

Research Highlight

Predicting Kinase Inhibitors Using Bioactivity Matrix Derived Informer Sets

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Prediction of compounds that are active against a desired biological target is a common step in drug discovery efforts. Virtual screening methods seek some active-enriched fraction of a library for experimental testing. Where data are too scarce to train supervised learning models for compound prioritization, initial screening must provide the necessary data. Commonly, such an initial library is selected on the basis of chemical diversity or by selecting an entire smaller library.

These approaches may not produce a sufficient number or diversity of actives.

An alternative approach is to select an informer set of screening compounds on the basis of chemogenomic information from previous testing of compounds against a large number of targets. We develop this Informer-Based-Ranking (IBR) approach using the Published Kinase Inhibitor Sets (PKIS) as the chemogenomic data to select the informer sets. Through new chemical screening experiments, we demonstrate the utility of IBR strategies in a prospective test.

Reference:

Zhang, H., Ericksen, S. S., Lee, C. P., Ananiev, G. E., Wlodarchak, N., Yu, P. & Wildman, S. A. (2019). Predicting kinase inhibitors using bioactivity matrix derived informer sets. *PLoS computational biology*, 15(8), e1006813.