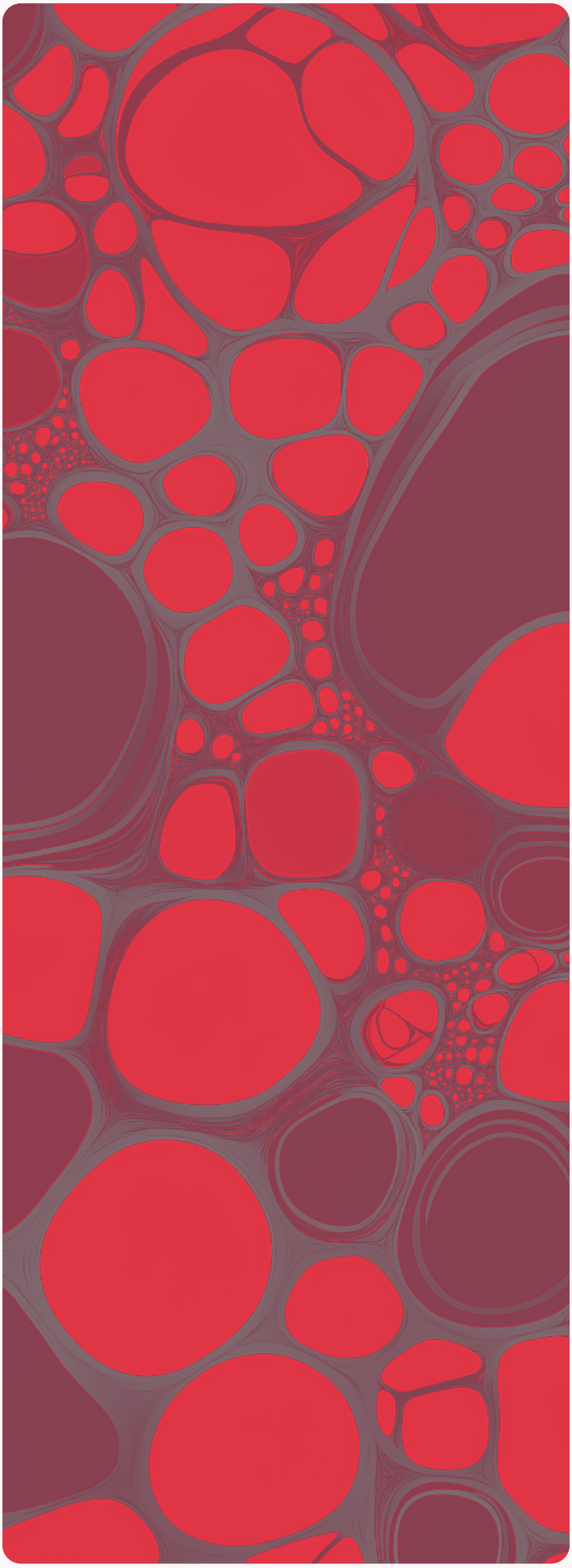

CERTARA

Simcyp™ PBPK Simulator

The Gold Standard in Population-based Physiologically Based Modeling and Simulation

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Simulate and Predict Drug Exposure

The Simcyp PBPK Simulator is the industry leader and most widely adopted platform for physiologically based pharmacokinetics (PBPK) modeling in drug development. Developed in collaboration with a consortium of 35+ of the top pharmaceutical companies worldwide, the Simcyp PBPK Simulator predicts drug behavior within the human body, aiding in various stages throughout drug R&D. This includes predicting first-in-human dose, optimizing clinical study designs, evaluating new drug formulations, predicting drug-drug interactions, and conducting virtual bioequivalence analyses.

10+ Global regulatory agencies that use the Simcyp PBPK Simulator

120+ FDA-approved novel drugs supported using the Simcyp PBPK Simulator in lieu of clinical studies

80% FDA-approved novel drugs leveraging PBPK in recent years used Simcyp

Key Areas of Application

The Simcyp PBPK Simulator can be used throughout the drug discovery and development processes and applied to small molecules, biologics, ADCs, generics, and new modality drugs.

