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NMR Driven conformational design - A powerful drug design tool

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Clear and detailed understanding of dynamic 3D small molecule in solution and the dynamic interchange of accessible low energy conformations have traditionally been predicted computationally or extrapolated from small molecule crystal structure data. The impact of a new quantitative and precise technology is described that provides detailed information of ligand conformations in solution. When coupled with activity data it gives unprecedented accuracy in describing pharmacophoric information that can deliver high impact, in for example, drug design contexts. The necessary experimental information required to define solution conformation is extracted from one & two-dimensional NMR data of ligand molecules in physiologically relevant solution conditions. In addition to driving drug design, conformational information on ligand molecules can be applied to broad settings in drug discovery enabling the identification of chemical equity independently of general screening approaches to template-hopping and virtual screening. Furthermore, it can significantly impact on small molecule drug design in Lead Generation and Lead Optimisation independently or in conjunction with computational chemistry or structure based drug design approaches. The presentation details the application of the technology and describes the use and impact with a number of case studies in the areas of structure based design and GPCR targeting settings.

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 joint AstraZeneca where he worked on all stages of drug discovery from target to candidate selection in medicinal chemistry as team leader and project manager. His keen interest in new technologies motivated a career move from big pharma to platform technology business in 2012 when he joint C4X Discovery. In his current role he is responsible for all internal drug discovery projects at C4X Discovery as well as continued development of the technology in the context of application to drug discovery.

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