

Bridging waters in the mucin runs

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So... DL will be upset that I'm putzing around even more with this data, but I'm curious about something.

Here's the back-story: Some other researchers did some MD runs and decided that the GalNAc's are held still by waters bridging the NAc's H and the nearest peptide backbone H. I looked through the already-equilibrated equilibration data, where waters were saved, and I do find that there is sometimes a bridging water. However, there is a water there about 38% of the time, but there is a 4-way interaction between the glycosidic O, the backbone O and those two H's 88% of the time.

My question: I wonder if the enhanced diffusive properties of the TIP3P waters are causing a water to be able to slip in that gap more often than one might otherwise expect. I don't know how I can tell this. But, I could calculate relevant J-coupling values for snapshots with and without the bridging water. Depending on the results, I can make a guess whether the water should be there less, or more, often. I still can't know for sure, but I can make more arguments. So, I suspect I'll do that. 😊

Also, I'll look for geometric changes when a bridging water is present.