Tautomeric Charge Microstates

All MCCE tools relevant to microstate analysis will start with "ms", like 'ms_top2pdbs" and "ms_hbond_percentages.py".

To use any microstate tools, MCCE needs to have the directory "ms_out", produced by "step4.py --ms". Read the steps 1 - 4 tutorial for more information about those runs.

sampled_ms_to_pdbs.py

Makes a sample PDB file, generated from a random sample of conformer microstates whose size is user-defined.