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Inhibitor design for blocking the protein-carbohydrate interactions

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Carbohydrate binding on protein is involved in many important biological processes. In this presentation, we shall report the research progresses in four cases: Inhibitors designed against glycogen phosphorylase via screening million compounds have been experimentally evaluated, leading to nine actives and two crystal complexes, helpful for controlling type 2 diabetes; screening of more than six million compounds against α-glucosidase, followed by molecular dynamics simulations and binding free energy calculations, suggested 10 hits for controlling the concentration of the postprandial blood glucose related to diabetes and the complications; molecular dynamics simulations were applied to the mannose and glucose bindings on flocculation proteins for helping design novel flocculation yeasts to improve yeast brewing production and possible binding modes of inulin on exo-inulinase were studied using Amber, via 100 ns molecular dynamics simulations, for understanding the hydrolysis mechanism and improving the efficiency in food additives and ethanol productions.

Biography

Shijun Zhong has completed his PhD from Xiamen University and Post-doctoral studies from Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences. He is a Professor at Dalian University of Technology. He has published more than 40 papers in reputed journals and has been serving as an Editorial Board Member of repute.

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