Computational biologists assist global network of researcher teams in developing new medicines

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Many years can pass before a newly developed medicine can enter the market. Computational biologists in Saarbrücken and Tübingen would like to speed up this long and tedious process. They have developed the software BALLView, with which new active agents can be conceptualized and visualized. Now international research teams can meet on the web and work with three-dimensional molecular models together on their monitors.

UNIVERSITÄT DES SAARLANDES

Researchers from the Center for Bioinformatics in Saarbrücken will present a prototype of the new platform together with the Saarland University Intel Visual Computing Institute at the CeBIT 2011 in Hanover from March 1st through the 5th at the Saarland University research booth (hall 9, booth B43).

“If you are looking to find the right key for a lock, you have to be able to spatially visualize it. It is no different for researchers who need to comprehend the chemical and spatial forms and structures of molecules in order to develop new medicines,” Andreas Hildebrandt explains. He leads the research group at Saarland University that, together with computational biologists in Tübingen, has developed the freely available Software BALL (Biochemical ALgorithms Library), to which the visualization component BALLView has been added. With the help of BALLView, you can dive into the 3D virtual world of active agent molecules, DNA and viruses. This better spatial view makes it easier for the viewer to find the “key agent molecule” which geometrically and chemically fits the three-dimensional “lock”, the so-called receptor molecule, in the human body.

International research teams from different fields are working together closely from different sites to better understand these complex mechanisms. “Up to now, they could not work on the same three-dimensional models simultaneously because of limited network capacities and problems with data security, among other things,” the bioinformatician explains. For this reason, the research team in Saarbrücken is expanding its software by so-called collaborative functions. These enable researchers to do complex molecular modeling together on the Internet, simultaneously. The 3D technology needed for this was developed by Professor Philipp Slusallek and his research team from the Saarland University Intel Visual Computing Institute and the German Research Center for Artificial Intelligence (DFKI). The expansion of ordinary web browsers allows complex 3D graphics to be displayed.

“This new web technology was integrated into the BALLView software. And now researchers can also share and exchange their ideas directly in a chat window in BALLView,” Hildebrandt explains. The software works with a special visualization method called ray tracing which very realistically displays the spatial structures of molecules with lighting, shadows and reflections. It can be looked at with the help of a virtual reality setup or simply on a standard 3D television set. “Two images are superimposed, allowing the viewer to see them with enormous depth through 3D glasses and get an extremely realistic spatial impression. He can also move the proteins and viruses directly on the screen as well as zoom into and edit individual sections,” says Andreas Hildebrandt, who will soon take on a professorship at the university in Mainz. Visitors to the computer trade fair Cebit can give this new technology a try on a 3D television.

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Information for radio journalists: If you would like to arrange a telephone interview with researchers and students from Saarland University in studio quality (Audio-ISDN-Codec), please contact Friederike Meyer zu Tittingdorf at the press office.

Weitere Informationen:
http://www.ballview.org

Kooperation international

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Zurück