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Application of QSPkR for prediction of key pharmacokinetic parameters

By Zhivkova, Zvetanka

Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Steady state volume of distribution, clearance and plasma protein binding | Over the last few decades quantitative structure - pharmacokinetics relationship (QSPkR) modeling established itself as a high throughput and reliable approach for prediction of the key pharmacokinetic parameters (PK) of new drug candidates at the very early stages of drug development process. Based on the principles of QSAR, QSPkR faces much more problems including the insufficiency of high-quality experimental PK data, the incomplete knowledge on the underlying mechanisms, and the lack of standardized procedures and acceptance criteria for high quality QSPkRs. This book summarizes the obstacles and challenges in QSPkR modeling and proposes a workflow for development of robust and predictive QSPkR based on the philosophy and the best practices in QSAR. Several published models for QSPkR prediction of the key PK parameters are briefly discussed. Personal results for QSPkR modeling of human body V_{ss} , CL and PPB with respect to the ionization state of the molecules are reported. The book could be equally helpful for both researchers in the field of drug design and students in pharmacy and related disciplines. | Format: Paperback | Language/Sprache: english | 136 pp.



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