Drug discovery could accelerate hugely with machine learning

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Drug discovery could be significantly accelerated thanks to a new high precision machine-learning model, developed by an international collaboration of researchers, including the University of Warwick.

The algorithm - partly devised by Dr James Kermode from Warwick's School of Engineering - can accurately predict the interactions between a protein and a drug molecule based on a handful of reference experiments or simulations.

Using just a few training references, it can predict whether or not a candidate drug molecule will bind to a target protein with 99% accuracy.

This is equivalent to predicting with near-certainty the activity of hundreds of compounds after actually testing them - by running only a couple dozen tests. The new method could accelerate the screening of candidate molecules thousands of times over.

The algorithm can also tackle materials-science problems such as modelling the subtle properties of silicon surfaces, and promises to revolutionise materials and chemical modelling - giving insight into the nature of intermolecular forces.

The approach, developed by scientists at the University of Warwick, the École polytechnique fédérale de Lausanne's Laboratory of Computational Science and Modelling, the University of Cambridge, the UK Science and Technology Facilities Council and the U.S. Naval

Research Laboratory, can also identify which parts of the molecules are crucial for the interaction.

Dr James Kermode, from the University of Warwick's Warwick Centre for Predictive Modelling and the School of Engineering, commented on the research:

"This work is exciting because it provides a general-purpose machine learning approach that is applicable both to materials and molecules.

"The research is expected to lead to a significant increase in the accuracy and transferability of models used for drug design and to describe the mechanical properties of materials."

The design of this algorithm, which combines local information from the neighbourhood of each atom in a structure, makes it applicable across many different classes of chemical, materials science, and biochemical problems.

The approach is remarkably successful in predicting the stability of organic molecules, as well as the subtle energy balance governing the silicon structures crucial for microelectronic applications, and does so at a tiny fraction of the computational effort involved in a quantum mechanical calculation.

The research illustrates how chemical and materials discovery is now benefitting from the Machine Learning and Artificial Intelligence approaches that already underlie technologies from self-driving cars to go-playing bots and automated medical diagnostics.

New algorithms allow us to predict the behaviour of new materials and molecules with great accuracy and little computational effort, saving time and money in the process.

'Machine Learning Unifies the Modelling of Materials and Molecules' is published in *Science Advances*. The research received funding from the Engineering and Physical Sciences Research Council.

Provided by University of Warwick