Glycan Stability and Flexibility: Thermodynamic and Kinetic Characterization of Nonconventional Hydrogen Bonding in Lewis Antigens

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Abstract	We provide evidence for CH-based nonconventional hydrogen bonds (H-bonds) for 10 Lewis antigens and two of their rhamnose analogues. We also characterize the thermodynamics and kinetics of the H-bonds in these molecules and present a plausible explanation for the presence of nonconventional H-bonds in Lewis antigens. Using an alternative method to simultaneously fit a series of temperature-dependent fast exchange nuclear magnetic resonance (NMR) spectra, we determined that the H-bonded conformation is favored by similar to 1 kcal/mol over the non-H-bonded conformation. Additionally, a comparison of temperature-dependent 13C linewidths in various Lewis antigens and the two rhamnose analogues reveals H-bonds between the carbonyl oxygen of the N-acetyl group of N-acetylglucosamine and the OH2 group of galactose/fucose. The data presented herein provide insight into the contribution of nonconventional H-bonding to molecular structure and could therefore be used for the rational design of therapeutics.
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