SimulationsPlus

ADMET Predictor®

AIDD

AI-DRIVEN DRUG DESIGN

The Artificial Intelligence-Driven Drug Design (AIDD) module, as part of our ADMET Predictor platform, automates the drug design process by integrating our advanced generative chemistry algorithms with our best-in-the-industry high-throughput PBPK (powered by the GastroPlus® ACAT model) and ADMET predictions.

Drug Design... Meet PBPK!

- AIDD can generate and evaluate up to 10 million molecules during an overnight run (8-core laptop computer), exploring a large portion of chemical space around the compound(s) or scaffold(s) of interest.
- AIDD also empowers chemistry and DMPK teams to control which part(s) of the molecule may be altered as part of the optimization and which should be maintained. You can also specify positions where substitutions can be applied, and control the chemistry based on synthetic feasibility constraints or a-priori knowledge about the target.
- A full suite of cheminformatics functionality is also included to provide you with the capabilities to visualize and analyze results from AIDD runs at any stage of the design process.

Industry-best ADMET and HT-PBPK predictions

AIDD is fueled by top performance property calculations:

- Top-ranked fully validated ADMET Predictor models
- High-throughput mechanistic PK (HTPK) simulations

Transparent model performance characteristics

For each of our models we provide key information about training sets, test sets, and performance statistics, including confidence estimates. Unlike other companies, you can judge for yourself the quality of each model before relying on the predictions involved in the AIDD generative process.

Incorporation of external models

Have a model that isn't included in our platform? Have a model that you like better than our equivalent? No problem! AIDD makes it easy to integrate your own models as part of the properties used in the multi-parametric optimization

simulations-plus.com/admetpredictor

Interested in collaborating?

Email us! info@simulations-plus.com

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