my software’s ability to produced correct ORCA calculations in the same way Avogadro can.

Propane:

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The two programs, respectively, produce different sets of cartesian coordinates for the molecule, however, they are correct relative to one-another, since the calculated values of the Single-Point Energy (SPE), from ORCA, is the same:

Avogadro generated SPE:

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CW4 – Molecular Dynamics generated SPE:



The two simulations output very slightly different values; however, this can be down to the individual simulation that is run on the computer. Two inputted files from Avogadro may return different energies on a simulation-by-simulation basis.

These simulations for propane took approximately 4 seconds to complete in each instance.

Let’s try a more complex molecule, take caffeine for example:

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Avogadro generated SPE:

CW4 – Molecular Dynamics generated SPE:



The runtime for these simulations is very similar as well with the elapsed time being approximately 2 minutes in both instances, yet again.