

Predictive Toxicology Software

Supporting prediction of drug-induced liver injury (DILI), QT risk, and off-target safety

Certara ToxStudio[®] is an intuitive, integrated suite of powerful in silico toxicology software tools that enables pharmaceutical, biotech, chemical, and agrochemical companies to rapidly answer “what-if?” questions, predict toxicological outcomes, assess compound safety, and generate regulatory-ready reports.

Make informed decisions with data-driven insights

Reduce reliance on animal testing

Streamline toxicology workflows

Modernizing preclinical safety



The challenge

Safety-related attrition continues to be a challenge in drug discovery and development. Existing options include investing in costly in vitro and/or in vivo studies, or waiting to find out in the clinic.



The solution: Certara ToxStudio

ToxStudio integrates innovative safety and toxicology platforms that use advanced analytics to minimize reliance on traditional in vivo testing which accords with the FDA's 2025 roadmap on New Approach Methodologies (NAMs).

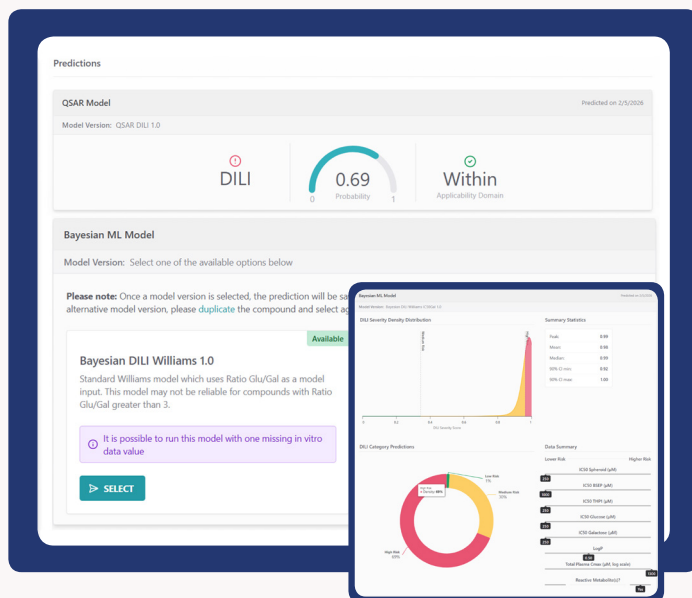
Software tools in ToxStudio

CERTARA[®] Libra[™]

AI-powered drug-induced liver injury (DILI) prediction software

Key features:

- **AI-powered QSAR (quantitative structure-activity relationship) modeling:** Identifies DILI hazards even before compound synthesis to prioritize safer chemical leads
- **Bayesian predictive model:** Integrates physicochemical data and in vitro assay data to flag potential DILI risks early

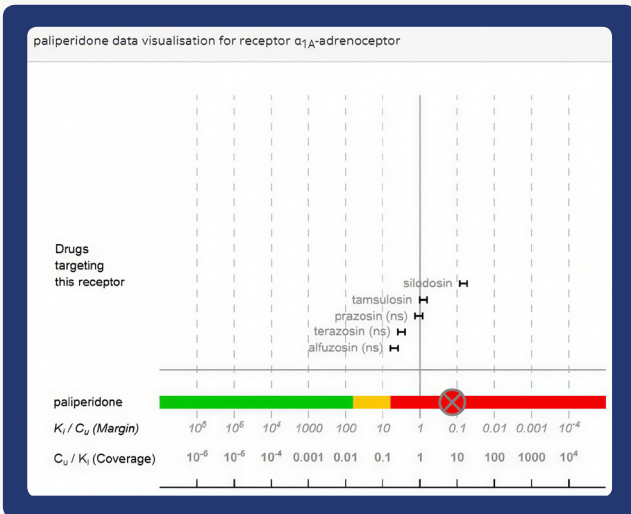


CERTARA[®] Secondary Intelligence[™]

Software to predict and analyze off-target pharmacology risks from secondary pharmacology screening assay data

Key features:

- **Extensive drug and receptor library:** Expertly curated list of over 1400 reference drugs and a consistent approach applied across 111 receptors to date, including full coverage of the consensus Bowes panel
- **Visualize quantitative analyses:** Compare test compound to reference drugs and evaluate likelihood of interaction at individual receptors with 'traffic light' visualization
- **Mechanistic insight:** More than 300 mechanistic safety pathways of note-worthy side effects associated with receptor interactions

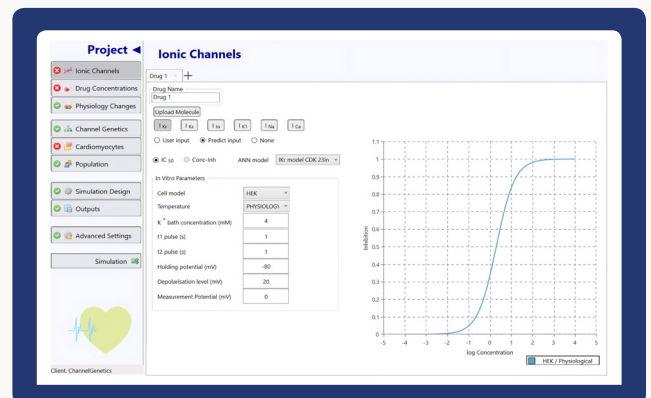


CERTARA[®] Cardiac Safety Simulator

Modeling & simulation platform to predict QT prolongation, available as a consultancy service

Key features:

- **QSAR modeling:** Predicts ion channel current inhibition with only the chemical structure
- **Advanced precision:** Evaluate up to 7 chemical entities (co-medications; metabolites)



Request a demo or contact us for more information

See ToxStudio in action



About Certara

About Certara Certara accelerates medicines using proprietary biosimulation software, technology and services to transform traditional drug discovery and development. Its clients include more than 2,600 biopharmaceutical companies, academic institutions and regulatory agencies across 70 countries. Visit certara.com | Copyright ©2026 Certara. All rights reserved.