Dr Chase Smith, Massachusetts College of Pharmacy and Health Sciences, gave this presentation at the "Guiding Optimal Compound Design and Development Symposium" held in Cambridge, MA, USA on 19 March 2015.

Abstract

The development of a 5-week long laboratory exercise that simulates an early stage drug discovery program and hit-to-lead optimization for use in an introductory course in the Pharmaceutical Sciences program at MCPHS University (Worcester/Manchester) will be discussed. Using the ADME QSAR module of the Stardrop™ software package, the students were introduced to triaging primary antimalarial screening data, evaluating calculated drug like properties and finally the selection of a hit series. The students then embarked on a hit-to-lead optimization through a decision making process involving improvement of the calculated drug like properties, improvement of metabolic stability using the web based SMARTCyp© algorithms and the calculation of analog activity using a QSAR model from the mobile application SAR Table©.

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