Super-sized tiny proteins

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What are the causes of illness? How can the effect of medication be improved? Molecular biologists can now gain new insights by the virtual simulations generated with a new type of software.

If it's a question of the efficacy of vaccines or the aggressiveness of toxins, researchers must be able to simulate and analyze the molecules involved in three dimensions. What do they look like? What is the three-dimensional structure of a protein? How can this structure be used to predict which molecules the protein interacts with? What function does it have? In the software applications most widely used today, the depiction of the simulated protein and the quality of the graphics leave a great deal to be desired - especially if larger molecules, consisting of thousands of atoms, have to be visualized and examined.

This is likely to get a lot easier with the arrival of “BioBrowser” a software application developed as part of a German Research Foundation project by researchers specialized in Visual Computing at Fraunhofer Austria in Graz. Based on research data of molecular biologists, the software automatically calculates and displays 3D models of complex proteins - at the push of a button, in high quality, and interactively.

Researchers can turn the molecule and look at it from every angle, enlarge it at will and select specific areas; the image is always razor sharp and users can switch between the most important variants. Visualized models can be very large and complicated - they often consist of 50,000 and more atoms. “When examining molecules, an enormous flood of data is generated that in itself makes little sense at all. BioBrowser converts this data into graphic images and makes the links between different molecules visible”, summarizes Dr. Eva Eggeling, Head of Visual Computing.

Interested researchers receive a download link on request that gives them direct free-of-charge access to the program. They can also arrange an appointment with colleagues in Graz to study the proteins on a large 3D projection screen. The Graz researchers are hoping this will give new drive to molecular biology and the development of medicines. At the moment they are working on extending and improving the user interface. Feedback from the first scientific users helps the Graz researchers decide whether they need to add other functions. The product is primarily directed at Austrian scientists, but can also be used worldwide. “We are also reckoning on enquires from other European countries, particularly from Germany and Switzerland”, explains Eggeling.

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