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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/fpocket-R.git
```

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

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