Mucin: 2. Generation of Topology and Input-Coordinate Files

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See the run-tleap.sh script. It was used to generate all the tleap input files.

It does these things for each pdb file that was modified per the last step:

1. Copies the pdb file to a temporary name.
2. Runs the appropriate tleap input script (see leapin* files below).
3. Moves the output from tleap to appropriately named files.

It also keeps a key for translating original pdb file names into parmtop and inpcrd file names. At the end, it removes any remaining temporary files.

Created: 19 Apr 2013 17:41:09 GMT , Updated: 22 Apr 2013 19:37:15 GMT

parms.zip

This archive contains all the force field information used for these simulations.
Created: 19 Apr 2013 15:35:23 GMT

leapin

This is the leap input script for the two glycosylated residues.
Created: 22 Apr 2013 19:27:25 GMT

leapin_protein

This is the leap input script for the unglycosylated protein.
Created: 22 Apr 2013 19:28:24 GMT

run_tleap.sh

Created: 22 Apr 2013 19:29:04 GMT