User Manual

With Conda installed, run the following commands in the terminal:

```
conda env create -f environment.yml
conda activate mol-env
conda install kivy -c conda-forge
easy_install networkx
```

Then, to run the program, use the following command:

```
python gui.py
```

General:
The action space should be a list of valid reactions in smarts format.
Starting Molecule list must be valid molecules in smiles format

GUI:

The GUI was designed with aesthetic buttons and drop-down list options which are very self-explanatory. So, it's very easy to start working with the GUI. Every button is labeled correctly and the functions as it should. We encourage exploration of the GUI.

Environment:

Working with our system's molecule environment is exactly the same as working with any other Open Ai's environments. Create the environment by calling gym.make('gym_molecule:molecule-v0'). This will create the environment with the default settings. Note that the GUI will do this automatically once it's started.

From here it's up to you, the user, to decide how you will implement your specific algorithm. You can call each function in the environment (reset,step,render) as needed inside your algorithm.

When calling the step function, provide it with the action selected by your agent. The step function will also return a tuple with the observations and associated rewards.

The reward function inside the environment has a default reward of 10 for demonstration purposes. This can be modified as you wish.

When the render function is called, a picture of the current state molecule will appear. Note that this will slow down the learning process.

An agent class with skeleton code has been provided for you to modify to your needs.

Table 1: Menu

When the program is first built and run, the above table (Table 1) which is the main menu appears. It contains all the variables which can be modified when running simulations in the environment. These variables are namely (from the top): Action Space, Starting Molecule, Rendering, Number of Environment loops and Number of Steps per Environment loop.
At the bottom right corner, 2 buttons are available which either creates the environment with the set variables or exit the environment and program.

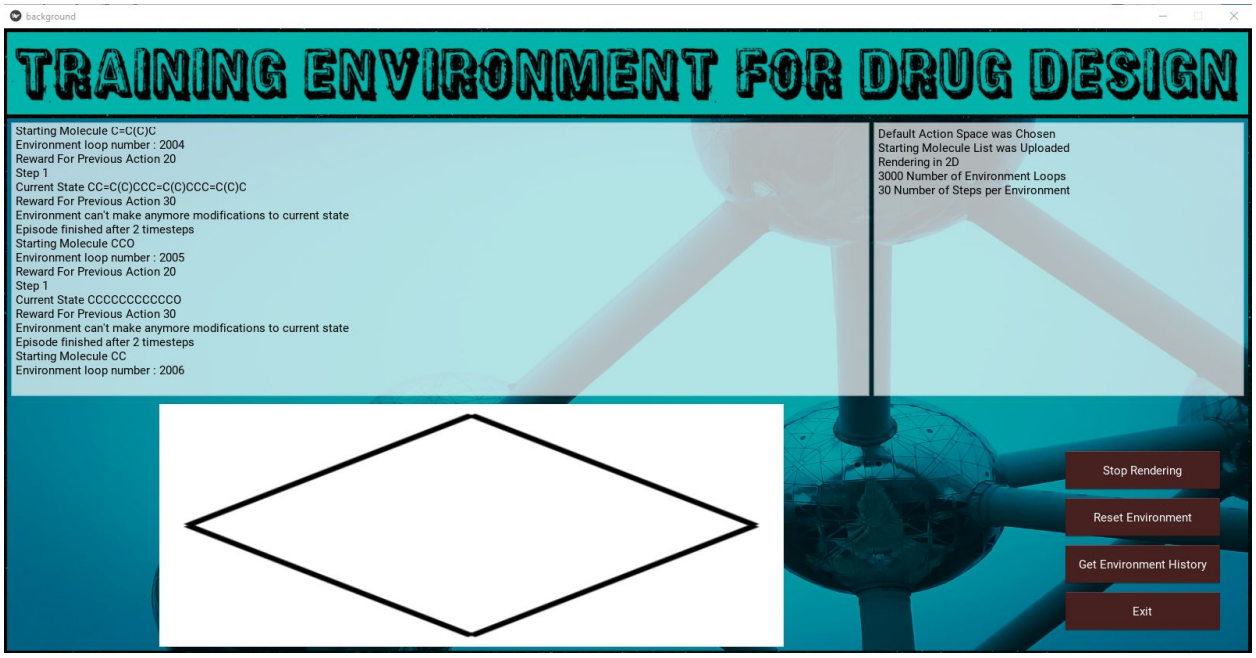

Table 2: Environment

When “Create Environment” is pressed in the Menu, the environment (Table 2) appears on the screen. On the top left box, the current state of the environment is printed along with the step number, environment loop number and the reward associated. The top right box contains information and variables about the ongoing simulation running in the environment such as the action space chosen, the starting molecule chosen, rendering enabled or disabled, the number of environment loops and the number of steps per environment loop. Furthermore, the bottom left window is the area where the rendering function takes shape and displays the image of the current state. Finally, this screen also has a set of control buttons on the right and has the following functionalities (from the top button): Enable/Disable Rendering, Reset the environment, Getting a History reaction list of the current ongoing simulation and the exit button.