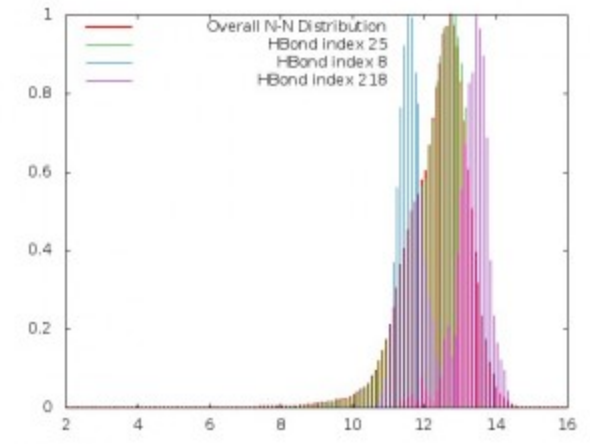
HBond plan making progress

July 7, 2013

Here is an expansion on the earlier post about this. Consider this plot:



This plot shows four distributions, all scaled so that the highest value is 1. The first plot, in red, is the distribution of N-N distances across the entire simulation. You can barely see it because it is almost completely covered by the distribution of distances when HBond "index 25" is present. That is, I took all the observed hydrogen bonds, gave them each a number, and found the N-N distance every time the bond was present. HBond 25 happens to have nearly the same distribution as the N-N distances across the entire simulation. This means that the bond is formed without regard to the N-N distance. And, this makes sense because it is within a single GalNAc residue (#12), and is defined by O4-HO4...O3. Unless there were some unusual hindrances, this bond should break and form independently of the N-N distance, and it appears to do that.

However, HBonds 8 and 218 behave differently. Bond index 8 appears mainly when the N-N distance is lower, while 218 appears mainly when it is higher.

Here are the bond descriptions:

Index	Type	Acceptor	Hydrogen	Donor	Frames	Fraction	Avg. N-N dist.
8	1	0VA_12@O2N	0VA_14@H3O	0VA_14@O3	5488	0.017	11.715
25	4	0VA_12@O3	0VA_12@H4O	0VA_12@O4	93433	0.294	12.399
218	1	0VA_14@O6	0VA_12@H4O	0VA_12@O4	1034	0.003	13.349

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The types are:

0 Glycan to its nearest amino acid
1 Glycan to another Glycan
2 Glycan to some other amino acid
3 Amino acid to another amino acid
4 Glycan to itself
5 Amino acid to itself

Note that 8 & 218 are between two different glycans.