Lecture Title:

Controlling Physicochemical Properties in Drug Design

Speaker:
Dr Klemens Hoegenauer (Novartis, Switzerland)

Abstract: The talk will explain why physicochemical properties are important for any drug, and in particular, drugs that are orally dosed and therefore need to overcome the absorption barrier. The necessity of a balanced lipophilicity profile for oral drugs will be discussed as they need to display both hydrophilic behavior (for solubility) and also lipophilic behavior (for membrane permeability). Different ways to measure or calculate lipophilicity, its role in desirability scoring systems and efficiency metrics will be presented. The last part of the talk will focus on molecules with Mw>500 and discuss the implications on property design.

Klemens Hoegenauer obtained his PhD with Professor Johann Mulzer in Vienna, Austria, working on the total synthesis of the alkaloid huperzine. After his graduation, he continued with a postdoctoral stay in the group of Professor Steven V. Ley in Cambridge, UK, where he spearheaded the efforts that led to the first total synthesis of thapsigargin and close analogs. He joined Novartis as a medicinal chemist in 2002, initially working at the Vienna site and since 2008 in Basel, Switzerland. He has worked on a number of anti-inflammatory hit-to-lead and lead optimization programs, including S1P agonists, PI3Kδ inhibitors and RORγt inhibitors. Since 2015, he supports the Hit Generation Sciences group as a Senior Medicinal Chemist focusing on the generation of first chemical matter for early projects covering the entire Novartis research portfolio. In 2018, Klemens became a scientific co-founder of the biannual “Alpine Winter Conference on Medicinal and Synthetic Chemistry” series in St. Anton, Austria.