Challenges and Limitations in the Studies of Glycoproteins: A Computational Chemist's Perspective

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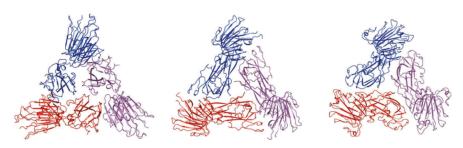
July 1, 2021

Abstract

Experimenters face challenges and limitations while analyzing glycoproteins due to their high flexibility, stereochemistry, anisotropic effects, and hydration phenomena. Computational studies complement experiments and have been used in characterization of the structural properties of glycoproteins. However, recent investigations revealed that computational studies face significant challenges as well. Here, we introduce and discuss some of these challenges and weaknesses in the investigations of glycoproteins. We also present requirements of future developments in computational biochemistry and computational biology areas that could be necessary for providing more accurate structural property analyses of glycopro-teins using computational tools. Further theoretical strategies that need to be and can be developed are discussed herein.

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