MOFF IDP Guide

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1. Setup template and pdb
    a. Run write_MOFF.py. Should be 2 arguments. The first is the pdb file you want to generate a pdb for. Current code only works with 1 protein in the pdb file, will look to improve that in the future. The second is the template file. Unless doing further development, this should be template_MOFF.top.
    b. The output should be a CA only pdb file and a template file. These will be input for gromacs
2. Generate a table potential
    a. Use smog to generate a table at the correct salt concentration. Follow their standard procedures. In the future, will add calculation of electrostatics to the MOFF table gen.
    b. Use convert_table.py to turn SMOG table into MOFF table. Takes 2 inputs. The first is the SMOG table used. The second is the corresponding output table at the same concentration. This output table will be the one used by gromacs.
3. Run simulation
    a. Minimize energy
    b. Place in an empty simulation box
    c. Run your simulation

Check out the Example folder for an example on how to do a simple simulation.

Starting in the example folder:

1. python ../Scripts/write_MOFF.py An16 ../Scripts/template_MOFF.top
2. python ../Scripts/ convert_table.py table_SMOG.xvg table_MOFF.xvg (used an ionic strength of 185 mM if you use this table)
3. Run the corresponding commands in Gromacs from job.pbs

Compatible with GROMACS 4.5

Email aplatham@mit.edu with any questions