Dr Jianling Wang gave this presentation at the International Symposium on Compound Design Technologies held in Shanghai, China on 21 November 2014.

Abstract

The high attrition rate in drug development and the deteriorated drugability as a result of the shifted chemical space of new therapeutic target for unmet medical needs have posed drastic challenges in current drug discovery and development. It has triggered the strategic transition in the past decade into parallel assessment of efficacy and comprehensive ADMET (absorption, distribution, metabolism, elimination and toxicity)/DMPK (drug metabolism and pharmacokinetics) properties of new chemical entities (NCEs) in the lead selection and optimization stages, to convert chemically a problematic NCE to an 'all-around' candidate. The emergence of such comprehensive *in silico, in vitro* and *in vivo* ADMET/DMPK tools is, by no means, indicative of the game being over, as the "more is better" type of "box-checking" profiling strategy is no longer viable and frequently leads to suboptimal productivity. This presentation will focus on the intelligent integration of comprehensive
in silico, in vitro
and
in vivo
ADMET/PK data and routine application of hypothesis testing, enabling to diagnose the causative within the interplay among multiple ADMET/DMPK properties, and to project the benefits over risks of a drug candidate in clinic. An overview of existing tools will be presented along with selected case studies.

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