XINNONG LI

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EDUCATION

Ph.D. of Pharmaceutical Sciences *05/2023 - 12/2026 (Expected)*
University at Buffalo, Buffalo, United States | GPA: 3.95/4.0

Master of Pharmacometrics and Personalized Pharmacotherapy *08/2021 - 05/2023*
University at Buffalo, Buffalo, United States | GPA: 4.0/4.0

Bachelor of Pharmacy *09/2016 - 07/2020*
Shenyang Pharmaceutical University, China | GPA: 3.66/4

RESEARCH EXPERIENCE

Machine Learning Enhanced Nonlinear Mixed-effect Model Selection Project *12/2022 - Present*
Ph.D. Thesis Project

- Designed the experiments to test the pyDarwin toolbox in single-objective nonlinear mixed-effect (NLME) model selection
- Contributed to the test and development of multi-objective optimization method in pyDarwin toolbox
- Evaluated the robustness and efficiency of all plug-in machine learning algorithms in pyDarwin package
- Successfully shortened the time in building NLME models from days to hours while ensuring the model robustness (validated against exhaustive search results) in user-defined search space

Female Reproductive Tract (FRT) Physiologically-based Pharmacokinetic Model Project *06/2023 - Present*
Ph.D. Thesis Project

- Developed and validated the Physiologically-based Pharmacokinetic (PBPK) model that includes uterine, cervical and vaginal spaces using the mrgsolve package in R
- Further expanded model structure to include fallopian tubes
- Participated in the building and optimization of R Shiny App of the FRT PBPK model
- Applied the general FRT PBPK model platform in simulating new compounds drug exposure

Drug Release Kinetic Model of Long-acting IUD *03/2024 - Present*
Ph.D. Thesis Project

- Developed in vitro drug release kinetic model of levonorgestrel (LNG) intrauterine devices (IUD) (Mirena, Kyleena, Skyla) using piecewise linear model
- Compared the combinations of various kinetic models and successfully plugged them in PBPK models and elevated the simulation accuracy

HPTN 083/084 Population Pharmacokinetic Model Project *01/2022 - 08/2022*
Master Thesis Project

- Developed population PK model of long-acting injectable cabotegravir (CAB-LA) in cisgender women, cisgender men, and transgender women populations based on HPTN 083/084 clinical trial data
- Evaluated the CAB-LA case-control drug exposure (e.g. area under curve (AUC)) within specific timeframes

PROFESSIONAL EXPERIENCE

Clinical Pharmacology and Pharmacometrics Intern *05/2025 - 08/2025*
Johnson and Johnson Innovatice Medicine

- Established base population pharmacokinetic (PopPK) model that can describe the CAR-T kinetic profiles using in-house clinical datasets
- Applied machine learning approach to identify covariates that contribute to the high variability of CAR-T therapy in vivo kinetics
- Established in-house pyDarwin platform for further exporation

PUBLICATIONS

Clinical Pharmacology and Therapeutics (2024)

- **Li X**, Sale M, Nieforth K, Bigos KL, Craig J, Wang F, Feng K, Hu M, Bies R, Zhao L. "pyDarwin: A Machine Learning Enhanced Automated Nonlinear Mixed-Effect Model Selection Toolbox" https://doi.org/10.1002/cpt.3114.

Journal of Pharmacokinetics and Pharmacodynamics (2024)

- **Li X**, Sale M, Nieforth K, Craig J, Wang F, Solit D, Feng K, Hu M, Bies R, Zhao L. "pyDarwin Machine Learning Algorithms Application and Comparison in Nonlinear Mixed-effect Model Selection and Optimization" https://doi.org/10.1007/s10928-024-09932-9

Expert Opinion on Drug Metabolism and Toxicology (2025)

- K Adams*, **X Li***, L Rohan, R Bies. "PBPK models of the female reproductive tract: current and future analysis" (* co-first author) https://doi.org/10.1080/17425255.2025.2470794

The Journal of Infectious Diseases (2025)

- Brett Hanscom; Mark Marzinke; **Xinnong Li**; Deborah J Donnell; Robert Bies; Craig W Hendrix; Zhe Wang; Carolina X Acuipil; Alex Rinehart; Jon COLLINS et al. "Estimation of prevention-effective CAB-LA concentrations among men who have sex with men (MSM) and transgender women (TGW) in HPTN 083" doi: 10.1093/infdis/jiaf561

Posters

- **X. Li**, A. Mazur, M. Sale, J. Craig, K. Nieforth, R. Bies. "Application of NSGA-II and pyDarwin in Multi-objective Optimization for Population Pharmacokinetic (PopPK) Model Selection" (2025, ACOP Poster)
- Hanscom B, Marzinke M, Bies R, Donnell D, Hendrix C, **Li X**, Wang Z, Acuipil C, Rinehart AR, Rooney J, Soto Torres L, McCauley MB, Grinsztejn B, Landovitz RJ – For the HPTN 083 study team. "Estimation of prevention-effective CAB-LA concentrations among MSM/TGW in HPTN 083" (2025, CROI Poster)
- M. Sale, **X. Li**, Y. Yu, A. Mazur, J. Craig, K. Nieforth, R. Bies. "Multi-objective Optimization for Population Pharmacokinetic Model Selection in pyDarwin" (2025, PAGE Poster)
- **X. Li**, T. Straubinger, G. Valicheria, Z. Zhang, S. Achilles, M. Donnelly, L. Zhao, E. Tsakalozou, B. Chen, L. Rohan, R. Bies, "Pharmacokinetic Model of Drug Delivery in the Female Reproductive Tract" (2024 ASCPT Presidential Trainee Poster)
- T. Straubinger, **X. Li**, G. Valicheria, Z. Zhang, S. Achilles, M. Donnelly, L. Zhao, E. Tsakalozou, B. Chen, L. Rohan, R. Bies, "Development of Graphical Interface in R Shiny for PBPK Model-based Prediction and Simulation of Drug Delivery in the Female Reproductive Tract" (2024, ASCPT Poster)
- **X. Li**, M. Sale, K. Nieforth, J. Craig, F. Wang, D. Solit, K. Feng, M. Hu, R. Bies, L. Zhao. "Performance of Machine Learning Algorithms for Model Selection" (2024, PAGE Poster)
- Y. Yu, A. Bekker, **X. Li**, R. Bies, R. Scott. "PBPK Model Prediction of Long-acting CAB and RPV Concentration in Pregnancy" (2023, CROI Poster)

Talks and Presentations

- FRT PBPK R Shiny app tutorial to FDA (2024)
- pyDarwin presentation to Pfizer (2024)
- pyDarwin presentation to Genetech (2025)
- pyDarwin presentation at Indiana CTSI Pharmacometrics Modeling and Simulation Symposium (2025)

TEACHING EXPERIENCE

Teaching Assistant

University at Buffalo

- pyDarwin Toolbox Applications in PopPK Modeling Lecture, PHC610(PopPK Modeling)
- Teaching assistant of PHC417/517 (Pharmacogenomics)
- Teaching assistant of PHC608 (Advanced PK/PD)

SKILLS

Technical: R, NONMEM, Python, WinNonlin, ADAPT,5, PK-SIM, Simcyp

HONORS & AWARDS

Presidential Trainee Award of ASCPT *2024*

Marilyn Morris Excellence in Pharmaceutical Sciences Fellowship Award *2023*