- First-in-human dose prediction
- Drug-drug interaction assessment – perpetrator and victim
- Dosing for specific populations – pediatrics, elderly, organ impairment, disease conditions, ethnic differences
- Absorption, food effect and formulation assessment
- Label claims in lieu of clinical studies and optimizing clinical study design
- Virtual bioequivalence analysis and formulations for complex generics
- Compound due diligence/risk analysis
- Evaluation of the impacts of extrinsic factors such as smoking and alcohol on drug performance
- Novel routes of administration – dermal, inhalation, long-acting injectable

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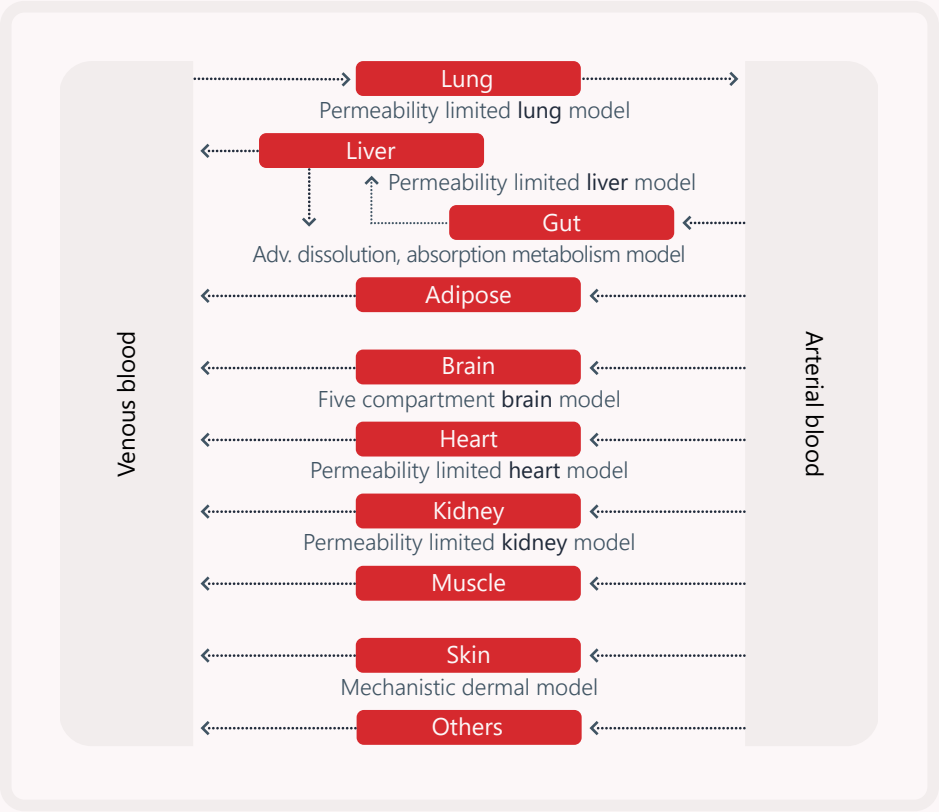
The Simcyp Difference

Simcyp PBPK models describe the behavior of drugs in relevant body tissues and organs. Each organ may be described by one or several physiological compartments. The concentration of the drug in each compartment is determined by combining systems data, drug data, and trial design information. The Simcyp PBPK Simulator includes a unique set of genetic, physiological and epidemiological databases that facilitate simulating virtual populations with different demographics, ethnicities, and disease states.

The Simcyp PBPK Simulator has the most advanced organ-specific PBPK models, driving use for a variety of applications from discovery to post-marketing.

The Simcyp PBPK Simulator is also accessible via our tech-enabled services. Certara's global Simcyp PBPK services team has 200+ years of combined experience using the Simcyp PBPK Simulator to support drug development and regulatory approval processes.

Additionally, the Simcyp PBPK Simulator is a part of full suite of PBPK solutions, including two additional platforms: Simcyp Discovery and Simcyp Biopharmaceutics.



Key Features

- Extensive libraries on demographics, developmental physiology, and drug elimination pathways.
- Advanced mechanistic organ models and compound files.
- Integrates in vitro data with in vivo outcomes to support informed decision making.
- Virtual population simulations reflect diverse demographics, ethnicities, and disease states.
- Includes 29 population libraries and over 100 small and large molecule models.
- Availability to support compound and population verification documents for regulatory submissions.

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Simcyp PBPK Simulator Version 24 Enhancements

Each year, new features and capabilities are added to the Simcyp PBPK Simulator. These feature enhancements are prioritized based in part on guidance from our scientific advisory board and consortium members, but also in recognition of trends in the regulatory and pharmaceutical R&D landscapes.

Biopharmaceutical capabilities and VBE module

Updated and expanded to include new features for predicting drug products food effects. Including refining gastric emptying model, a gastric emptying covariate model, a fast stomach emptying (Magenstrasse) model, and a drug-lipid interaction model, all aimed at improving the simulation of drug absorption under various meal conditions.

Expanded library for DDI

Version 24 includes new and upgraded compound files for enzymes and transporters for broader DDI capabilities. Further, providing qualification documentations for transporter-mediated DDI in the gut, liver and kidney.

