Huge plots of H-bonds in mucins

June 20, 2013

I'm working on option 3 from <u>the previous post</u>.

The HBONDS-Avg* files tell me how many H-bonds were observed in each type of simulation. These aren't all the possible ones, just the observed ones.

I used this to get the numbers:

From /runset/ANALYSIS/HBOND: wc HBONDS-Avg_t* | sort -n

...then take the largest file-length number at left minus 1 (for the table header).

N-acetyl-galactosylated (d4g): 255 hbonds
Mannosylated (d4m): 390
un-glycosylated (protein): 189

Obviously, there are too many to really make into a table. But, those numbers include all h-bonds, even if they are only present in 1 frame out of the many frames considered. So, the next thing is to decide how to choose a cutoff.

Here is a plot showing, in order from highest to lowest, the fraction of the run during which each H-bond was present. This is for simulation number 1 in the d4g runset.

I'm inclined to cut off at around 1% (fract=0.01), at least to start. I can also ignore H-bonds to the end groups. For T1, the combination of those drops the number from 236 total bonds to 70. That moves things back into the realm of graphing possibility.

Bad thing: Apparently, cpptraj doesn't, by default, plot each H-bond per frame. Dammit. So, I'll have to do something else to work around this... Maybe just write a program. Sigh.