Building 3-D models of molecules with RealityConvert

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Denis Fourches wants to make the search for new drugs faster and less expensive. So he uses powerful computers to help model interactions between chemical compounds and biological targets to predict the compound's effectiveness, thus narrowing the field of potential drug candidates for testing and saving researchers time and money. Now he has a new tool in his arsenal – a computer program that will allow anyone to rapidly create three-dimensional models of molecules for 3-D printing as well as augmented and virtual reality applications, making it easier to study these complex biomolecular structures.

"Large and complex biomolecules like proteins make it difficult for researchers and students to accurately visualize their structure or how they might interact with a given compound," says Fourches, assistant professor of chemistry at NC State. "But if we can easily build an accurate 3-D model of the protein into a virtual reality or augmented reality environment, we can enable a much better perception of the geometrical and structural characteristics of that molecule."

RealityConvert is a software tool that converts molecular objects – such as proteins and drugs – to high quality 3-D models. It generates 3-D molecular and biomolecular models in standard file formats that are compatible with the vast majority of augmented and virtual reality programs as well as 3-D printing tools. The conversion is fast and the program is specifically geared toward generating models for various chemicals and small proteins. Fourches is already utilizing the program with his undergraduate organic chemistry students. RealityConvert is

open access and freely available to the public.

"The ultimate goal of RealityConvert is to facilitate and boost the development of augmented reality and virtual reality content for bioinformatics and cheminformatics applications," Fourches says. "These technologies allow for stunning and immersive experiences, offering untapped opportunities for both research and education purposes."

The latest version of the program is available on Fourches' GitHub platform and on its website.

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