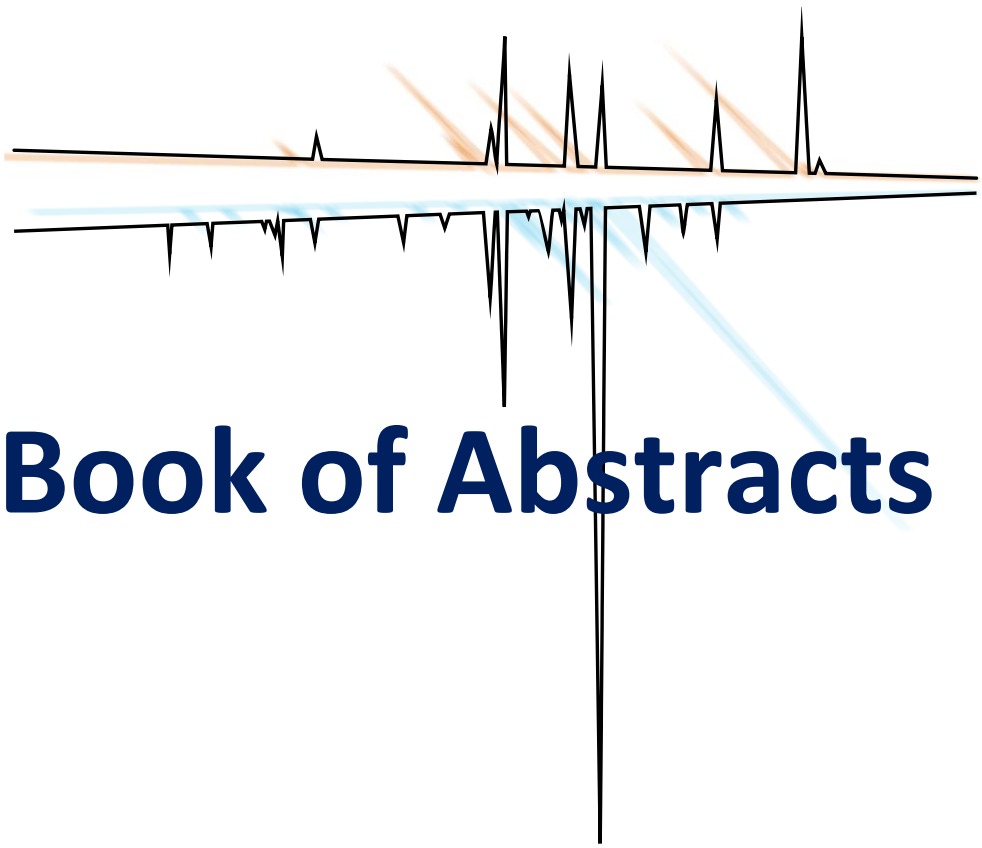
10th IAPC Meeting

Tenth World Conference on Physico-Chemical Methods in Drug Discovery & Sixth World Conference on ADMET and DMPK



Book of Abstracts

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&
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Highlight on the benefits of PBPK modeling: A link between drug properties and its in vivo performance

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Physiologically based pharmacokinetic (PBPK) modeling or more recently also known as physiologically based biopharmaceutics modeling (PBBM) is a computer-aided (*in silico*) biopharmaceutical tool, designed to mechanistically describe bioperformance of a drug and predict its absorption and systemic availability. PBPK/PBBM was quickly adopted by pharmaceutical companies and medical regulatory agencies, its scope has expanded over the years, and nowadays PBPK/PBBM represents an essential tool in various phases of drug and formulation development (1).

A major advantage of PBPK modeling over traditional *in vitro* and preclinical animal studies is the ability to link the physicochemical properties of a drug to its dissolution, absorption and disposition in a target patient or population, taking into account specific physiological conditions. This is accomplished through linked differential equations that describe simultaneous or sequential dynamic processes that a drug undergoes in the body following different routes of administration. PBPK predictions can refer to various physiological or disease states, so this unique approach can support personalized pharmacotherapy and drug/dose/dosing regimen selection in different patient populations or individual patients (2).

Although PBPK modeling can rely solely on the *in silico* generated data regarding drug's properties (i.e., predicted based on the chemical structure of a drug), the prediction accuracy can be significantly improved with experimentally obtained input values. Therefore, any improvement in experimental drug characterization methods will inevitably lead to more reliable PBPK predictions.

To illustrate the concept and implementation of PBPK modeling, this presentation will provide basic information on the structure of a PBPK model, and emphasis will be placed on case studies describing the interplay between drug-specific and physiologically relevant parameters that determine drug performance *in vivo*. Selected examples will be used to demonstrate how PBPK predictions can be used in conjunction with *in vitro* data on drug properties to answer clinically relevant questions, such as selecting appropriate drug therapy in bariatric patients, and assessing the impact of changes in gastric pH resulting from impaired gastric secretion or co-administration of proton pump inhibitors on drug dissolution, potential gastrointestinal precipitation and concomitant oral absorption.

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References

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