Molecular Modeling and Structure-Based Drug Design and Discovery of Renin Inhibitors

Abstract

Renin is a specific enzyme that plays a very important role in human body’s blood circulation system and regulates the blood pressure. Renin inhibitors are potential drugs that can be used to treat hypertension disease. By following a series of systematic structure-based drug design principles with molecular modeling, innovative ideas, and persevering hardworking, Aliskiren, the first-in-class renin inhibitor, was discovered and developed successfully by Ciba-Geigy scientists as a highly effective medicine to treat patients with high blood pressure. In this seminar, the invention and development of Aliskiren from the initial molecular modeling to its chemical synthesis will be presented.

References
(1) http://renin-research.blogspot.com/.