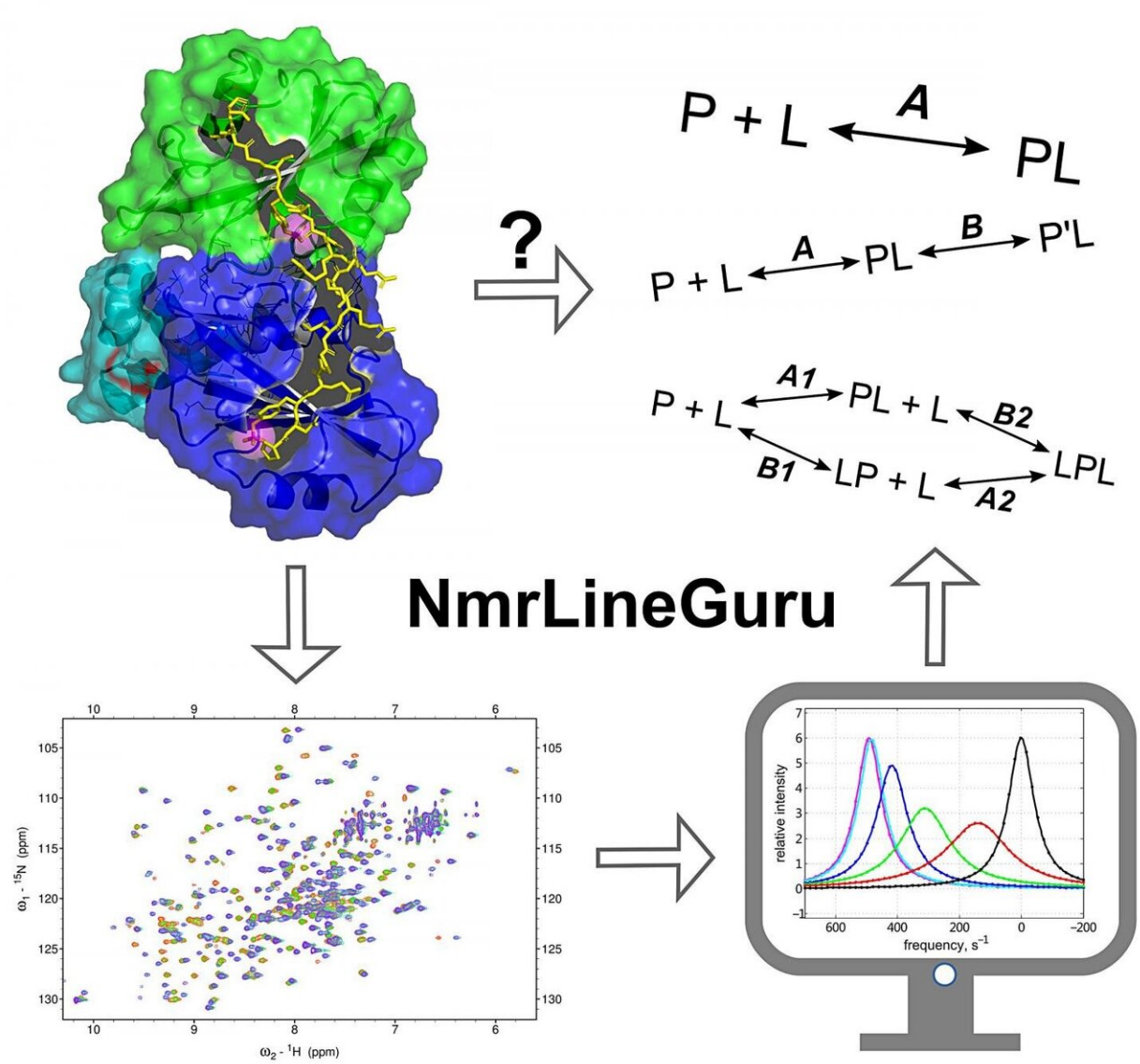
Site search: A digital approach to proteins and cancer

