fpocket Analysis Pipeline Demo

Preparation

```
conda activate fpocketR
cd ~/Weeks_Lab/fpocket4/fpocketR/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

```
python -m fpocketR -pdb 7ELR.pdb
```

or

```
python -m fpocketR -pdb 7ELR
```

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 (input: XAN).

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

```
bash fpocketR_batch_submitter.sh
```

NOTE: Analyses run from bash scripts must specify ligand name in command line (use the -l or --ligand options).

Contents of shell file

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

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

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

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

- Specify upto 2 chain ids (eg. A,B) for discontiguous RNAs (-c, --chain).
- Specify the chain containing the ligand of interest (-l, --ligand).

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

- Specify *fpocket* parameters to use default parameters (optimized for proteins) or your own parameters (-m, --m; -M, --M, -D, --D; -i, --i; -A, --A; -p, --p).

```
-pdb 3E5C.pdb -nsd 3E5C.nsd -l SAM -m 3.4 -M 6.2 -D 2.4 -i 15 -A 3 -p 0
```

- Specify no ligand for apo structure analysis (-l, --ligand).
- Analyze all NMR states (-s, --state).

```
-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, --dpi).
- Specify a custom name for the output directory (-o, --out).

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

fpocket-R options

Input options	**Description**
-pdb, --pdb STRING (Required)	Specify a path to a .pdb file, .cif file, or 4 charater PDB indentification code to run fpocketR.
-nsd, --nsd STRING	Specify an .nsd file or other secondary structure file for generating secondary structure figures.
fpocket parameter options	**Description**
-m, --m FLOAT	Sets fpocket -m flag. Specifies the minimum radius for an a-sphere. (Default: 3.0)
-M, --M FLOAT	Sets fpocket -M flag. Specifies the maximium radius for an a-sphere. (Default: 5.7)

fpocket parameter options	Description
-i, --i INT	Sets fpocket -i flag. Specifies the minimum number of a-spheres per pocket. (Default: 42)
-D, --D FLOAT	Sets fpocket -D flag. Specifies the a-sphere clustering distance for forming pockets. (Default: 1.65)
-A, --A INT	Sets fpocket -A flag. Specifies the number of electronegative atoms required to define a polar a-sphere (Deafult: 3).
-p, --p FLOAT	Sets fpocket -p flag. Speciefies the maximum ratio of apolar a-spheres. (Default: 0)

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

Analysis settings	Description
-s, --state INT	Specify a particular NMR states/model for analysis. Set to 0 for all. (Default: NONE)
-c, --chain STING	Specify the chain(s) IDs conatining RNA (case sensitive). List upto 2 chains seperated by a comma (eg. A,B). (Default: A)
-l, --ligand STRING	Specify the three character residue name of desired ligand.
-lc, --ligandchain STRING	Specify the chain containing the ligand of interest. (Default: same as first RNA chain.)
-off, -offset INT	Specify the offset between the structures in the input pdb and nsd files. Manual input is required for use with .cif files. (Default: will gather offset from pdb header.)
-qf, --qualityfilter FLOAT	Specify the minimum fpocket score for a pocket to pass the quality filter. (Default: 0.0)

Figure settings	Description
-dpi, --dpi INT	Specify 3D figure resolution (dots per linear inch). (Default: 300)
-zoom, --zoom INT	Specify zoom buffer distance to set the feild of view for 3D figures. (Default= 10)

Figure settings	Description
-cp, --connectpocket BOOLEAN	Visually connects pockets in 2D figures. (Default: False)
-al, --alignligand BOOLEAN	Align output structures to input structure. Useful for multistate analysis. (Default: True)