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Molecular recognition via hydrogen bonding in glycine with α/β-glucopyranosoide complexes: A DFT and Fourier transform infrared spectroscopy

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Molecular recognition by specific targets is at the heart of the life processes. It has been shown that the interactions between carbohydrates and proteins mediate a broad range of biological activities, starting from fertilization, embryogenesis, and tissue maturation and extending to such pathological processes as tumor metastasis. Glycine is one of the amino acid which fuels cancer cells and rapidly dividing cancer cells require the amino acid glycine but proliferating noncancerous cells did not show this reliance, suggesting that inhibiting cells' ability to take up or metabolize glycine or extracting the glycine from cells may be an effective anticancer strategy. The physicochemical nature of sugar-protein interaction has been a matter of debate for years. Herein, we undertake the DFT calculation to optimize the geometry of n-octyl-α/β-d-glucopyranosid with glycine and used the atoms in molecules (AIM) approach to characterize the nature of the intermolecular hydrogen bonds. Interactions between n-octyl-α/β-d-glucopyranosid and glycine were analysed by temperature-dependent FTIR spectroscopy as well. Our results show that the complex of glycine with glucopyranoside has proved to contain many of the molecular features associated with protein-carbohydrate interactions. All OH groups and the ring oxygen atoms of the bound sugar are involved in the formation of hydrogen bonds. Most of the hydrogen bonds exhibit nearly optimal geometries. The CHs of the sugar chain participate in the formation of the CH…π interactions with the nitrogen of the glycine molecule. Indeed, in the complexes of sugar-binding proteins, all the polar groups (OHs and ring oxygen) of the bound monopyranosides are involved in the formation of hydrogen bonds. We have provided experimental and theoretical evidence on the formation of complexes between glycine with glucopyranoside by arrays of multiple hydrogen bonds. Whilst the hydrogen bonds formed between O-H4 group and the Glycine in these complexes seem to be the strongest in this work, the presence of multiple hydrogen bonds may help stabilise of the complexes.

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