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Comprehensive prediction of drug-protein interactions and side effects for the human proteome

Identifying unexpected drug-protein interactions is crucial for drug repurposing. We develop a comprehensive proteome scale approach that predicts human protein targets and side effect of drugs. For drug-protein interaction prediction, FINDSITEcomb, whose average precision is ~30% and recall ~27%, is employed. For side effect prediction, a new method is developed with a precision of ~57% and a recall of ~24%. Our predictions show that drugs are quite promiscuous with the average (median) number of human targets per drug of 329 (38), while a given protein interacts with 57 drugs. The result implies that drug side effects are inevitable and existing drugs may be useful for repurposing with only ~1,000 human proteins likely causing serious side effects. A killing index derived from serious side effects has a strong correlation with FDA approved drugs being withdrawn. Therefore, it provides a pre-filter for new drug development. The methodology is free to the academic community on the DR. PRODIS (DRugome, PROteome, and DISeasome) webserver at http://cssb.biology.gatech.edu/dr.prodis/. DR. PRODIS provides protein targets of drugs, drugs for a given protein target, associated diseases and side effects of drugs, as well as an interface for the virtual target screening of new compounds. Successful applications of the methodology to treat Chronic Fatigue Syndrome, to identify novel antibiotic leads and promising anti-seizure drugs are described.

Biography

Jeffrey Skolnick is the Director of the Center for the Study of Systems Biology in the School of Biology at the Georgia Institute of Technology, USA. He is also the Mary and Maisie Gibson Chair & Georgia Research Alliance Eminent Scholar in Computational Systems Biology. Among his awards is the SURA 2014 Distinguished Scientist Award, an Alfred P. Sloan Research Fellowship and he is a Fellow of the American Association for the Advancement of Science and the Biophysical Society. He is the author of over 355 publications, has an h-index of 76 and has served on numerous Editorial Boards.

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