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...

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Let’s imagine that we have developed a drug with very good potency for some cancer therapy. However, with time, many patients start developing resistance to the drug due to some particular point mutation as a result of the high metabolism of the cancer cells. Or let’s imagine that some specific treatment for a virus has lost its efficacy due to some viral...

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