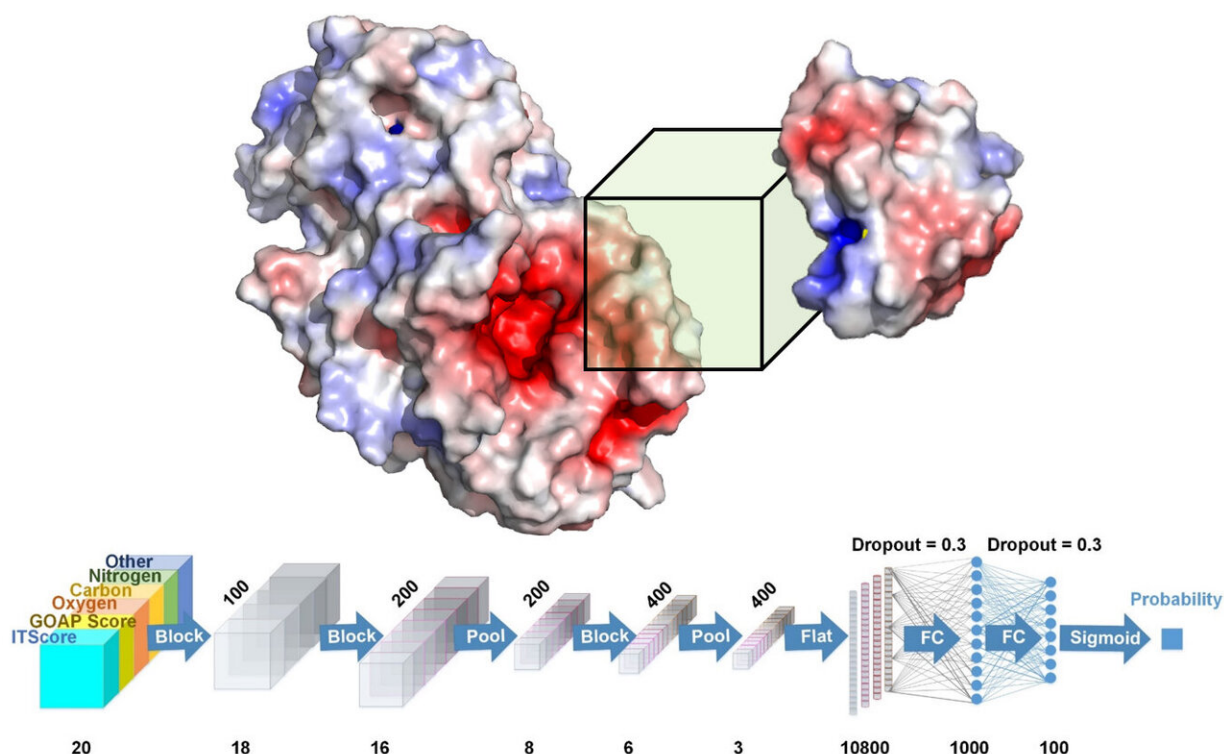# Deep learning, 3-D technology to improve structure modeling, create better drugs

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DOVE, created by Purdue researchers, captures structural and energetic features of the interface of a protein docking model with a 3D box and judges if the model is more likely to be correct or incorrect using 3D convolutional neural network. Credit: Daisuke Kihara/Purdue University

Proteins are often called the working molecules of the human body. A typical body has more than 20,000 different types of proteins, each of

which are involved in many functions essential to human life.

Now, Purdue University researchers have designed a novel approach to use deep learning to better understand how proteins interact in the body—paving the way to producing accurate structure models of protein interactions involved in various diseases and to design better drugs that specifically target protein interactions. The work is released online in *Bioinformatics*.

"To understand molecular mechanisms of functions of protein complexes, biologists have been using experimental methods such as X-rays and microscopes, but they are time- and resource-intensive efforts," said Daisuke Kihara, a professor of biological sciences and computer science in Purdue's College of Science, who leads the research team. "Bioinformatics researchers in our lab and other institutions have been developing computational methods for modeling protein complexes. One big challenge is that a computational method usually generates thousands of models, and choosing the correct one or ranking the models can be difficult."

Kihara and his team developed a system called DOVE, DOcking decoy selection with Voxel-based deep neural nEtwork, which applies deep learning principles to virtual models of protein interactions. DOVE scans the protein-protein interface of a model and then uses deep learning model principles to distinguish and capture structural features of correct and incorrect models.

"Our work represents a major advancement in the field of bioinformatics," said Xiao Wang, a graduate student and member of the research team. "This may be the first time researchers have successfully used deep learning and 3-D features to quickly understand the effectiveness of certain protein models. Then, this information can be used in the creation of targeted drugs to block certain protein-protein

interactions."

More information: Xiao Wang et al, Protein Docking Model Evaluation by 3D Deep Convolutional Neural Networks, *Bioinformatics* (2019). DOI: 10.1093/bioinformatics/btz870

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