Team develops speedy software designed to improve drug development

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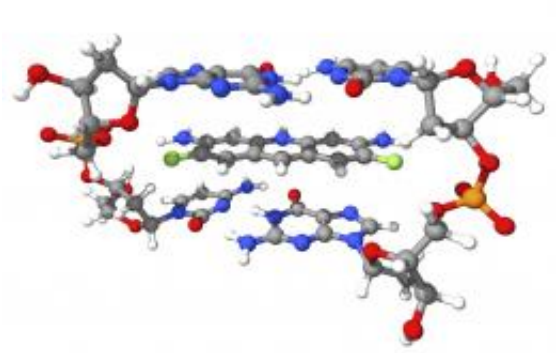


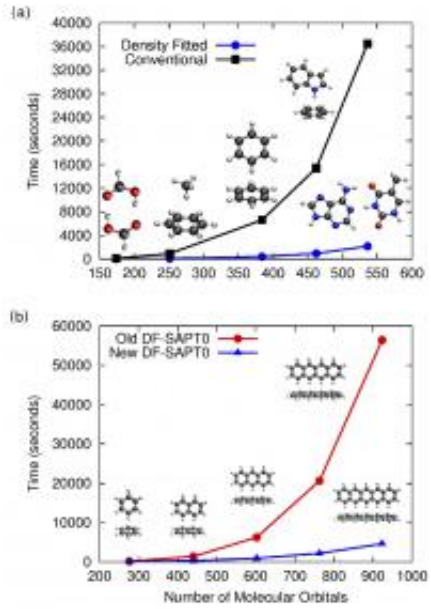
Computer Program Quickly Analyzes Molecular Interactions I

(PhysOrg.com) -- Creating new, improved pharmaceuticals is sometimes very similar to cracking the code of a combination lock. If you have the wrong numbers, the lock won't open. Even worse, you don't know if your numbers are close to the actual code or way off the mark. The only solution is to simply guess a new combination and try again.

Similarly, when a newly created drug doesn't bind well to its intended target, the drug won't work. Scientists are then forced to go back to the lab, often with very little indication about why the binding was weak. The next step is to choose a different pharmaceutical "combination" and hope for better results. Georgia Tech researchers have now generated a computer model that could help change that blind process.

Symmetry-adapted perturbation theory (SAPT) allows scientists to study interactions between molecules, such as those between a drug and its target. In the past, computer algorithms that study these noncovalent interactions have been very slow, limiting the types of molecules that can be studied using accurate quantum mechanical methods. A research team headed by Georgia Tech Professor of Chemistry David Sherrill has developed a computer program that can study larger molecules (more than 200 atoms) faster than any other program in existence.

“Our fast energy component analysis program is designed to improve our knowledge about why certain molecules are attracted to one another,“ explained Sherrill, who also has a joint appointment in the School of Computational Science and Engineering. “It can also show us how interactions between molecules can be tuned by chemical modifications, such as replacing a hydrogen atom with a fluorine atom. Such knowledge is key to advancing rational drug design.”



Computer Program Quickly Analyzes Molecular Interactions II

The algorithms can also be used to improve the understanding of crystal structures and energetics, as well as the 3D arrangement of biological macromolecules. Sherrill's team used the software to study the interactions between DNA and proflavine; these interactions are typical of those found between DNA and several anti-cancer drugs. The findings are published this month in the *Journal of Chemical Physics*.

Rather than selling the software, the Georgia Tech researchers have decided to distribute their code free of charge as part of the open-source computer program PSI4, developed jointly by researchers at Georgia Tech, Virginia Tech, the University of Georgia and Oak Ridge National Laboratory. It is expected to be available in early 2012.

"By giving away our source code, we hope it will be adopted rapidly by researchers in pharmaceuticals, organic electronics and catalysis, giving them the tools they need to design better products," said Sherrill.

Sherrill's team next plans to use the software to study the noncovalent interactions involving indinavir, which is used to treat HIV patients.

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