



## Scientists at IRB Barcelona and BSC publish the world's largest video database of protein motions

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By EurekAlert

After four years of conducting intensive calculations in the supercomputer MareNostrum at the Barcelona Supercomputing Center, scientists headed by Modesto Orozco at the Institute for Research in Biomedicine (IRB Barcelona) have published a new video database on protein motions. Called MoDEL, this new database holds more than 1,700 proteins and is partially accessible via the Internet to researchers worldwide. MoDEL has been developed to study the basic biology of proteins and to aid in the design of new pharmaceutical agents.

"Nowadays we design drugs as if the proteins against which they are to act were static and this goes a long way against the development of new drug therapies because this is not a true scenario. With MoDEL this problem is solved by providing a user from 10,000 to 100,000 photos per protein, and these confer movement to these structures and allow a new approach," says Orozco, head of the "Molecular modelling and bioinformatics" group at IRB Barcelona, director of the Laboratory of the Barcelona Supercomputing Center and full professor at the University of Barcelona. According to this study, pharmaceutical companies are already using the MoDEL strategy to develop the first drugs against cancer and other diseases which could become available this year.

### A project in expansion

The scientists that develop MoDEL work from an international catalogue of static protein structures (approximate 40,000) in the Data Bank (PDB). "1,700 videos of proteins from the 40,000 that make up the PDB may appear to be a small number, but in fact structures in the PDB are very similar. Therefore, following internationally established similarity criteria, we have selected 1,700 proteins with a known structure".

But for Modesto Orozco the most relevant point is that MoDEL is now covering more than 30% of human proteins of pharmaceutical interest, that is to say, those that are potential targets of a new drug. "We obtained this data by considering that we are in fact covering more. However, MoDEL will continue to grow and this can be achieved by a well established process". According to the researchers, the main objective is to focus on relevant proteins in human cancer and 3 years cover 80% of pharmaceutical targets.

In order to undertake the MoDEL project, Orozco and his group are supported by resources provided by IRB Barcelona SuperComputing Center, the Marcelino Botín Foundation, the Fundación Genoma España, the National Bioinformatics Programme and European projects.

### SOURCE

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