

Multiple PDB MCCE Runs (pro_batch)

p_batch is a program included in MCCE, under the folder MCCE_bin. It accepts a directory containing ".pdb" files, and runs MCCE with identical settings on each protein file. Usage: p_batch protein_dir [custom_script.sh] By default, default_script.sh is created by p_batch at run time, if it does not exist. The default scripts calls for steps 1-4 of MCCE to be run at level 1, assumes a dielectric constant of 8 with NGPB as the Poisson Boltzmann solver, and sets entropy control on. Another tool is available called "pro_batch". This behaves very similarly to p_batch, though the file pro_batch creates by default has more features for heavy users.