Integrated Interface for Computational Apparatus
User's manual

EikiMeg

alpha 1.0 (Last update: 22/08/28)

Contents

Part I

About IICA

1   What is IICA?

IICA(Integrated Interface for Computational Apparatus) is a python-based tool aimed at enabling to utilize computer softwares without any complicated procedures. With IICA, one can carry out computational works.

It consists of 'Central' and some 'Application's, each of which are linked to other softwares such as Autodock vina.

Recommended system requirements for Central is following:

- Bash environment (Ubuntu or WSL)

- Python 3.7.13

- Tkinter 8.6.12 (python package)

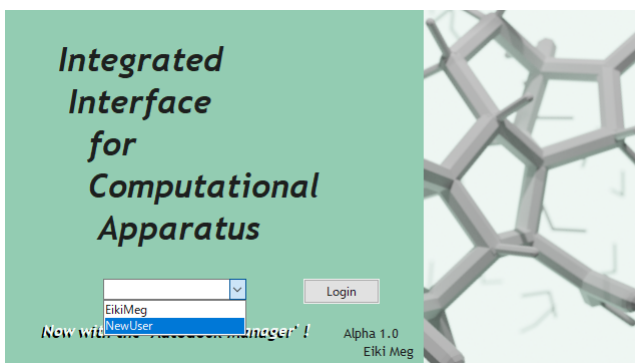Others are needed in some Applications. (See each sections in Part II)

IICA is developed by Eiki Meguro (or, EikiMeg) alone. If you find any issues, don't hesitate to contact me. Also, requests on feature are welcome.

2   Usage of Central

2.1   User registration (First time only)

After determining your username (String without spaces), type 'Reg' in command the line, then you will be asked username. Follow the directions and when you see a message 'User {Your_Username} is ready. Welcome to IICA!', registration is complete. Make sure IICA recognize you as a new user in login screen.
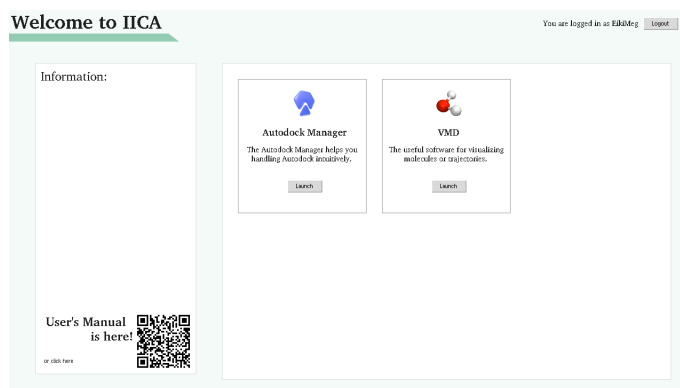

'NewUser' is recognized as a new user.

2.2   Entering IICA Central

To launch IICA, simply type 'IICA' in the command line. Select your user from the drop-down list and click 'Login' to proceed.

Then you'll see a screen as below:

IICA Central

Part II

Applications in IICA

3   Autodock Manager

Requirements:

- Pymol 2.4.1 (python package)

In progress...