Mucin analysis files

December 23, 2013

I can't find anything...

Here is a list of directories and contents in the ANALYSIS directory. I'll do the GalNAc (d4g) directory first because that has the most stuff in it. If there are significant differences for the Mannose or unglycosylated directories, I can add them later.

GalNAc

/RESEARCH/DLIVE/d4g/ANALYSIS

- **2D_J-Coupling**
  - Directory containing information relevant to the 2D J-coupling calculations. Also contains some binned data.
  - No subdirectories
  - File types:
    - i_j (i and j are numbers)
      Phi and Psi values for position i in run j
    - BINS_i_j
      Binned values for i_j
    - JOUT_i_j
      2D J-coupling values for each pair in i_j
    - JOUT_i_ALL*
      2D J-coupling values at position i for all runs, plus some stats info
    - DATA and GRID are convenient, for doing the 2D calc (are symlinks)
- **ANGLES**
  - Various angle measurements
  - No subdirectories
  - File types:
    - PDB_PhiPsi_all.dat
      phi and psi angles from the original NMR structures
    - Phi_Karplus_i_tj.dat and Theta_Karplus_i_tj.dat
      Phi and Theta angles measured for use in typical (not 2D) J-coupling calcs. Here, for position i and run j.
    - PhiPsi_tj.dat
      Phi and Psi values, both for backbone and glycosidic linkage, for run j. Each of the four positions is included in the one file.

- **DIST**
  Various distance measurements
- **EQUIL**
  - Energetics information to establish equilibration prior to production.
  - One subdirectory
    PLOTS
    Plots of the energetics info
- **GalNAc**
  Various analyses specific to the O-GalNAc'd peptides
- **GalNAc.bak.2013-09-04**
  Old version of the previous. Can probably go now.
- **HBOND**
  Files related to general H-Bond analyses (not shared bonds).
- **JCOUP**
  Output files from standard, 1D J-coupling calculations.
- **MANUAL**
  - Temporary space for manual analysis while I figure out how I want to do something
  - Subdirectories:
    - **old**
    - **ANGLES**
    - **DIST**
    - **THR_back**
- **PDB**
  Information relevant to the pdb files received from David.
- **PhiPsi_Bins**
  Binned Phi-Psi data (protein and sugar) for making plots.
- **PLOTS**
  Files relevant to plots.
- **PTRAJ_INPUTS**
  Files used as input to ptraj or cpptraj.
- **RADIAL**
  Files relevant to radial distribution calculations.
- **RMSD**
  Files relevant to RMSD calculations.
- **SUMMARIES**
  Data summaries that don't seem to go anywhere else.
- **WAT_BOND**
  Analysis related to finding shared/bridging H-bonds with water.