

Software to more accurately predict structure of a drug, reduce drug discovery losses

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A Purdue-based startup is developing molecular modeling simulation software that could help pharmaceutical companies more accurately predict the crystal structure of a drug once produced, helping maintain a consistent drug quality and save costs when developing new drugs.

Lyudmila Slipchenko, associate professor in Purdue's Department of Chemistry, and Pradeep Kumar Gurunathan, a graduate student in chemistry, co-founded the company Simplexity Simulations LLC to commercialize the software.

The company's work is based on finding a computationally efficient method to predict polymorphism, or the ability of solid material to exist in two or more forms or crystal structures.

"Polymorphism is a big problem in the pharma industry, a multibillion dollar problem. In the '90s there was a drug called Ritonavir used to treat retroviral diseases including HIV/AIDS. It was a pretty successful drug in clinical trials, but once it went to production, the polymorph, or internal crystal structure of that drug, changed and became inactive and useless," Gurunathan said. "When the internal crystal structure of a drug changes into different forms, various important drug outcomes - like drug efficacy, bioavailability and even toxicity - also change. Pharmacists think they are developing a drug in one form, when, in fact, the drug ends up being something else. Aside from the chemical consequences, companies also endure huge losses when this occurs because of the time and money it takes to develop a particular drug,

which, once it hits shelves, may not be of any use."

Simplexity Simulations software deals with crystal structure prediction so drug developers and pharmacists can understand how a drug will change once it is produced.

"We have a unique technology called the [effective fragment potential method](#), which accurately describes various non-bonding interactions between molecules. Our software could more accurately predict internal energies and chemical stability of different polymorphs," Slipchenko said. "We believe this technology can be applicable to [crystal structure prediction](#) and help the pharmaceutical industries understand what interactions drug components will have before spending the time and money in developing them."

Technology used by Simplexity Solutions has been licensed through the Purdue Research Foundation Office of Technology Commercialization. Simplexity Simulations is a member of the Purdue Startup Class of 2016. Purdue has 27 startups based on Purdue intellectual property that were launched in the 2016 fiscal year.

Simplexity Simulations' product could be used on its own or as a supplementary product to other software programs.

"If we can demonstrate that our product improves a drug's success then, obviously, a company could be interested in using it," Gurunathan said. "They also can use our product as a subsidiary to improve their chances of [drug](#) success. For example, if you want to browse the internet you can use Internet Explorer, Google Chrome or Firefox, it generally doesn't matter. However, in a computer you can have all three programs installed but only use one of them, or use them for different purposes. Similarly, our software can be used as a supplement to other software programs."

The company is seeking funding and plans to beta test the product before going to market.

"Our first step, once we receive funding, is to transfer the technology we have into an end user readable format. That entails writing software code, which will make the product marketable," Slipchenko said. "We plan on sending our product to people in the area who are ready to test the software. Once we do that and prove it's successful, we want to market it to big pharma companies."

Gurunathan credits Purdue Foundry, an entrepreneurship and commercialization accelerator located in the Burton D. Morgan Center for Entrepreneurship in Purdue's Discovery Park, with getting the company off the ground.

"We received the National Science Foundation i-Corps funding for the initial customer discovery process, which allowed us to meet and talk with a lot of potential customers," he said. "The i-Corps program put us in touch with Purdue Foundry, where we found two incredible entrepreneur-in-residence mentors who've been helping us conduct customer discovery and guide us on the next steps. Their expertise and network contacts in the pharma industry and their systematic approach towards startup development have helped us immensely."

Provided by Purdue University

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