



Showcasing research from Professor Cheng's laboratory, Department of Pharmaceutical and Artificial Intelligence Sciences, School of Medicine, Shanghai Jiao Tong University, Shanghai, China.

GlycanInsight: an open platform for carbohydrate-binding pocket prediction and characterization

GlycanInsight is an open platform for carbohydrate-binding pocket prediction and characterization. To provide insight into carbohydrate-protein interaction, it predicts carbohydrate-binding pockets on a protein structure, analyzes pocket characteristics, and suggests putative binding ligands. On the benchmark dataset of experimental structures, GlycanInsight achieves a high Matthews correlation coefficient of 0.63, outperforming existing tools, and maintains robust performance on AlphaFold2-predicted structures. By integrating precise prediction with automated structural annotation and ligand retrieval, GlycanInsight facilitates mechanistic studies and rational design of glycan-targeted therapeutics. The platform is freely accessible at <http://www.glycaninsight.cn/>.

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See Mingyue Zheng, Xi Cheng *et al.*, *Chem. Sci.*, 2025, **16**, 10264.