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Nota di contenuto	Biosimulation in Drug Development; Contents; Preface; List of Contributors; Part I Introduction; 1 Simulation in Clinical Drug Development; 1.1 Introduction; 1.2 Models for Simulations; 1.3 Simulations in Clinical Drug Development: Practical Examples; 1.3.1 Predicting the Outcome of Phase I Studies of Erythropoietin Receptor Agonists; 1.3.2 Simulations for Antimicrobial Dose Selection; 1.3.3 Optimizing the Design of Phase II Dose Finding Studies; 1.3.4 Predicting the Outcome of Phase III Trials Using Phase II Data; 1.4 Conclusions; 2 Modeling of Complex Biomedical Systems; 2.1 Introduction 2.2 Pulsatile Secretion of Insulin 2.3 Subcutaneous Absorption of Insulin; 2.4 Bursting Pancreatic -Cells; 2.5 Conclusions; 3 Biosimulation of Drug Metabolism; 3.1 Introduction; 3.2 Experimental Approaches; 3.2.1 Animal Test Models; 3.2.2 Microbial Models; 3.3 The Biosimulation Approach; 3.4 Ethical Issues; 3.5 PharmBiosim - a Computer Model of Drug Metabolism in Yeast; 3.5.1 General Concept; 3.5.1.1 Chemical Abstraction; 3.5.1.2 Biological Abstraction; 3.5.2 Initial Steps - Experimental Results; 3.5.2.1 Dehalogenation (Pathways

II and III); 3.5.2.2 Retro-Claisen Condensation (Pathway IV)
3.5.2.3 Ester Hydrolysis (Pathway VI)3.5.2.4 Competing Pathways and Stereoselectivity; 3.6 Computational Modeling; 3.6.1 Selection of the Modeling Software; 3.6.2 SBML-compatible Software; 3.6.2.1 Cellware; 3.6.2.2 Copasi; 3.6.2.3 Ecell; 3.6.2.4 JigCell; 3.6.2.5 JSim; 3.6.2.6 Systems Biology Workbench; 3.6.2.7 Virtual Cell; 3.6.2.8 XPPAUT; 3.6.3 CellML-compatible Software; 3.6.4 Kinetic Model; 3.6.4.1 Methods; 3.6.4.2 Model Derivation; 3.6.4.3 Results; 3.6.5 Stoichiometric Model; 3.6.5.1 Methods; 3.6.5.2 Model Derivation; 3.6.5.3 Results
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5.2.1.1 Full-Scale Mechanistic Gray-Box Modeling

Sommario/riassunto

This first comprehensive survey to cover all pharmaceutically relevant topics provides a comprehensive introduction to this novel and revolutionary tool, presenting both concepts and application examples of biosimulated cells, organs and organisms. Following an introduction to the role of biosimulation in drug development, the authors go on to discuss the simulation of cells and tissues, as well as simulating drug action and effect. A further section is devoted to simulating networks and populations, and the whole is rounded off by a look at the potential for biosimulation in industrial dru
