

## Researchers Use AI to Develop Tool for Predicting Cancer Nanomedicine Outcomes

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Nanomedicines may offer clinicians a way to deliver precise, targeted therapy directly to tumors without damaging surrounding tissue. Yet, progress in the development of new drugs that treat cancer at the nanoparticle level has been frustratingly slow. Good results in animal models haven't necessarily translated to clinical success in humans, in part because of low delivery efficiency of nanoparticles to tumors.

Now, with the support of a new \$1.3 million grant from the National Institute of Biomedical Imaging and Bioengineering of the National Institutes of Health, researchers led by Zhoumeng Lin, B.Med., Ph.D., DABT, CPH, are building a tool that can offer drug researchers insight into how well a new nanoparticle-based cancer therapy will work, even before a drug enters animal testing.

"This project will provide a tangible tool to improve the design of nanoparticles to accelerate clinical translation of cancer nanomedicines from animals to humans in order to benefit cancer patients," said Lin, an associate professor in the department of environmental and global health at the [UF College of Public Health](#) and Health Professions and a member of UF's Center for Environmental and Human Toxicology and Center for Pharmacometrics and Systems Pharmacology.

Another anticipated benefit is the reduction or elimination of animal experimentation for new nanomedicines that are determined to have low delivery efficiency, Lin added.

Lin joined the university this summer from [Kansas State University](#). He is the first faculty member in PHHP hired under UF's artificial intelligence initiative, which seeks to make the university a national leader in AI. Lin's expertise is in the development and application of computational technologies to address research questions related to nanomedicine, animal-derived food safety assessment, and environmental chemical risk assessment.

To build their predictive model of nanoparticle cancer therapies, researchers will use an AI technology known as artificial neural network and train it with hundreds of datasets from physiologically-based pharmacokinetic (PBPK) computer models. PBPK models describe the absorption, distribution, metabolism and excretion of a drug in the body using mathematical equations, and they can be used to predict the concentration of a drug following different therapies.

“In this project, we will integrate PBPK modeling with AI approaches to build an AI-assisted smart model that can predict delivery efficiency of nanoparticles to tumors,” Lin said. “This approach is new in the fields of nanomedicine, pharmacology and toxicology.”

Next, Lin’s co-investigator, Santosh Aryal, Ph.D., an associate professor in the department of pharmaceutical sciences and health outcomes at the University of Texas at Tyler, will conduct pharmacokinetic lab experiments using nanoparticles. The data from these experiments will be used to validate and/or optimize the new AI-PBPK model.

“We are excited about this collaboration and hope this will further open up novel avenues in cancer nanomedicine development,” Aryal said.

For the project’s final outcome, the team will convert the smart model into a publicly available web-based interface for use by nanomedicine researchers.

“This project addresses a crucial problem of low delivery efficiency of cancer nanomedicines, which has been a critical barrier to progress over the last 20 years,” Lin said. “This will greatly improve our fundamental understanding of the key factors of nanoparticle tumor delivery.”

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