Drug Design for high school students, high school teachers and the public at large

Blatter Marie-Claude1,5, Daina Antoine2, Baillie Gerritsen Vivienne1, Marek Diana4,6, Palagi Patricia M.5, Xenarios Ioannis1,3,4,6, Schwede Torsten7,8, Michielin Olivier2,3,9,10, Zoete Vincent2


SIB Swiss Institute of Bioinformatics, Switzerland

Our aim is to introduce, in an engaging and challenging way, concepts such as 3D structure, protein function, diseases and the role played by bioinformatics in drug discovery and development.

Our workshop involves…

1. a short film produced by Studio KO graphic designers, which introduces the key notions for drug design (protein target, disease, ligand, docking, …)

2. the ‘manual docking’ of 3D-printed small molecules into a 3D-printed structure representing the target protein on a one-to-one scale, and ‘manual docking’ with a camera system (leap motion)

3. tools embedded into a user friendly freely accessible web interface: www.atelier-drug-design.ch participants can design new ‘virtual’ molecules, visualize their binding mode and estimate their affinity for the target protein, which they can then compare with existing drugs

4. direct links to expert tools for predicting possible targets (SwissTargetPrediction) as well as important properties of the molecule in order to evaluate its potential of becoming a drug (SwissADME)

5. pen and pencil activities to understand how a computer encodes chemical structures (fingerprints) and how similarities between molecules are calculated.

The workshops give a simple yet realistic picture of how bioinformatics is used to design drug candidates. Hands-on sessions are for cancer (target BRAF and IDO1) and pain (target COX) treatments. Over 200 people attended our pilot workshops. Many of them, even with a very limited knowledge of chemistry, were inspired by the challenge to sketch a molecule whose properties – compared to well-known drugs - they could perhaps improve, in competition with other participants. According to a first evaluation (n=35), the participants (over 16 years) really appreciate using bona fide bioinformatics tools. Those interested in science for their future studies also appreciated discovering a new professional field. The workshops are currently given by 2 public labs: ‘Chimiscope’ in Geneva and ‘l’Éprouvette’ in Lausanne. There will soon be an English and German version of the workshops, which will broaden the area to the whole of Switzerland as well as abroad. Interested? Please, contact us!