H-bond analysis for mucins

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Based on a look at H-bonding analysis from one of the GalNAc simulations, using the expanded angle definitions significantly increased the number of H-bonds found. I'm looking at:

/e05/lachele/RESEARCH/DLIVE/d4g/ANALYSIS/HBOND/HBONDS-Avg_t9.dat

...and in the top 20 H-bonds, only two would have made the cpptraj default cutoff of 135 degrees. I suppose that's ok.

There's an awful lot of data. I need to figure out how to summarize it. The point of these simulations is to determine the effect of glycosylation on peptide length/rigidity. So, there are a number of possibilities:

- Count H-bonds of varying types, by fraction:
    - Glycan to attachment THR
    - Glycan to neighboring THR
    - Glycan to other amino acids
    - Glycan to other glycan
    - Amino acid to other amino acid
- Correlate peptide length with H-bonds.

The first option is pretty simple to do. The second one could be done a number of ways. I'm thinking to do this:

1. Do the first option above: Find out which H-bonds are most prevalent across all the simulations and structures for each of the three fragment types.
2. For the top 10 or 20 most populated H-bonds, get the average peptide length for all frames where that bond is populated.
3. Might as well just make a huge plot... On one axis, have each category of H-bond. On the other, have the peptide length (might need to bin just to cut down data hugeness). Put a dot for each length/bond combination.
4. Come up with some sort of scoring function. For example, the average length thing in point 2, above, but maybe something more clever.

I'll do 1-3 for now. I'm really curious about 3.

Also... I do have to address the bonds mentioned in other papers.