

Computer-aided Drug Design

Dmitri Kireev

Center for Integrative Chemical Biology and Drug Discovery, UNC Eshelman School of Pharmacy, University of North Carolina, Chapel Hill, NC 27513

Drug discovery is a long, uncertain and costly process. Computational methods play an increasingly important role in speeding it up and improving the odds of success. In this overview, we will first introduce the basics of drug discovery – the paradigm, milestones and respective deliverables, as well as technologies used. We will then introduce and provide details on major computer-aided techniques and give examples of their application.