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Conformational Design and its importance in drug discovery

One of the key drivers in applied medicinal chemistry which is often referred to is property based multifactorial design, at the core of which is the endeavor to harmonize a number of workflows into one. Optimization of potency, selectivity as well as ADMET properties is complex as a result of its high degree of multi-dimensionality and interdependences. Throw into the mix the question how conformations of molecules impact on properties of molecules and it becomes an almost intractable problem to solve rationally it seems.

However, it is argued that detailed understanding of molecular shapes as well as the impact factors which lead to diverse conformational behaviors and the targeted manipulation of shape preferences, conformational design, are potentially an important opportunity to harness efficiencies and could make designs more effective.

The talk will aim to make a case why conformational design is important, assesses some of the principals, which rationalize targeted manipulation of conformational preferences and the impact of them on biological properties of molecules.

Biography

Thorsten Nowak completed his PhD from the University of Cambridge (UK) in the areas of aldol methodology and natural product synthesis. In 1996, he joined AstraZeneca where he worked on all stages of drug discovery in medicinal chemistry as Team Leader and Project Manager. His keen interest in new technologies motivated a career move in 2012, when he joined C4X Discovery. Since he joined C4X, he has been instrumental in expanding the capabilities of C4X into applied drug discovery. In his current role as Head of Medicinal Chemistry, he is leading the chemistry group and is responsible for all internal drug discovery efforts conducted at C4X as well as program work with our pharmaceutical partners.

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