To-Do list for the bridging water issue

September 18, 2014

I need to do these things to properly deal with the bridging water issue.

1. Determine the extent to which the smaller (~57 ns total) set of frames with waters saved represents the conformational space of the ~1 us worth of frames without the waters saved.
    1. I expect it to be a reasonable representation, particularly of the most populated states, for the GalNAc variants. Since my concern is with the most populated states, that should be ok.
    2. I don't expect it to be sufficient for the Man or unglycosylated variants, but I'm not concerned with them for this problem.
    3. To do this, I essentially have to re-do all the analyses on the smaller set of data. Because I'm tired and busy and this has already taken 3 years, I'll just copy code and make minor changes. The programmer in me shudders at this, but I'll get over it. Even having to do it that way makes my head hurt. There are so many files. Even with docs and scripts, it's a lot. It will be very easy to make mistakes.
        1. After doing the initial H-H vs O-O analysis (see post following this one), it is obvious that this will all go a lot faster if I save a version of the equilibrated data without waters. So, I think I'll do step three first because that step will necessarily generate that sort of file.
2. Calculate the various quantities of interest, particularly j-couplings, for situations with and without the bridging water.
    1. On second thought, the j-couplings might not be that useful. Hard to guess.
3. Save these trajectories from the with-waters frames, without waters (mostly):
    1. All frames from all simulations.
    2. The following also get saved on a per-GalNAc-site basis. That is, there will be at least 4 of each of the following:
        1. All frames within the general 4-way area.
        2. All frames with a bridging water. These get saved with the bridging water.
        3. All frames in the 4-way area without a bridging water.
4. I would like to also run a gas-phase, water-dielectric simulation, and I might do that. If the 4-way is maintained there, then the water is less likely to be maintaining the rigidity of the peptide.