Visualizing the structures of molecules

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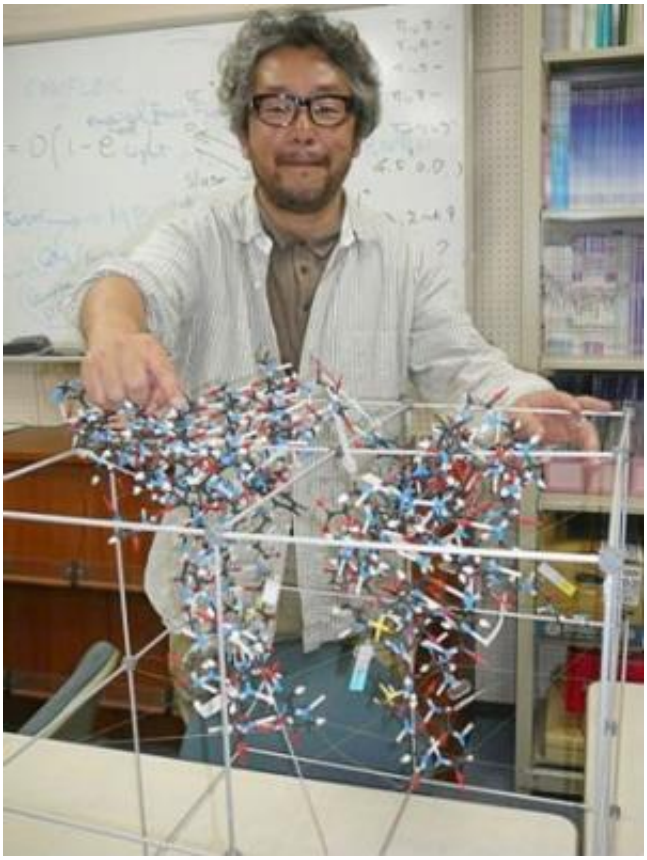

Credit: Hitoshi Goto

Hitoshi Goto and colleagues have developed high performance molecular simulation tools to study the 3D arrangement of molecules, enabling better design of medicinal and agricultural drugs which are more effective and fewer side effects.

"We've developed high performance molecular simulation tools and a graphical user interface for researchers to study the conformation—the three-dimensional structural arrangement of molecules, and this is enabling us to design medicinal and agricultural drugs that are more effective and have fewer side-effects," says Goto. The tool-set has been commercialized under the brand name CONFLEX/BARISTA, for which Goto wrote the algorithms.

He explains that CONFLEX, together with its graphical user interface BARISTA, enables researchers to visualize the possible spatial arrangements of atoms in a molecule and therefore more easily study their chemically important (energetically stable) molecular formations. This in turn can reveal how a particular arrangement or conformation influences a molecule's chemical behavior. For instance, HIV inhibitors can be better understood and studied with the aid of 3-D graphical representations provided by the software.

Another area of Goto's research involves the development of methods to predict crystal structures in instances of molecular structures having more than one crystalline form: a phenomenon known as polymorphism.

"When a molecule can be crystallized with different packing forms, a part of the grown crystal may show unexpected physical, chemical and biological (medicinal) properties," says Goto. For instance, a second crystal structure of aspirin has recently been discovered, which is slightly different to the commonly known standard structure. Goto's crystal simulation technology can be used to calculate the energies bound up in such a polymorphic structure, an understanding that can help research chemists predict its medicinal effects.

CONFLEX is currently available at version 6. Goto and his lab co-workers have been working on new algorithms that will help researchers search for new crystal structures, an endeavor that normally requires the

use of expensive X-ray equipment. "This function will be available in a few months in version 7 of CONFLEX," says Goto. "Developing these algorithms is very complex and time consuming. In fact, I've been working on them for over a decade, for it's involved a lot of trial and error. So I'm pleased this feature is now ready to be distributed."

Provided by Toyohashi University of Technology