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 with these four steps:

Step 1: Make PDB file into MCCE PDB

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

`$ step1.py 1DPX.pdb`

Step 2: Create side chain conformers

This step makes alternative side chain locations and ionization states.

`$ step2.py`

Step 3: Calculate 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 &`
- `For more exhaustive work, we recommend using tools like p_batch to process many runs at once in the background.`

Jupyter notebook

Here is a Jupiter note book template: mcce.ipynb

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