Keystone Symposia Conference: Computer-Aided Drug Design

(Steamboat Springs, Colorado, USA 29.3.-3.4.2008)

I had an opportunity to visit the springlike Rocky Mountains in the beginning of April, and to take part in one of the key meetings in molecular modeling and drug design in 2008. The meeting was arranged in a small ski resort, North-West of Denver, Colorado by a non-profit organization of Keystone Symposia.

It could be argued that the plenary speakers were top notch, both from academia and industry. Graduate students delivered none of the short talks, which was a little discrepancy from the classic European meetings. Next, let's focus on the main topics of the meeting.

The apparent pitfalls of molecular docking was clearly recapped by several speakers, and it seems that the field is moving more and more towards applying free energy-based methods and not only consensus scoring but consensus docking too to evaluate affinity rank order of ligands. Clearly, another hot topic was the consideration of the ligand efficiency when choosing lead molecules for further development. Several big pharma companies presented positive results from their fragment-based campaigns where ligand efficiency calculations were used along with X-ray and NMR structure determination.

Holger Gohlke showed some preliminary results of their new flexible docking method, which is based on elastic potential grids. If and when this software will be available, it is something to be tested on our own projects for sure as well. An interesting talk about millisecond-scale protein molecular dynamics was delivered by David E. Shaw. Their software and hardware solutions might be groundbreaking in large-scale simulations.

My contribution to the meeting was a poster presentation titled "Guiding Ligands in Fatty Acid Amide Hydrolase: Assessing the Penalty Values in Fragment-Guided Docking of Phenyl Carbamates". A few of the participants at the poster session were eager to learn how the method was implemented. After the discussion with a few partakers, I am convinced the presented docking method will be used in further FAAH studies.

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