

# Resource Summary Report

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## Simulations Plus

RRID:SCR\_003946

Type: Tool

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### Proper Citation

Simulations Plus (RRID:SCR\_003946)

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### Resource Information

**URL:** <http://www.simulations-plus.com/>

**Proper Citation:** Simulations Plus (RRID:SCR\_003946)

**Description:** Commercial developer of Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) and Physiologically-Based Pharmacokinetic (PBPK) modeling and simulation software for the pharmaceutical and biotechnology, industrial chemical, cosmetic, herbicide, and food ingredient industries. Their software allows pharmaceutical scientists to predict certain key potential endpoints and dynamics, in silico, thereby reducing research & development costs and helping clients make better projects decisions sooner. Consulting services: Their team of highly-skilled scientists is available to assist with your discovery and development activities on a project-by-project basis. They now offer expanded pharmacodynamic modeling services, NONMEM analysis, and regulatory report writing assistance. Their ultimate goal is to develop tools and systems which bridge PBPK modeling with clinical trial data analysis. Training workshops & User Groups: they offer hands-on introductory and advanced training workshops in the United States, Europe, and Asia throughout the year.

**Synonyms:** Simulations Plus Inc.

**Resource Type:** commercial organization

**Keywords:** pharmaceutical, modelling, simulation, pharmacodynamic, biotechnology, chemical, cosmetic, food ingredient, herbicide, drug development, drug, pharmacokinetic

**Funding:**

**Availability:** License required

**Resource Name:** Simulations Plus

**Resource ID:** SCR\_003946

**Alternate IDs:** nlx\_158339, ISNI: 0000 0004 0506 5380, grid.418738.1, Wikidata: Q7521341

**Alternate URLs:** <https://ror.org/02p0yhm49>

**Record Creation Time:** 20220129T080221+0000

**Record Last Update:** 20250420T014159+0000

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## Ratings and Alerts

No rating or validation information has been found for Simulations Plus.

No alerts have been found for Simulations Plus.

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## Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We found 32 mentions in open access literature.

**Listed below are recent publications.** The full list is available at [FDI Lab - SciCrunch.org](#).

Pansari A, et al. (2024) A tutorial on physiologically based pharmacokinetic approaches in lactation research. CPT: pharmacometrics & systems pharmacology, 13(11), 1841.

Chaturvedi K, et al. (2023) Identification of the Putative Binding Site of a Benzimidazole Opioid (Etazene) and Its Metabolites at  $\mu$ -Opioid Receptor: A Human Liver Microsomal Assay and Systematic Computational Study. Molecules (Basel, Switzerland), 28(4).

Komura H, et al. (2023) The Trends and Future Prospective of In Silico Models from the Viewpoint of ADME Evaluation in Drug Discovery. Pharmaceutics, 15(11).

Yuan Y, et al. (2023) Pharmacokinetics of Novel Furoxan/Coumarin Hybrids in Rats Using LC-MS/MS Method and Physiologically Based Pharmacokinetic Model. Molecules (Basel, Switzerland), 28(2).

Scior T, et al. (2023) Targeting the Human Influenza a Virus: The Methods, Limitations, and Pitfalls of Virtual Screening for Drug-like Candidates Including Scaffold Hopping and Compound Profiling. Viruses, 15(5).

Frechen S, et al. (2022) Quality Assurance of PBPK Modeling Platforms and Guidance on Building, Evaluating, Verifying and Applying PBPK Models Prudently under the Umbrella of Qualification: Why, When, What, How and By Whom? *Pharmaceutical research*, 39(8), 1733.

Punt A, et al. (2022) Predictive Performance of Next Generation Physiologically Based Kinetic (PBK) Model Predictions in Rats Based on In Vitro and In Silico Input Data. *Toxicological sciences : an official journal of the Society of Toxicology*, 186(1), 18.

Ooka M, et al. (2022) Identification of environmental chemicals that activate p53 signaling after in vitro metabolic activation. *Archives of toxicology*, 96(7), 1975.

Koczurkiewicz-Adamczyk P, et al. (2022) Cinnamamide derivatives with 4-hydroxypiperidine moiety enhance effect of doxorubicin to cancer cells and protect cardiomyocytes against drug-induced toxicity through CBR1 inhibition mechanism. *Life sciences*, 305, 120777.

Acquah FA, et al. (2021) Simulations of Promising Indolizidine- $\alpha$ - $\beta$  Nicotinic Acetylcholine Receptor Complexes. *International journal of molecular sciences*, 22(15).

Alagumuthu M, et al. (2021) Structure-Based Design of Novel Peptidomimetics Targeting the SARS-CoV-2 Spike Protein. *Cellular and molecular bioengineering*, 14(2), 177.

Krzywik J, et al. (2021) An insight into the anticancer potential of carbamates and thiocarbamates of 10-demethoxy-10-methylaminocolchicine. *European journal of medicinal chemistry*, 215, 113282.

Fatima K, et al. (2021) Neomenthol prevents the proliferation of skin cancer cells by restraining tubulin polymerization and hyaluronidase activity. *Journal of advanced research*, 34, 93.

Rajpoot S, et al. (2021) Dual targeting of 3CLpro and PLpro of SARS-CoV-2: A novel structure-based design approach to treat COVID-19. *Current research in structural biology*, 3, 9.

Tsantili-Kakoulidou A, et al. (2021) Drug-like Properties and Fraction Lipophilicity Index as a combined metric. *ADMET & DMPK*, 9(3), 177.

Rácz A, et al. (2021) Machine learning models for classification tasks related to drug safety. *Molecular diversity*, 25(3), 1409.

Djokovic N, et al. (2021) An Integrative in silico Drug Repurposing Approach for Identification of Potential Inhibitors of SARS-CoV-2 Main Protease. *Molecular informatics*, 40(5), e2000187.

Krache A, et al. (2021) Preclinical Pharmacokinetics and Dosimetry of an  $^{89}\text{Zr}$  Labelled Anti-PDL1 in an Orthotopic Lung Cancer Murine Model. *Frontiers in medicine*, 8, 741855.

Wu F, et al. (2020) Computational Approaches in Preclinical Studies on Drug Discovery and Development. *Frontiers in chemistry*, 8, 726.

Clark RD, et al. (2020) Design and tests of prospective property predictions for novel antimalarial 2-aminopropylaminoquinolones. *Journal of computer-aided molecular design*, 34(11), 1117.