Informatics and modeling supports drug safety

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Abstract

High attrition rates and the failure of late stage compounds due to toxicity issues are forcing pharmaceutical companies to evaluate drug safety at an earlier stage, as well as in a more structured manner. Developing and applying computational models and informatics tools are a crucial part of current Drug Safety. This presentation will provide insight into the complexity of Safety data and give examples of how the data can be utilised depending on data quality and data structure. Emphasis will be mainly on supporting drug projects in the earlier phases up to clinical testing, with examples ranging from simple rule-based systems and QSAR models of screening data to modelling of more complex in vivo and clinical data.