Workshop D2

Computer-Aided Drug Design explained in a few simple steps (Drug Design Workshop)

Dr. Marie-Claude Blatter[1], A. Daina[1], V. B. Gerritsen[1], D. Marek[1], P. M. Palagi[1], O. Michielin[1], V. Zoete[1]

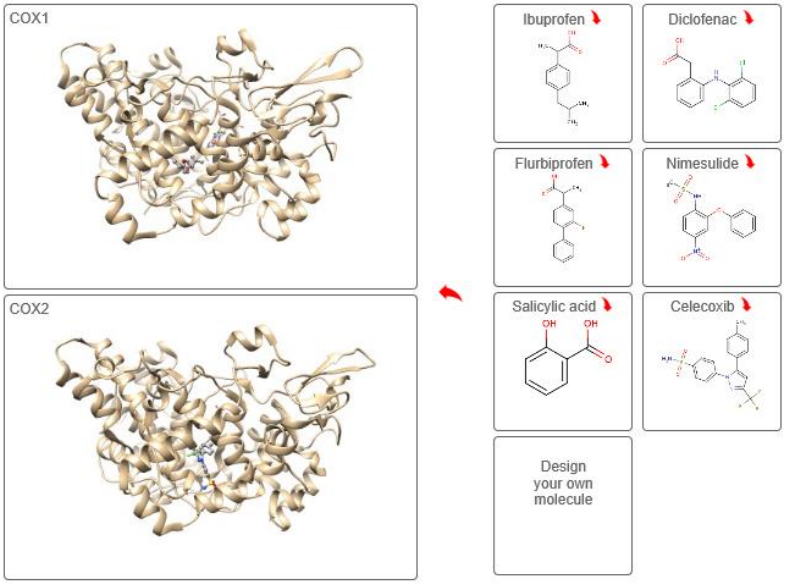
[1] Swiss Institute of Bioinformatics, 1, rue Michel Servet, 1211 Geneva 4, Switzerland

Marie-Claude.Blatter@sib.swiss

www.drug-design-workshop.ch

The aim of the workshop is to acquire a simple yet realistic picture of how bioinformatics is used to design drugs today. Participants will acquire sufficient knowledge and practice to help their students design new drug candidates. Perhaps with therapeutic properties even better than those of existing drugs! Examples are taken from drugs or drug candidates for the treatment of cancer and pain.

After a very short in troduction on the biological context (protein 3D-structure, protein function and diseases) and basic drug design concepts, participants will be invited to design their own drugs, *in silico*. For this, they will model the interactions between the drug and the target protein and predict other potential target proteins as well as some pharmacological properties of the molecule by using web-based tools that are developed by the SIB Swiss Institute of Bioinformatics. These tools are embedded into a user-friendly interface (www.drug-design-workshop.ch), which is freely accessible, without login; videos, documentation and pedagogical materials on the subject are also available on the site.



In parallel, participants will be able to test the manual docking of 3D-printed small molecules into a 3D-printed protein, itself representing the drug target true to scale.