December 11 2019, by Chris Adam



Purdue University researchers developed software, called NmrLineGuru, to help

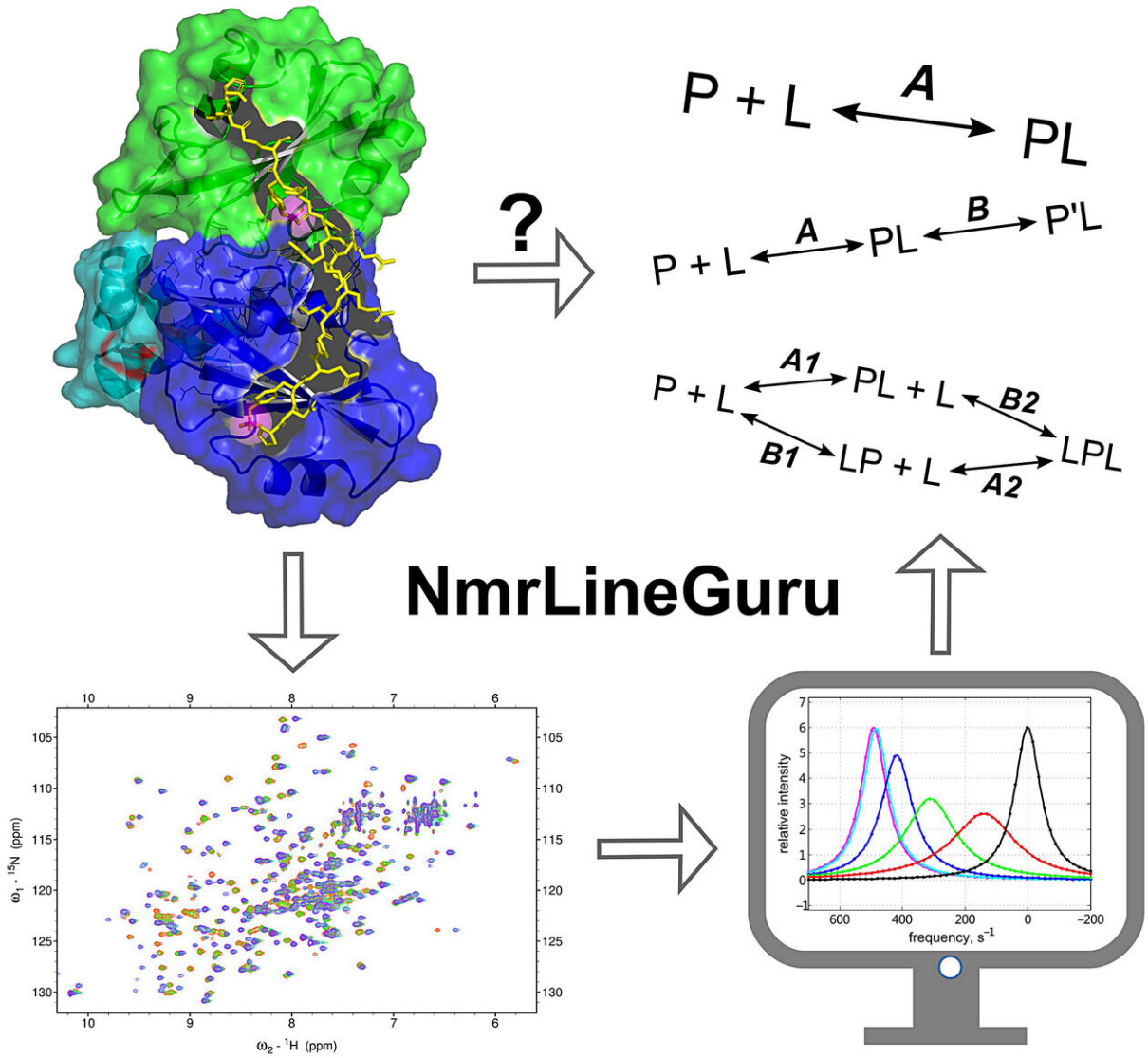
scientists study specific information about proteins. Credit: Purdue University/Chao Feng

What if scientists could create more effective drugs to treat cancers and other diseases by better targeting specific sites on proteins in the body?

That's the primary question researchers in the Purdue University laboratory of Carol Post, a distinguished professor in Purdue's College of Pharmacy, are trying to answer. They have developed software called NmrLineGuru to move researchers closer to the answer. Their work is published in the Nov. 5 edition of *Scientific Reports*.

Chao Feng, a postdoctoral researcher in Post's lab, who helped lead the research team, said, "We created software for fast 1D nuclear magnetic resonance lineshape simulation and analysis with multistate equilibrium binding models. It enables researchers and scientists to study much more specific information about proteins that are linked to serious diseases to help in the drug discovery process."

Proteins play a crucial role in the growth of cancer in the body by stimulating molecules responsible for tumor growth. The graphical user interface software developed at Purdue can help researchers quickly understand, through simulated models, how certain proteins bind with other molecules in the body.



Purdue researchers developed software, called NmrLineGuru, to help scientists study specific information about proteins. Credit: Purdue University

"Our work stems from a deep understanding of the need in the drug discovery field for better and faster solutions to understand biological functions of proteins and molecules in the body," Feng said.

The Purdue software supports the most common two-, three-, and four-state binding models used in the drug discovery industry to study such interactions between the proteins involved in a disease state and the molecules that bind to them. The software takes the information submitted by the user and creates specific model information about protein interactions.

More information: Chao Feng et al, NmrLineGuru: Standalone and User-Friendly GUIs for Fast 1D NMR Lineshape Simulation and Analysis of Multi-State Equilibrium Binding Models, *Scientific Reports* (2019). DOI: 10.1038/s41598-019-52451-8

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