Mucin: 1. PDB file preparation

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The PDB's as received from David Live needed minor modifications before they could be used in tleap (a program used to set up files to be used as starting points for simulations). The steps below describe the modifications made. The modifications are also described in the included script. The script was used to alter the mannosylated and n-acetyl-galactosylated peptides. Analogous steps were performed by hand for the unglycosylated protein. Also attached are sample pdb files before and after for each of the three systems (d4g, d4m and prot).

For all three systems:

1. If any hydrogen atom has the character H as the 13th or 14th character, remove it. It does not conform with the force field's (ff's) templates and will be reinserted in a reasonable location.

2. Change the name of atom CA in ACE to be CH3 (to conform with ff templates).

3. Change the name of the NH2 to NHE (same reason).

For both O-linked peptides:

1. Change the name of residue THR to OLT so that it will be properly treated by the GLYCAM_06h-1 ff.

2. Insert a blank line after the residue NHE.

For the mannosylated peptide:

1. Change the residue name MAN to 0MA (zero-M-A) for compatibility with GLYCAM_06h-1.

2. Insert a blank line after each line in the MAN/0MA reside that contains atom O3 (for proper processing in tleap).

For the n-acetyl-galactosylated peptide:

1. Change the residue name GNC to 0VA (zero-V-A) for compatibility with GLYCAM_06h-1.

2. Insert a blank line after each line in the GNC/0VA reside that contains atom O6 (for proper processing in tleap).

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alter_pdbs.sh

This is the script file used to alter the mannosylated and n-acetyl-galactosylated peptides.
Created: 28 Feb 2013 20:04:50 GMT

prot_fn1.pdb

An original peptide pdb file.
Created: 28 Feb 2013 20:06:42 GMT

prot_fn1_tleap.pdb

A peptide pdb file altered for use in tleap (with the force fields).
Created: 28 Feb 2013 20:07:50 GMT

d4m_fn01.pdb

An original manosylated peptide file.
Created: 28 Feb 2013 20:13:26 GMT

d4m_fn01_tleap.pdb

A mannosylated file altered for tleap.
Created: 28 Feb 2013 20:13:57 GMT

d4g_fn1.pdb

An original n-acetyl-galactosylated file.
Created: 28 Feb 2013 20:14:29 GMT

d4g_fn1_tleap.pdb

An n-acetyl-galactosylated file altered for tleap.
Created: 28 Feb 2013 20:14:59 GMT