

A simple MCCE example of pH titration

Run MCCE

Prepare a working directory:

```
$ mkdir test_lysozyme  
$ cd test_lysozyme
```

Get a pdb file

```
$ getpdb 1dpx
```

You now have a pdb file 1DPX.pdb in the working directory.

The simplest way to run mcce is do these four steps:

Step 1 convert PDB file into MCCE PDB

This step proof reads the structure file and cuts terminal residues and complex cofactors into smaller ones if necessary.

```
$ step1.py 1DPX.pdb
```

Step 2 make side chain conformers

This step makes alternative side chain locations and ionization states.

```
$ step2.py
```

Step 3 make energy table

This step calculates conformer self energy and pairwise interaction table.

```
$ step3.py
```

Step 4 Simulate a titration with Monte Carlo sampling

This step simulates a titration and writes out the conformation and ionization states of each side chain at various conditions.

```
$ step4.py
```

Notes

Command help "-h"

- For more detailed command usages, use "-h" switch in each command above.

Run in background

- Some steps take hours to finish, so it is recommended to run at the background. For example:

```
step3.py > run.log &
```

Jupyter notebook

Here is a Jupyter note book template: [mccee.ipynb](https://github.com/mccee/mccee/blob/master/notebooks/mccee.ipynb)

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