

Toward Systems Chemical Biology

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Reductionist approach has been a key factor in the success of modern life sciences. However recently there is a need to also establish a more comprehensive approach to integrate such separately developed components. The increasing availability of data related to genes, proteins and their modulation by small molecules has provided a vast amount of biological information leading to the emergence of systems biology and the broad use of simulation tools for data analysis. However, there is a critical need to develop cheminformatics tools that can integrate chemical knowledge with these biological databases and simulation approaches, with the goal of creating systems chemical biology.

The introduced article is a successful example for the creation of a systems chemical biology platform, and its use for predicting adverse drug effects. The research uses the most complete collection of data sources currently available.

紹介論文

Gaining Insight into Off-Target Mediated Effects of Drug Candidates with a Comprehensive Systems Chemical Biology Analysis

Josef Scheiber, et al. (Novartis Pharma AG, Basel, Switzerland)

J. Chem. Inf. Model. 2009, 49, 308–317

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We present a workflow that leverages data from chemogenomics based target predictions with Systems Biology databases to better understand off-target related toxicities. By analyzing a set of compounds that share a common toxic phenotype and by comparing the pathways they affect with pathways modulated by nontoxic compounds we are able to establish links between pathways and particular adverse effects. We further link these predictive results with literature data in order to explain why a certain pathway is predicted. Specifically, relevant pathways are elucidated for the side effects rhabdomyolysis and hypotension. Prospectively, our approach is valuable not only to better understand toxicities of novel compounds early on but also for drug repurposing exercises to find novel uses for known drugs.

参考論文

Systems chemical biology Tudor I Oprea, et. al. (University of New Mexico)

Nature Chem. Biol, 3,8, 447-450 (2007)