Enhanced support for Biologics

Version 24 incorporates movement of soluble targets and drug-target complexes throughout the body and extending the target shedding model, enabling the specification of membrane-bound targets across various tissues and within plasma. Furthermore, a TMDD model is implemented for small molecules.

Expanded Trial Design support

New features to enhance speed and ease of use for designing and simulating clinical trials.

Specific Populations modeling

Enhanced capabilities for pediatric, pregnancy, and lactation populations.

Performance and Usability

Modernized UI, cloud computing add-on, Ask Simcyp help chat, and incorporating chemical structure based predictors.

Routes of Administration

Improved functionality for long-acting injectables, inhalation, and ocular routes.

Simcyp Expansions

Further to the work of the Simcyp Consortium, the Certara Simcyp team develops specialized modules that are connected to the Simcyp PBPK Simulator and require additional licensing.

- Simcyp Animal
- Simcyp Pediatric
- Simcyp In Vitro Analysis (SIVA) Toolkit
- Simcyp Long Acting Injectable (LAI)
- Simcyp Lactation
- Virtual Bioequivalence
- Simcyp Biologics
- Simcyp Designer

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Trusted by Industry, Academic, and Regulatory leaders

Since 2001, the Simcyp Consortium has served as a collaborative research center for PBPK and mechanistic modeling. In addition to its 35+ industry members, leading academic institutions from around the globe, and 11 regulatory bodies, including the US Food and Drug Administration are affiliates of the Consortium.

Members gain access to the latest version of the Simcyp PBPK Simulator, guide its ongoing development, and benefit from Simcyp experts' advice, training, and educational programs. Hundreds of peer-reviewed papers are based on the Simcyp PBPK Simulator, demonstrating its impact in drug development, clinical pharmacology, toxicology and other key scientific areas.

Smaller companies can gain access to the Simcyp PBPK Simulator via licensing or consulting services, without needing to join the Consortium.

PBPK Modeling used to Support Label Claims

120+ novel drugs used the Simcyp PBK Simulator in lieu of clinical studies across a variety of modalities and therapeutic areas.

Oncology

AbbVie	Venclexta *(venetoclax)*
Agios	Tibsovo *(ivosidenib)*
Amgen	Blincyto *(blinatumomab)*
Amgen	Lumakras *(sotorasib)*
Ariad	Alunbrig *(brigatinib)*
Ariad (Takeda)	Iclusig *(ponatinib)*
AstraZeneca	Calquence *(acalabrutinib)*
AstraZeneca	Lynparza *(olaparib)*
AstraZeneca	Tagrisso *(osimertinib)*
AstraZeneca	Truqap® *(capivaserib)*
Beigene	Brukinsa *(zanubrutinib)*
Biohaven	Nurtec *(rimegepant)*
BluePrint Medicines	Ayvakit *(avapritinib)*
Celgene	Inrebic *(fedratinib hydrochloride)*
Daiichi Sankyo	Turalio *(pexidartinib)*
Daiichi Sankyo	Ezharmia *(valmetostat tosilate)*
Daiichi Sankyo	Vanflyta® *(quizartinib dihydrochloride)*
Deciphera	Qinlock *(ripretinib)*
Eisai	Lenvima *(lenvatinib)*
EMD Serono	Tepmetko *(tepotinib hydrochloride)*
Genentech	Alecensa *(alectinib)*
Genentech	Cotellic *(cobimetinib)*
Genentech	Gavreto® *(pralsetinib)*
Genentech	Polivy *(polatuzumab vedotin-piiq)*
Genentech	Rozlytrek *(entrectinib)*
Incyte	Pemazyre *(pemigatinib)*
Janssen	Balversa *(erdafitinib)*
Janssen	Lazcluze *(lazertinib)*
Janssen	Erleada *(apalutamide)*
Lilly	Retevmo *(selpercatinib)*
Lilly	Verzenio *(abemaciclib)*
Loxo	Jaypirca *(pirtobrutinib)*
Loxo Oncology	Vitrakvi *(larotrectinib)*
Menarini/Stemline	Orserdu *(elacestranto)*
Mirati	Krazati *(adagrasib)*
Novartis	Farydak *(panobinostat)*
Novartis	Kisqali *(ribociclib succinate)*
Novartis	Scemblix *(asciminib)*
Novartis	Odomzo *(sonidegib)*
Novartis	Vijoice *(alpelisib)*
Novartis	Rydapt *(midostaurin)*
Novartis	Tabrecta *(capmatinib)*
Novartis	Zykadia *(ceritinib)*
Novartis	Jakavi *(ruxolitinib)*
Pfizer	Daurismo *(glasdegib)*
Pfizer	Ibrance® *(palbociclib)*
Pfizer	Bosulif *(bosutinib)*
Pfizer	Lorbrena *(lorlatinib)*
Pharmacyclics	Imbruvica *(ibrutinib)*
PumaDiabetic	Nerlynx® *(neratinib)*
Sanofi	Jevtana *(cabazitaxel)*
Seattle Genetics	Tukysa *(tucatinib)*
Servier	Voranigo *(vorasidenib)*
Spectrum	Beleodaq *(belinostat)*
Springworks	Ogsiveo® *(nirogancent)*
Takeda	Exkivity *(mobocertinib)*

