[Overview]
This is a program of ab initio molecular orbital method and the density functional theory. Specifically, the Hartree-Fock theory, the 2nd-order Møller-Plesset perturbation, and the Kohn-Sham method are implemented.

[Install]
Make sure your mac has an Apple Silicon M series SoC. For macs with intel CPU, there is a separate distribution file. When you download the Zip file, it will be automatically expanded and you will find a folder named "Quantum_Chemistry". Move this folder to a place you like. Since we work in it, it's better under your home, not in the "Application" folder. Do not change the name and relative location of the folders under the "Quantum_Chemistry". Otherwise, the program will not work properly.

At this stage, calculation programs(*.exe) in the "Bin" folder are available. You can go to the "Bin" with the terminal and run, for example, as "./H2O.exe arguments". As for the arguments, if you run the program with no arguments, usage will be displayed. However, it is easier to use the GUI frontend described below than to use these programs directly.

Files "quantum.exe" and "editor.exe" in the "Gui" folder are the frontend body. For these frontends to work, "GTK+3", "VTE3", and "adwaita-icon-theme" are required. If any of these are not installed on your mac, install them all. You can use any package manager. Use the one you have used so far. For example, for Homebrew, run "brew install vte3" in the terminal and so on.

Since there are shell scripts "01_Quntam.sh" and "02_Editor.sh" in the "Run" folder which launch these frontends, usually, to launch the frontend, go to the "Run" folder and run the script. You can run these scripts from the terminal. But, if you want to run them by double-clicking with the Finder, right-click to open "Get Info" and set the "Open with this application" item to "Terminal". It may already be set, but if not, set it. You can find "Terminal" in "Utilities" under "All Applications" under "Others". This completes the installation.

[Uninstall]
Delete the folder "Quantum_Chemistry". That's it.

[How to use], [Caution], [Arbitrary Molecule], [History]
See README file for Windows because thses are the same on the Windows.