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Conformational Study of Hydroxy Protons in G_{A1} by NMR Spectroscopy

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Investigation of the structure of the gangliosides has proven to be very important in the understanding of their biological roles such as regulation of differentiation and growth of cells. Unexchanged hydroxyl protons and amide protons in ganglioside are protrude farther from the carbon backbone than the C-linked protons and provides nOe contacts with other protons which can provide additional distance constraints in structural determination. Also, they can provide important informations about the hydrogen bondings existed in G_{A1}. A reduction in temperature susceptibility has been commonly accepted as an indicator of reduced interaction with solvent, due to the intramolecular hydrogen bonding. Also, the vanishingly small $^{3}J_{IH3,IOH3}$, $^{3}J_{IVH2,IVOH2}$ coupling constants (< 2 Hz) indicate that these OH protons are involved in strong hydrogen bondings. The NOE contacts including the exchangeable protons provide the long range constraints in structural determination of G_{A1}. We can conclude that ring IV should be stacked underneath the galactose(II) ring, and acetamide group in GalNAc(III) appears to be surrounded by ring II and ring IV. Therefore, G_{A1} have a folded structure even though it does not have sialic acid which forms a stable hydrogen bonding in most of the gangliosides.