

[Subject category: Health and medicine]

A QUANTUM LEAP IN DRUG DISCOVERY

Chemists at the University of Bristol are using high-performance computing to help speed up the process of designing potential new drugs.

The drug industry relies heavily on computational chemistry: vast libraries of candidate drug molecules are screened against their targets in a computer and those that show promise are then selected for further development.

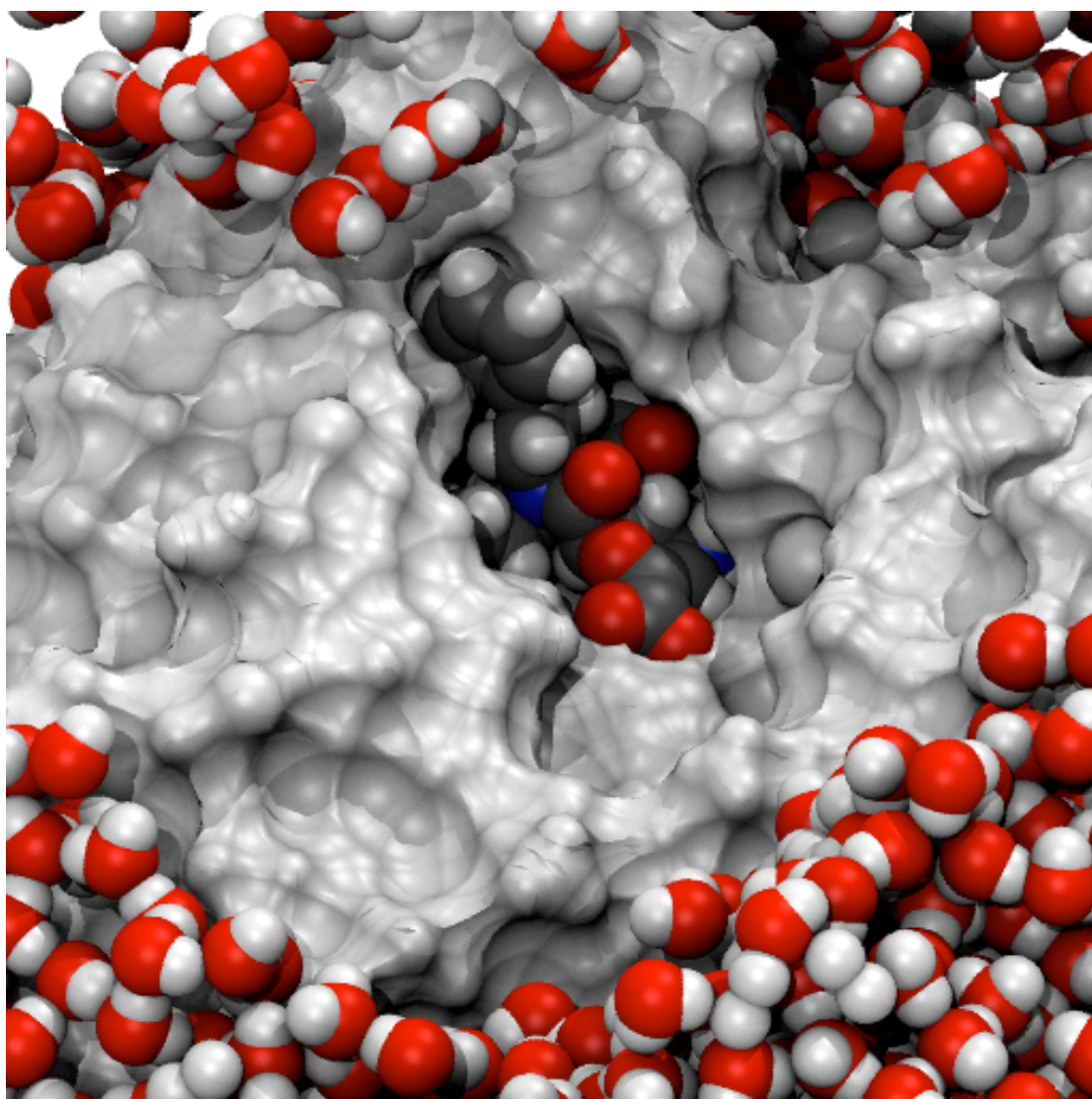
However, current approaches to the problem, based upon classical molecular mechanics, have limitations for this later developmental stage because the calculations consider atoms as balls and the interactions between them as springs; ultimately this is not highly reliable.

At the molecular scale classical mechanics starts to break down and the rules of quantum mechanics take over, where particles behave as waves and the physics of the system becomes unpredictable and complex. Dr Manby and his team are looking to unravel the quantum mechanical interactions between a drug molecule and its target, providing a much more accurate picture of the system's behaviour. However, the calculations needed are extremely complex and require new computational approaches.

The researchers have teamed up with Bristol-based computer chip designer ClearSpeed Technology plc, who produce an innovative chip that contains 100 processor cores, which allows extremely fast processing while consuming relatively little power. By combining new software with this novel computer technology, the computationally expensive calculations should be feasible. "Ultimately we believe that the quantum mechanical approach is the way to get a much more accurate idea of how a drug might interact with a protein and that the kind of computational chemistry we are developing will hopefully take us towards that goal," Dr Manby says.

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Bind tightly...a drug displaces water molecules as it binds to a protein