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An Insight into the Conformational Dynamics of Glycan through Molecular Dynamics Simulation

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Abstract : Glycan of glycolipids and glycoproteins is playing a significant role in living systems particularly in molecular recognition processes. Molecular recognition processes are attributed to their occurrence on the surface of the cell, sequential arrangement and type of sugar molecules present in the oligosaccharide structure and glyosidic linkage diversity (glycoinformatics) and conformational diversity (glycoconformatics). Molecular Dynamics Simulation study is a theoretical-cum-computational tool successfully utilized to establish glycoconformatics of glycan. The study on various oligosaccharides of glycan clearly indicates that oligosaccharides do exist in multiple conformational states and these conformational states arise due to the flexibility associated with a glycosidic torsional angle (φ,ψ) . As an example: a single disaccharide structure NeuNacα(2-3) Gal exists in three different conformational states due to the differences in the preferential value of glycosidic torsional angles (φ,ψ). Hence establishing three dimensional structural and conformational models for glycan (cartesian coordinates of every individual atoms of an oligosaccharide structure in a preferred conformation) is quite crucial to understand various molecular recognition processes such as glycan-toxin interaction and glycan-virus interaction. The gycoconformatics models obtained for various glycan through Molecular Dynamics Simulation stored in our 3DSDSCAR (3DSDSCAR.ORG) a public domain database and its utility value in understanding the molecular recognition processes and in drug design venture will be discussed.

Keywords : glycan, glycoconformatics, molecular dynamics simulation, oligosaccharide
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