fpocket Analysis Pipeline Demo

Preparation

```
conda activate fpocket-R
cd ~/Weeks_Lab/fpocket4/fpocket-R_7.0/demo
```

Navigate to a working directory that contains a .pdb file(s). Secondary structure drawings such as .nsd file(s) are optional.

Run from terminal

```
../fpocket-R_7.0.py -pdb 7ELR.pdb
```

This argument will run fpocket, analyze pockets, and make 3D figures.

The user will be prompted to input ligand name since multiple heteroatoms are detected.

Run batches of files through fpocket-R using a bash script

```
bash fpocket-R_7.0_job_submitter.sh
```

Analyses run from bash scripts must specify ligand name in command (-l)

Contents of shell file

- Specify an nsd file to create 2D figures (-nsd).
- Specify a three character ligand residue name for holo structure analysis (-l).

  ```
  -pdb 3E5C.pdb -nsd 3E5C.nsd -l SAM
  ```

- Specify the chain id of the RNA, if not chain A (-c).

  ```
  -pdb 2GDI.pdb -nsd 2GDI.nsd -l TPP -c X
  ```

- Specify upto 2 chain ids (eg. A,B) for discontiguous RNAs (-c).

```
-pdb 1YKV.pdb -nsd 1YKV.nsd -l DAI -c A,B
```

- Specify no ligand for apo structure analysis (-l).
- Analyze all NMR states (-s).
- Align all outputs to the input .pdb file (-al).

```
-pdb 6MCI.pdb -nsd 6MCI.nsd -l no -s 0 -al
```

- Specify the resolution for 3D figures to decrease render time or increase quality (-dpi).
- Specify a custom name for the output directory (-o).

```
-pdb 7EZ0.pdb -nsd 7EZ0.nsd -l no -c N -dpi 50 -o group_I_intron
```

fpocket-R options

Input options	**Description**
-pdb STRING (Required)	Specify a .pdb file to run fpocket.
-nsd STRING	Specify an .nsd file for generating secondary structure figures.
-a STRING	Specify a directory contianing fpocket outputs for analysis (without running fpocket).
-s INT	Specify a particular NMR states/model for analysis. Set to 0 for all. Default: NONE
fpocket options	**Description**
-m FLOAT	Sets fpocket -m flag. Specifies the minimum radius for an a-sphere. Default: 3.0
-M FLOAT	Sets fpocket -M flag. Specifies the maximium radius for an a-sphere. Default: 5.7
-i INT	Sets fpocket -i flag. Specifies the minimum number of a-spheres per pocket. Default: 42
-D FLOAT	Sets fpocket -D flag. Specifies the a-sphere clustering distance for forming pockets. Default: 1.65
-p FLOAT	Sets fpocket -p flag. Speciefies the maximum ratio of apolar a-spheres. Default: 0
Output options	**Description**

Output options	Description
-o STRING	Specify name of fpocket output parent directory name. Default: fpocket-R_out_{fpocket parameters}
-n STRING	Specify name prefix for fpocket_out and analysis_out subdirectories.
-y	Overwrites output files and directories with same name.

Analysis settings	Description
-l STRING	Specify the three character residue name of desired ligand.
-c STING	Specify the chain(s) IDs conatining RNA. List upto 2 chains seperated by a comma (eg. A,B). Default: A
-lc STRING	Specify the chain containing a ligand. Default: same as specified RNA chain.
-off INT	Specify the offset between the structures in the input pdb and nsd files. Default: will gather offset from pdb header.
-qf FLOAT	Specify the minimum fpocket score for a pocket to pass the quality filter. Default: 0.1
-df FLOAT	Specify distance filter (Angstroms) for identifying nucleotides near pockets. Default: 4.5

Figure settings	Description
-dpi INT	Specify 3D figure resolution (dots per linear inch). Deafult: 300
-zoom INT	Specify zoom buffer distance to set the feild of view for 3D figures. Deafult= 10
-cp	Visually connects pockets in 2D figures. Deafult: False
-al	Align output structures to input structure. Useful for multistate analysis. Default: True