The Sixth European Workshop in Drug Design (VI EWDD)

Siena, Italy, 3rd to 9th June 2007

The EWDD workshop is held every two years in the countryside surrounding the town of Siena in Tuscany, central Italy. This year the workshop venue was a former monastery of Certosa di Pontignano which dates back to the 14th century. Purpose of the workshop is to be a meeting place for top experienced scientists and students around the world. The agenda contained lectures over a range of topics within computational chemistry plus a computer workshop.

In total there were 25 talks which were held in the morning sessions. I found most of them interesting. Especially I liked the talks by Jonathan Mason (Lundbeck Research, Denmark), Thierry Langer (University of Innsbruck, Austria) and Michael Kaiser (UCSF, USA).

Mason's talk handled the molecular similarity of small molecules in regard to their functional similarity. He also talked about an interesting virtual screening method called FLAP which they have co-developed. The method allows protein-protein, protein-ligand and ligand-ligand comparison making it applicable to a variety of research projects.

Langer talked of pharmacophore development in which his group is specialized. He discussed the construction of pharmacophores by using either a set of ligands or a protein crystal structure as a starting point. In addition to the theoretical part of the talk he gave examples of virtual screening projects done in his group using pharmacophores.

Kaiser introduced a work where he had used structural similarity of small molecule ligands to relate proteins to each other. This way, novel links can be found between proteins that are missed with traditional methods based on protein sequence or structure data. The approach had also been used to find unknown targets for existing drugs.

In the afternoons, the students were divided in three groups each of which worked on a particular research project for the whole week. The first group, in which I participated, was run by Thierry Langer where students constructed a pharmacophore model for thrombin inhibitors and later validated it. In the second group the students were asked to construct a comparative model of a protein and run molecular dynamics with it. The students in the third group used GRID interaction fields for virtual screening.

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