

Predicting Metabolic Side Effects Of Transported Drugs

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BACKGROUND

Drug clearance is the important process by which a drug and/or its metabolites are eliminated from an organism. When drug clearance is excessive, efficacy of the drug may not be achieved; when drug clearance is inadequate, toxicity to the organism may result. Members of the solute carrier (SLC) and ATP-binding cassette (ABC) “drug” transporter families have well-established roles in absorbing, distributing, and eliminating xenobiotics such as drugs. In addition, there is growing evidence for suggesting that these transporters also transport metabolites, nutrients, signaling molecules, and antioxidants at the organismal and cellular levels. Competition of drugs with metabolites at the level of transporters involved in absorption, distribution, and elimination of drugs and metabolites can lead to major metabolic side effects over the long term. Owing to the tremendous clinical importance of these transporters, there is a need to combine metabolic reconstruction (systems biology) methods with computational (pharmaceutical) chemistry, as well as wet lab validation to study these transporters of the SLC and ABC family and drug-induced metabolic changes.

TECHNOLOGY DESCRIPTION

Researchers at the University of California have developed a method of predicting, based on a drug or other small molecule structure, the likely impact on transporter-mediated metabolism. The present invention is able to predict potential competition of drugs with non-drug metabolites in the absorption, distribution and elimination of drugs and metabolites. This would be useful for companies repurposing drugs or prioritizing leads, and possibly, useful clinically to predict metabolic complications in patients on multiple drugs and thus help with choosing the proper drugs in the hospital and clinic. The present invention uses a combination of metabolic reconstruction (systems biology) methods with computational (pharmaceutical) chemistry, as well as wet lab validation.

APPLICATIONS

The invention can be used to evaluate the role of drug transporters in many diseases affecting metabolism, including kidney and liver disease as well as diabetes. It can also be used to predict the consequences of drug-metabolite interactions at the level of the transporter. The invention may also be useful clinically to predict metabolic complications in patients on multiple drugs and thus help with choosing the right drugs in the hospital and clinic environment.

PATENT STATUS

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OTHER INFORMATION

KEYWORDS

drug clearance, pharmacokinetics,
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CATEGORIZED AS

- **Medical**
 - Diagnostics
 - Other
 - Research Tools
 - Therapeutics
- **Research Tools**
 - Other

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