

## Mucin: 3. MD simulation

### 1. Page 1

See below for the run control files specific to each set of simulations.

Overview of the simulation protocols.

1. Steepest descent minimization for 10,000 cycles.
2. Heat from 5.0 to 300.0 degrees C over 20,000 steps, each 0.002 ps, using the weak coupling algorithm in NVT conditions with constraints on bonds containing hydrogen.
3. Equilibrate for 1,000,000 steps (0.002 ps) at NPT (1 atm, 300 K) using Langevin dynamics to maintain temperature and isotropic position scaling to maintain pressure. Bonds including hydrogens were constrained.
4. To collect data, continue using the equilibration conditions for another 50,000,000 steps. To conserve disk space during these runs, coordinates for water molecules were not recorded. Coordinates were written out every 5000 steps (each nanosecond).

Notes:

\* For the mannosylated and unglycosylated residues, coordinates for a few additional atoms were accidentally saved (see the prod\*.in files). These extra coordinates are deleted in the curation phase.

\* During the runs, a hardware malfunction corrupted a small number of data frames. These were

Created: 10 Feb 2013 04:26:14 GMT , Updated: 22 Apr 2013 20:14:13 GMT

min.in

The minimization protocol used for all runs.

Created: 22 Apr 2013 20:15:47 GMT

heat1.in

The heating file used by the unglycosylated and mannosylated runs and runs 1-16 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:38:30 GMT

heat2.in

The heating file used by runs 17-32 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:44:29 GMT

equil1.in

The equilibration file used by the unglycosylated and mannosylated runs and runs 1-16 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:45:14 GMT

equil2.in

The equilibration file used by runs 17-32 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:45:48 GMT

prod1.in

The production file used by the mannosylated runs and runs 1-16 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:51:59 GMT

prod2.in

The production file used by runs 17-32 of the N-acetylgalactosylated runs.

Created: 22 Apr 2013 20:52:38 GMT

prod\_protein.in

The production file used by the unglycosylated runs.

Created: 22 Apr 2013 20:53:13 GMT