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NON-TARGET BASED DRUG DESIGN

Most drugs exert their effects via multi-target interactions, as hypothesized by polypharmacology1. While these multi-target interactions are responsible for the clinical effect profiles of drugs, current methods have failed to uncover the complex relationships between them. Here we introduce an approach which is able to relate complex drug-protein interaction profiles with effect profiles. Structural data and registered effect profiles of all small-molecule drugs were collected and interactions to a series of non-target protein sites of each drug were calculated. Statistical analyses confirmed a close relationship between the effect and interaction profiles. Based on this relationship, the effect profiles of drugs can be revealed in their entirety, and hitherto uncovered effects can be predicted in a systematic manner.