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Put shape back into chemistry: How important is conformational design?

The spotlight in drug discovery and design has been firmly centred on “quality” and “efficiency” in an endeavour to improve productivity and reduce high development attrition rates. In particular, much attention has been focused on measured and predicted drug property optimization because this is expected to significantly impact both the quality and the efficiency of drug design. With such a dominating focus, it is right to ask if other important aspects of drug design are being generally overlooked by the medicinal and computational chemistry community. This presentation aims to make a case for the increasingly clear importance (and therefore necessary adoption) of conformational design in harmony with property optimization.

It is argued that the impact of creatively applied conformational design based on a validated experimental foundation will lead to a number of benefits and can be far reaching. For example, limiting shape diversity whilst gaining a deep understanding of shape giving structural features presents a complementary approach to property based design. It will lead to a tighter integration of the highly complementary medicinal and computational chemistry workflows. And importantly, it will provide undoubtedly a driver to re-invigorate the development and creative exploitation of experimental methods aimed at describing and predicting the conformational behaviour of small molecules in solution. Hence, conformational design based on experimental evidence offers new drivers for innovation in drug discovery.

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 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 joined 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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