

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

Oyku Balli¹, Vladimir Uversky², Serdar Durdagi³, and Orkid Coskuner-Weber⁴

¹Turkish-German University

²University of South Florida

³Bahcesehir Universitesi

⁴Turkish-German University Faculty of Science

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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 glycoproteins using computational tools. Further theoretical strategies that need to be and can be developed are discussed herein.

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