MD Simulations

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David Live provided several NMR-derived structures of mucin fragments with varying degrees of glycosylation. Each of these was used as the initial structure for at least one molecular dynamics simulation.

There were 48 structures for the unglycosylated peptide. Each was used as the initial structure for an independent simulation.

There were 36 structures for the mannosylated peptide. Each was used as the initial structure for an independent simulation.

There were 16 structures for the N-acetylgalactosylated peptide. Each was used as the initial structure for two independent simulations. The two were given different initial random seeds so that they would sample different conformational spaces.

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The MD Simulations of the Mucin Fragments entailed these steps (see protocols within this project for details).

0. Set up run environment. Make directories, copy files, etc.

1. PDB file preparation. It was necessary to make minor adjustments to the PDB file formats before they could be processed by the pre-simulation software tleap.

2. Generation of topology and input-coordinate files. The PDB files from step 1 were used as input to tleap. This protocol also contains information about force field choice, counter ion insertion and water box size, among others.

3. Molecular dynamics simulations using files generated in step 2.

4. Data curation. The data needed some minor modifications before it would be easily usable.

5. Data analysis. Finally, the data were analyzed in a number of ways.

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