

Instructions for Installing ORCA, Multiwfn, and Python on Windows

Step 1. Install ORCA 5.0.3 for Windows

- Visit the ORCA website and download version 5.0.3 for Windows (https://www.orcasoftware.de/tutorials_orca/first_steps/install.html)
- Unzip the file to the location of your choice, which will be referred to as "ORCA Location" in these instructions.
- Set the PATH variables by following the instructions on the ORCA website (https://www.orcasoftware.de/tutorials_orca/first_steps/trouble_install.html#path-variable). You will need to add the address of "ORCA Location" to the PATH variables. This step is important to ensure that ORCA is accessible from any directory in your command prompt.

Step 2. Install Multiwfn program version 3.8

- Download the program from the Multiwfn website (http://sobereva.com/multiwfn/misc/Multiwfn_3.8_dev_bin_Win64.rar)
- Unzip the file to the location of your choice, which will be referred to as "Multiwfn Location" in these instructions.
- Set the PATH variables by adding the address of "Multiwfn Location" to the PATH variables. This step is important to ensure that Multiwfn is accessible from any directory in your command prompt.

Step 3. Install Python

- Download the Windows installer for Python from the official website. Make sure to choose a version equal to or greater than version 3.7 (<https://www.python.org/downloads/windows/>)
- Run the downloaded file (.exe) in administrator mode and follow the prompts to complete the installation.
- Select "Add Python to PATH" and install.

By following these instructions, you should have successfully installed ORCA, Multiwfn, and Python on your Windows machine. Make sure to test each program to ensure that they are working correctly.