Characterization of π-carbohydrate interaction through molecular dynamics simulations

Woicickoski, C[1,2], Verli, H.[1,2]

[1]Centro de Biotecnologia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil
[2]Faculdade de Farmácia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil

Protein-carbohydrate interactions play important roles in many biologic processes. The carbohydrate recognition may occurs through a series of non covalent interactions between the carbohydrate face and aromatic side chains from amino acid residues, in a π-carbohydrate interaction already investigated through techniques as NMR, IR, molecular modeling and X-ray crystallography. Nevertheless, few data exist explicitly pointing to the contribution of π-carbohydrate interactions to the determination of protein structure, folding and conformation as a part of the molecule conformational ensemble. In this context, the current work intends to characterize the contribution of π-carbohydrate interactions on the secondary structure content and preference in a 12-amino acids peptide model through molecular dynamics simulations in explicit solvent. The simulations were performed using GROMOS96 force field in GROMACS simulation suite during 0.1μs, starting from a completely misfolded molecule. The π-carbohydrate interaction was previously described by NMR techniques to occur in this system between the *O*-linked carbohydrate and the side chain of a Trp residue. Several monosaccharide residues and amino acid side chains were modified in order to evaluate its influence on the peptide conformation. The results obtained demonstrate an adequate folding of the peptide, from a misfolding state, to the solution conformation according to NMR data in the simulation time scale. Additionally, the identification of the influence of π-carbohydrate interactions within the glycopeptides may represent an important contribution in the structural and functional studies of glycoconjugates based on force field calculations. Supported by CNPq Universal (472174/2007-0), CAPES and FAPERGS.

Keyword: Carbohydrate, Molecular dynamics, Protein Folding