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Oncology continued

Takeda	Fruzaqla® *(fruquintinib)*
Taiho	Lytgobi *(futibatinib)*
Verastem	Copiktra *(duvelisib)*

Rare Disease

Agios	Pyrukynd *(mitapivat)*
AkaRx (Eisai)	Doptelet *(avatrombopag maleate)*
AstraZeneca	Koselugo *(selumetinib)*
Aurinia	Lupkynis *(voclosporin)*
Genentech	Enspryng *(satralizumab)*
Genentech	Evrysdi *(risdiplam)*
Global Blood Therapeutics	Oxbryta *(voxelotor)*
Intercept	Ocaliva *(obeticholic aciNined)*
Ipsen	Sohonus® *(palovarotene)*
Kadmon	Rezurock *(belumosudil)*
Merck	Welireg *(belzutifan)*
Mirum	Livmarli *(maralixibat)*
Mitsubishi Tanabe	Dysval *(valbenazine)*
Novartis	Isturisa *(osilodrostat)*
Peloton/Merck	Welireg *(belzutifan)*
PTC Therapeutics	Emflaza *(deflazacort)*
Sanofi Genzyme	Cerdelga *(eliglustat tartrate)*
Sun Pharmaceutical Inc.	Leqselvi *(deuruxolitinib)*
Travere	Filspari *(sparsentan)*
Vertex	Symdeko *(tezacaftor/ivacaftor)*
Vertex	Trikafta *(elexacaftor/ivacaftor/tezacaftor)*

Central Nervous System

AbbVie	Rinvoq *(upadacitinib)*
AbbVie	Qulipta *(atogepant)*
Alkermes	Aristada *(aripiprazole lauroxil)*
Alkermes	Lybalvi *(olanzapine/samidorphan)*
Eisai	Dayvigo *(lemborexant)*
Idorsia	Quviviq *(daridorexant)*
Janssen	Ponvory *(ponesimod)*
Kyowa Kirin	Nourianz *(istradefylline)*
Lilly	Reyvow *(lasmiditan succinate)*
Novartis	Mayzent *(siponimod fumaric acid)*
Pfizer	Zavzpret *(zavegepant)*
UCB	Briviact *(brivaracetam)*

Infectious Disease

Gilead	Veklury *(remdesivir)*
Janssen	Olysio *(simeprevir)*
Merck	Pifeltro *(doravirine)*
Merck	Prevymis *(letermovir)*
Nabriva	Xenleta *(lefamulin acetate)*
Novartis	Egaten *(triclabendazole)*
Pfizer	Paxlovid® *(nirmatrelvir, ritonavir)*
Tibotec	Edurant *(rilpivirine)*
ViiV	Cabenuva Kit *(cabotegravir/rilpivirine)*

Gastroenterology

AstraZeneca	Farxigo *(dapaglifoxin)*
AstraZeneca	Movantik *(naloxegol)*
Helsinn	Akynzeo *(fosnetupitant/palonosetron)*
Phathom	Voquezna TriplePak *(vonoprazan/amoxicillin/clarithromycin)*
Shionogi	Symproic *(naldemedine)*
Shire	Motegrity *(prucalopride)*

Cardiovascular

Actelion (J & J)	Opsumit *(macitentan)*
BMS	Camzyos *(mavacamten)*
Johnson & Johnson	Xarelto *(rivaroxaban)*
Pfizer	Revatio *(sildenafil)*

Endocrine

AbbVie	Orilissa *(elagolix)*
Astellas	Veozah® *(fezolinetant)*
Esperion	Nexetol *(bempedoic acid)*
Janssen	Invokana *(canagliflozin)*
Lilly	Olumiant *(baricitinib)*
Lilly	Mounjaro *(tirzepatide)*
Merck	Steglatro *(ertugliflozin)*

Other

Galderma	Aklief *(trifarotene)*
Gilead	Livdelzi *(seladelpar)*
Takeda	Livtencity *(maribavir)*

Learn more about Simcyp: Advanced technology solutions support all PBPK applications

Learn more

About Certara

Certara accelerates medicines using proprietary biosimulation software, technology and services to transform traditional drug discovery and development. Its clients include more than 2,000 biopharmaceutical companies, academic institutions and regulatory agencies across 70 countries.