세미나 초록

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소속	보로노이
발표 주제	분자설계 연구방법을 이용한 신약개발
발표 내용	Since the first attempts at structure-based drug design about four decades ago, molecular modelling techniques for drug design have developed enormously, along with the increasing computational power and structural and biological information on active compounds and potential drug target molecules. Nowadays, molecular modeling can be considered an integral component of the contemporary drug discovery and development process. Rational, target-based drug development projects benefit significantly from understanding the essential ligand–receptor interactions for designing a potent and efficacious drug that binds to the desired target. In this presentation, I will provide an overview of molecular modeling methods with special focus on their successful application towards receptor-ligand binding model predictions and hit identification study using a virtual screening method.