

PBPK Modeler / Computational Toxicologist III

ScitoVation is the premier startup company for scientists who want to explore cutting-edge research and make a significant impact in the toxicology industry. You will be part of a highly-sought-after team of thought leaders and collaborators who are dedicated to finding innovative solutions to assess the safety of chemicals and products. Our team is driven by using the best science in chemical safety to improve risk assessment and decision making for clients. We are also at the forefront of developing next generation new approach methodologies (NAMs) and spearhead the efforts required to get key-stakeholder buy in ranging from regulatory bodies to pharma organizations. It's an exciting time to join our organization with many companies prioritizing Next Generation Risk Assessment and few that deliver on its requirements. With a vision of being THE trusted source in chemical safety & assessment – while elevating human and environmental health and well-being, do you have what it takes to join our team and make your mark?

Job Overview:

ScitoVation is a small research and development team with the mission of developing and implementing approaches to revolutionize the way we understand the impact of chemicals on our health. We work with companies---both Fortune 500 and smaller groups--to help with decision making about what chemistries are appropriate for their products. While animal testing is the de facto standard for establishing chemical safety, our team is building computational and cell-based methods for safety assessment that are more economical and more relevant to human health.

As a PBPK modeler/Computational Toxicologist, you will be responsible for developing groundbreaking research to achieve this mission. Your expertise in physiologically based pharmacokinetic (PBPK) modeling and scientific programming will advance the science in non-animal toxicology testing. You will help our partners leverage pharmacokinetic modeling, bioinformatics, computational biology, cheminformatics, and data science to advance their research programs and their product stewardship goals. Your collaborations with our in vitro assay development team will create creative, integrative approaches to chemical safety testing in a research environment that is truly unique.

ScitoVation is recognized as having a high level of expertise in PBPK modeling that brings value to the client. As a PBPK modeler, you will be part of a multidisciplinary team working on the development of models that best fit the client needs. You will help predict exposure from one species to another, capture human variability by including Monte Carlo analysis in pharmacokinetic models, estimate a response from varying exposure conditions and across life-stages or vulnerable populations, such as children, the elderly, or those working in specific occupations. You will also perform route-to-route extrapolation, conduct high-dose to low-dose extrapolation to predict concentration in blood and tissue for exposure at different doses and estimate population daily exposure intakes that are consistent with blood or urine measures found in biomonitoring surveys by doing reverse dosimetry. In addition, you will employ pharmacodynamics (PD) models coupled with PBPK models to predict both dose-response and time-course for the development of adverse effects.

Accountable for:

- 1. Executing high-quality scientific research in PBPK modeling consistent with ScitoVation's vision
- 2. Planning, designing, developing, and applying pharmacokinetic and PBPK models—as well as in vitro to in vivo extrapolation (IVIVE)—to solve real-world chemical risk assessment challenges.
- 3. Applying bioinformatics, pharmacokinetics, biological models, data science, and biostatistics to support human safety and risk assessment of chemicals and drugs
- 4. Interpreting in vitro ADME studies, mammalian pharmacokinetic and metabolism studies



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- 5. Using scientific programming expertise to develop scripts to manipulate, analyze, and integrate big data from a variety of resources, both internal and external.
- 6. Developing computational pipelines for implementing dosimetry models utilizing best-practices approaches implemented in scientific programming languages such as R and python.
- 7. Scientific communication with clients providing expertise and developing business opportunities
- 8. Contributing to publications in high-quality scientific and technical journals
- 9. Formulating, articulating and critically evaluating scientific hypotheses
- 10. Identifying and integrating relevant internal and external data and knowledge resource to enable data mining in biological context
- 11. Analyzing biological data; curating reference datasets and annotations
- 12. Building prototype tools for analysis and data sharing

Education and Experience:

Master's Degree or PhD in a relevant field (e.g., toxicology, engineering, mathematics, biology, bioinformatics, molecular biology) with two years of post-graduate research experience in an academic, government, and/or industry position.

Hands-on knowledge of PBPK modeling.

Systems biology expertise, a general knowledge of cell and molecular biology, and understanding of the general principles of pharmacokinetic modeling, RNA sequencing, structure-activity relationships, and other computational toxicology techniques

Demonstrated proficiency with relevant general-purpose coding languages, such as R.

Familiarity with simulation languages commonly used in PBPK modeling (e.g., Berkeley Madonna, PKSim, GastroPlus, and/or Matlab).

Familiarity with team-based software tools

Competencies and Behaviors:

- Experience developing, parameterizing, and validating physiologically based pharmacokinetic (PBPK)
 modeling; employing PBPK models for chemical safety decision making applications, including forward
 dosimetry, species-to-species extrapolation, and in vitro-to-in vivo extrapolation.
- A working understanding of the principles of toxicology and risk assessment.
- Excellent scientific programming skills, with experience employing tools including R, python, JavaScript, and MySQL for solving computational challenges.
- Excellent writing, organization, and verbal communication skills
- Inherently creative, able to bring fresh ideas to his/her own work and the work of others
- Self-motivated and willing and able to take a primary leadership role in one or more projects
- Capable and comfortable with critically evaluating the ideas and work of themselves and of others
- Effectively communicate and work with stakeholders with disparate career backgrounds and motivations
- Detail conscious, organized
- Excellent time management skills
- Anticipate problems and implement mitigation strategies
- Efficient, driven, willing to go the extra mile
- Positive team player and collaborator