### **Readme**

### **I. Prerequisites**

1. Download and install Anaconda (Download link: [https://www.anaconda.com/](https://www.anaconda.com/" \t "https://www.doubao.com/chat/_blank)).
2. Download the code compressed package chatcof\_interactive.zip (Download link: [https://github.com/anney10000/chatcof/releases/tag/v1.0](https://github.com/anney10000/chatcof/releases/tag/v1.0" \t "https://www.doubao.com/chat/_blank)).
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. In Jupyter Lab, locate the extracted folder and view the database.py and synthesis.db files.
3. Create a new Python 3 Notebook.
4. Enter %run database.py. If "Load Done" appears, the startup is successful.
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.