Molecular modelling studies in drug discovery

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Abstract

Modern drug discovery remains a high-risk, resource-intensive enterprise, where candidate failure is frequently precipitated by unfavorable pharmacokinetic and toxicological profiles. Molecular modeling offers powerful strategies to accelerate hit identification and optimize lead compounds with enhanced pharmacological profiles. Nevertheless, ensuring reliability requires methodological validation. This guest lecture covers the critical workflow steps, technical considerations, and best practices in structure-based ligand discovery procedures.

About the presenter

Prof. Akdemir's primary research interests focus on the discovery and design of new drug candidate compounds. To this end, he integrates molecular modelling and molecular pharmacology in his studies. Following his PhD (VU University Amsterdam, The Netherlands), he served as a computational chemist at a drug development company.

In 2011, he was appointed in the Department of Pharmacology (Bezmialem Vakif University, Faculty of Pharmacy, Istanbul, Türkiye). He assumed the role of Vice Dean of the Faculty of Pharmacy in 2013. During his tenure, he contributed to the development of the pharmacy curriculum and founded the *Drug Discovery and Development* master's and PhD programs, as well as the Computer-Aided Drug Design Research Laboratory. As the Institutional Erasmus+ Coordinator, he secured Erasmus and Erasmus+ charters and established numerous bilateral agreements.

He joined the academic staff at Istinye University Faculty of Pharmacy (Istanbul) in 2023 and was appointed Acting Dean in July 2023. As of October 2025, he has taken up a position in the Department of Pharmacology at Istanbul Kent University Faculty of Pharmacy. Prof. Akdemir has authored 77 articles and 5 book chapters and holds a Scopus H-index of 25.