fpocket-R

fpocket-R is a modified version of fpocket 4.0 and is optimized for finding, characterizing, and visulizing drug-like RNA-ligand binding pockets.

Installation with Conda

Windows Users:

1. fpocket-R requires a Unix/Linux to run properly, this mean that Windows users need to activate the Windows Subsystem for Linux (WSL).

   - WSL is build-in to Windows 10 and 11 and allows users to easily run conda and fpocket-R using a Linux virtual machine.

   - Guide to installing WSL and Ubuntu

   - Once WSL is activated on your computer, use WSL/Ubuntu to install conda and fpocket-R using the installation instructions for Linux.

Linux, Unix, MacOS, and WSL users:

2. Install conda on a Unix/Linux-based system

   - Guide to install conda

     - **macOS users:** Regular installation > macOS

     - **Windows users:** User WSL/Ubuntu to install conda: Regular installation > Linux

     - **Linux users:** You can figure it out

Linux, Unix, MacOS, and WSL users with conda installed:

3. Open your terminal and navigate to the directory where you would like to install the fpocket-R and RNAvigate packages (optional).

   - **Tip for new Windows (WSL) users:** You can navigate to your Windows file system in the WSL command line by using the following command:

     ```
     cd /mnt/c/Users/<your-user-name>
     ```

4. Clone the RNAvigate and fpocket-R GitHub repositories. (RNAvigate is a dependancy for fpocket-R)

   ```
   git clone https://github.com/Weeks-UNC/RNAvigate.git
   git clone https://github.com/Weeks-UNC/fpocketR.git
   ```

5. Create fpocket-R conda eviroment and install fpocket-R and RNAvigate.

```
cd fpocketR
conda env create -f env.yml
conda activate fpocketR
conda develop .
cd ../RNAvigate
conda develop .
```

Demo

Demonstration of fpocketR usage