eDrug: Drug eDesign: Building the next generation of software solutions for drug design

Description

Computer simulations are taking over in design processes. Nevertheless, complex projects will largely benefit from human intuition and team-work. We combined computer and human power into the next generation of fully interactive computational tools for drug design.

The goal of eDRUG was to prove the potential of this novel computational solution in the (then) current pipeline of drug development and raise prospective interest in the pharmaceutical industry. We aimed to merge human knowledge with state of the art affordable computational resources to create an interactive and (capable of) intuition-guided software solution.

The idea was set on three technological pillars: 1) the PELE software allowing fast biophysical characterization of drug-target interactions; 2) advances in computational hardware providing more computational performance in reduced space, requiring lower power consumption and acquisition cost, and 3) better graphical devices allowing a richer and faster human (team) data analysis and software interaction.

The goal matched with the increasing and future needs from pharmaceutical companies to improve rational drug design (in response to cell/virus mutations, personalized medicine, etc.). One worldwide leading pharmaceutical company, anda local biotech SME, was counseling the developing team and testing the prototypes, to meet a product that fulfills industry expectations.

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