Readme

I. Prerequisites

1.Download and install Anaconda (Download link: https://www.anaconda.com/).

2.Download the code compressed package chatcof\_interactive.zip (Download link:https://github.com/wchou93/chatcof\_interactive).

3.Create a folder at any location (e.g., a "Jupyter" folder on your desktop), place the compressed package into it, and extract the contents.

II. Usage Instructions

1.Open Anaconda Navigator, select Jupyter Lab, and start it.

2.On the left side of the popped-up Jupyter Lab web window, find the path where the chatcof\_interactive folder was placed. Open it, and you will see several files such as datebase.py.

3.Click the blue "+" icon in the upper left corner, select "python3 (ipykernel)" under the first Notebook option, and a new window will pop up.

4.Enter %run database.py. If -Load Done- appears after running, it means the program has been successfully launched, and you can start querying and making predictions.

5.Enter the compound name, CAS number, or SMILES expression to query the formula. You can also predict the dosage ratio of ligand 1 and ligand 2, the name and dosage of the solvent, the name and dosage of the additive, as well as the temperature and time.

Frequently Asked Questions

To stop the query: In Jupyter, click Kernel → Restart to restart the kernel.