Join us for our webinar

In Silico Transporter Modeling and its Role in Computational Toxicology

Presented by Matt Segall and Gerhard Ecker

Thursday 29 April, 4.00pm UK – 8.00am PDT, 11.00am EDT

Transmembrane Transport Proteins not only play a significant role in ADME, they are increasingly linked to toxicity.
In this webinar, Gerhard Ecker, from Phenaris, will outline computational approaches to predict the transporter interaction profile of compounds to minimise the risk of failures in drug development.

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Matt Segall
Optibrium

Gerhard Ecker
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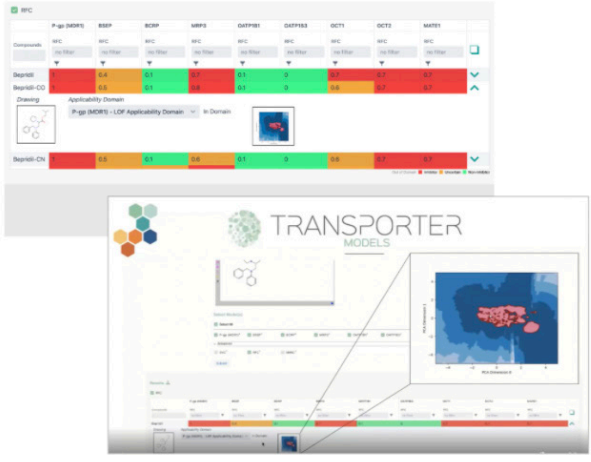
We will present classical machine learning models as well as deep learning approaches, with the latter being applied to overcome insufficient size and imbalance of toxicity datasets. This combined use of structure-based methods for prediction of molecular initiating events and machine learning have led to a model for mitochondrial toxicity.

We will also demonstrate the latest integration of StarDrop with the Phenaris Transporter Model Platform.



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