

Restarting the mucin analysis

128.192.9.183/elin/lachele/2013/06/20/restarting-the-mucin-analysis

June 20, 2013

Happily, I've had the analysis scripts written for a long time. I've been trying to decide how best to automate calculation of the SDM (standard deviation in the mean). I've also been trying to get that paper written so I can publish it and then reference the technique, but that's another post. I think I'll just use the method I was previously for now (I can change it later if I need to). That is, I find the value where the difference is minimized, using straight-line intercept calculations, between using method 1 and method 2. That should certainly be close enough for this situation. I just need a decent number.

Here are the script files I use for analysis. They should be called from each runset/ANALYSIS directory (see info included with the [first post in this series](#)). Call them in the order listed (the two J-coupling scripts can probably be switched if need be).

1. make cpptraj files for analysis
 - requires runset/cpptraj_setup.bash
 - Also runs cpptraj and ptraj
2. do Karplus
 - calls J-Couplings.pl
3. do 2D J-coupling
 - calls src/extract_data/make_phi_psi_files
 - calls src/2D_JCOUPLING/InterpolateJ
 - requires src/2D_JCOUPLING/grid_x_y_J_12_14
4. do SDM
 - requires runset/REFRESH_SETUP
5. get timings sizes
 - requires runset/REFRESH_SETUP

I just re-ran all the scripts. Next up is figuring out what to do with the H-bonding information. Then, I need to make plots.

Regarding the H-bonding analysis, I used information from [this paper](#). Since cpptraj gets the distances between heavy atoms, I used 3.0 Å as the distance cutoff. This is what was suggested by the paper and also cpptraj default. I used 100-180 degrees for the angle limits. These limits are suggested by the paper. cpptraj uses 135 as a default. In [another paper](#), there was a study of H-bonding from a similar simulation. But, they didn't say how they defined H-bonding. So, I'm not sure how to compare to their results.

PS: Wordpress is not good at making mixtures of ordered and unordered lists...

