WATsiteOnTheFly

Ahmadreza Ghanbarpour, Amr H. Mahmoud, and Markus A. Lill

Download and set up example

Download 4fm8.tar.gz file from

https://pharma.unibas.ch/fileadmin/user_upload/pharma/Research_groups/Computational_Pharmacy/Bilder/Research/4fm8.tar.gz

to any folder, e.g. /home/*username*/WATsiteOnTheFly_example/

[change *username* to your user name]

```
cd /home/username/WATsiteOnTheFly_example/
tar zxf 4fm8.tar.gz
```

The folder contains the following essential files for WATsiteOnTheFly prediction:

- 4fm8: Coordinates of zero point of grid box in which hydration information will be predicted. Currently the box size is fixed to 24x24x24 $Å^3$.
- prot_amber.prmtop: Amber topology file based on protein_amber_aligned.pdb.
- protein_amber_aligned.pdb: PDB file containing coordinates of protein structure.

For generating own example, those files need to be generated by user first.

Download and initiate docker image

```
docker pull lilllab/watsite_on_the_fly:version1.0
```

```
docker run -it  -v
/home/cresset/Desktop/WATsiteOnTheFly_example:/WATsiteOnTheFly_examp
le lilllab/watsite_on_the_fly:version1.0 /bin/bash
```

(in this way the working directory is mapped from inside to outside of docker image)

Change to directory `/WATsiteOnTheFly_example` (which contains example 4fm8):

```
cd /WATsiteOnTheFly_example
```

Run WATsiteOnTheFly

```
conda activate ml
python  /water/export/master.py  -i  /WATsiteOnTheFly_example/  -d
/water/export/example/  -l  /WATsiteOnTheFly_example/  -s  4fm8  -o
/WATsiteOnTheFly_example/ -z /WATsiteOnTheFly_example/4fm8/
```

Visualization using PyMOL

Due to license issues, PyMOL is not installed as part of the WATsiteOnTheFly docker image. To visualize the results, please open new terminal and change again into folder /home/*username*/WATsiteOnTheFly_example/

```
cd /home/username/WATsiteOnTheFly_example/
```

Download create_figure_watsite.py from https://pharma.unibas.ch/fileadmin/user_upload/pharma/Research_groups/Computational_Pharmacy/Bilder/Research/create_figure_watstie-py

Start PyMOL with prepared create_figure_watsite.py script

```
pymol create_figure_watsite.py
```

In PyMOL:

```
create_figure_watsite 4fm8, 0UQ, 4
```

Different occupancy and free energy isosurfaces can be toggled on and off by selecting objects on the right panel of PyMOL.