

Deep Origin deploys AI-powered ADMET models across drug discovery programmes

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Four organisations are using Deep Origin's in silico safety prediction models across millions of compounds, while wet-lab results will feed back into the system to expand model performance.



Deep Origin and partners in the Pharmacological Research and Evaluation through Digital Integration and Clinical Trials Simulation (PREDICTS) consortium announced that their new drug safety prediction models are now being implemented by four organisations in a pilot programme.

The in silico ADMET (absorption, distribution, metabolism, excretion, toxicity) models will be used to assess and filter millions of compounds to prioritise the drug candidates worth advancing.

PREDICTS is part of the Advanced Research Projects Agency for Health (ARPA-H) Computational ADME-Tox and Physiology Analysis for Safer Therapeutics (CATALYST) programme, which is led by Program Manager Michael Patterson.

The programme aims to revolutionise preclinical drug safety prediction by developing human-based models that accurately estimate toxicity and safety profiles for drug candidates.

If successful, CATALYST will enable safer and faster drug development, particularly for rare disease populations. Robust modelling will also capture more representative physiologies and help meet the targets of the U.S. Food and Drug Administration's Modernization Act.

The Deep Origin-led PREDICTS consortium was awarded an up to \$31.7 million Other Transaction Agreement from ARPA-H in 2025 to develop in silico models to more accurately predict drug safety and toxicity.

Now, roughly one year since the start of the work, the first models are in the hands of drug developers.

ADMET-NOW: In silico platform of 77 predictor models for ADME and toxicity

Of the 77 machine learning-based models in development, 62 are now available to pilot participants.

The models predict absorption, distribution, metabolism, excretion and toxicity – the ADMET properties that determine whether a molecule will survive preclinical development.

The four organisations now implementing these models span antivirals, antibacterials, oncology and immune-mediated disease.

ImmVue is developing small molecule, allosteric compounds targeting tyrosine kinases to modulate lymphocyte functions.

Sanford Burnham Prebys is conducting research across cancer, neuroscience, immunology and children's diseases.

Synko is developing broad-spectrum antivirals based on its Synthetic Carbohydrate Receptors small molecule platform.

SyzOnc is developing small molecule modulators of targets that simultaneously control cancer cell proliferation, extracellular matrix architecture and immune cell function in matrix-rich solid tumours.

Public ADMET datasets are small, with a few thousand molecules for most endpoints.

When the ADMET safety models developed by the consortium are tested in partner laboratories, the experimental results will be shared back to assess performance and continue adding to the training data.

"These organizations have computational teams that have chosen to run our predictors because they see their potential," said Natalie Ma, Ph.D., Co-Founder and Chief Business Officer of Deep Origin.

"Because they send their lab results back, every program that uses the models will make the next one better."

Togo foundational chemistry model enables model building across data-sparse scenarios

Every ADMET-NOW model is built on Togo, Deep Origin's foundational chemistry model.

Togo is trained across a wide range of molecular and protein-ligand tasks and produces descriptors that allow a new property model to be trained on fewer than 1,000 data points, which is the situation for many ADMET endpoints.

To date, 62 property-specific models have been developed, with 89% outperforming the best-performing model identified in the literature, including genotoxicity, human ether-à-go-go-related gene inhibition and drug-induced liver injury.

Virtual humans for safety assessment and toxicology prediction as the next frontier

Beyond ADMET-NOW, Deep Origin is developing Virtual Human Avatars of Toxicology to increase the human-relevance of safety predictions in preclinical development.

Deep Origin distinguishes the virtual human from "digital twins", which only infer outcomes from statistical averages of patient parameters.

The virtual human is fine tuned to simulate special populations and biological situations, including physiological traits, comorbidities, mutations and other specific transcriptomic, proteomic or cellular states.

The virtual human uses organ models to simulate the physical and chemical events inside a body to predict drug safety by tracking pharmacokinetics and permeability, liver metabolism, drug and metabolite interactions with proteins, and the impacts of these actions within affected cells.

The organ models are connected rather than running in isolation, because toxicity often manifests as a result of a chain of events.

Liver, kidney, intestine, blood coagulation and bone marrow organ models that make up the virtual human are in advanced development.

"As far as we know, no one has built a mechanistic model of a whole human body for toxicology," said Michael Antonov, Co-Founder and Chief Executive Officer of Deep Origin.

"The Deep Origin team is making great progress building a virtual human with ARPA-H's support."

The PREDICTS consortium is led by Deep Origin and includes Ginkgo Bioworks, ImmVue Therapeutics, MIDO LLC, Netrias, Sanford Burnham Prebys and Tessel Biosciences.

Additional specialists span computational biology, toxicology and drug development.