学术报告

Prediction of drug-protein interactions in the druggable human proteome

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Venue: Room 111, Center for Applied Mathematics

Abstract: Protein-drug interactions drive the therapeutic and undesired effects for a significant majority of the drugs. About 96% of therapeutic targets of drugs are proteins and 93% of all drug-target interactions involve proteins. However, our knowledge of the landscape of drug-protein interactions (DPIs) is very limited. Computational prediction of drug-protein interactions facilitates research in drug discovery, characterization, repositioning and repurposing. This talk surveys modern DPI databases and predictive tools. We focus primarily on similarity-based methods that do not require knowledge of protein structures, allowing for druggable genome-wide predictions of DPIs. We provide an in-depth look 35 high-impact similarity-based predictors that were published in the last decade. We also summarize results of a comprehensive comparative analysis of predictive performance of seven types of representative similarity-based predictors, which relies on a novel benchmark database. Finally, we reveal our new webserver for DPI predictions, CONNECTOR.

欢迎大家参加!