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DRUG DOSAGE OPTIMIZATION BASED ON MACHINE LEARNING AND MECHANISTIC MODELING

Keywords Model-informed drug development, Drug Dosage Optimization, Machine Learning, Mechanistic Modeling, Agent-Based Modeling, Pharmacometrics

INVENTION NOVELTY

The novelty of the technology lies in its unique approach to drug dosage optimization, which combines machine learning techniques with mechanistic modeling. Unlike traditional methods, which often rely solely on empirical data or simplistic models, this approach integrates advanced computational algorithms with detailed mechanistic understanding of drug action and big datasets.

VALUE PROPOSITION

By leveraging machine learning and mechanistic modeling, we provide pharmaceutical companies with the tools to predict drug effects more accurately, optimize dosing regimens, and identify patients who are most likely to benefit from specific treatments. Additionally, our technology reduces reliance on costly and time-consuming empirical testing, minimizing the need for animal and human experiments.

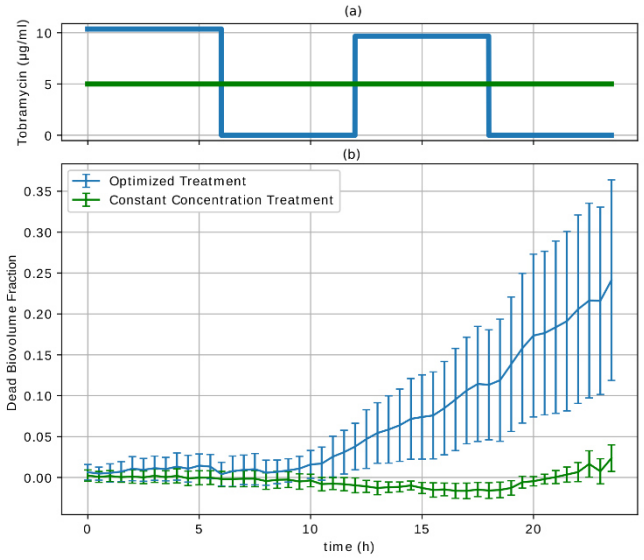

Figure1. Experimental results of PA biofilm treatment with Tobramycin. (a) shows the concentration of antibiotics in time. The green line corresponds to the constant treatment and blue line to the dosage deployment pattern suggested by results of simulation. (b) shows the proportion of dead biovolume in the treated biofilm (subtracted dead biovolume in the untreated control). The optimized deployment eradicates the PA biofilm more efficiently. © Helmholtz-Zentrum für Infektionsforschung

TECHNOLOGY DESCRIPTION

Our online Model-Informed Drug Development (MIDD) software has two core modules. The **Prediction Module** employs a diverse range of modeling techniques, including PK/PD models, Agent-Based models, and Machine Learning, to predict drug effects with unprecedented accuracy and generality across various drugs. Integrated with optimization algorithms such as differential evolution and genetic algorithms, the **Optimization Module** provides users with efficient tools to explore and identify optimal dosage regimens, enhancing decision-making in drug development. Hosted on cloud platforms like Microsoft Azure, our user-friendly interface enables seamless data upload, visualization of critical features, and streamlined analysis of multi-modal data, empowering drug development experts to accelerate research and optimize therapeutic outcomes. In a proof-of-principle study the *in silico* driven selection of dosing regimens to optimize antibiotics treatment against *Pseudomonas aeruginosa* (PA) biofilms was shown to improve treatment by 22 %. Using the biologically-informed Prediction Module in combination with the Optimization Module, designed to maximize the proportion of dead biovolume, demonstrated the ability to improve current therapeutic approaches.

COMMERCIAL OPPORTUNITY

The technology is available for in-licensing. Additionally, the services can be customized to specific therapeutic areas and drug candidates.

DEVELOPMENT STATUS

The technology has undergone initial proof-of-concept studies and validation experiments. A prototype is under development.

HZI HELMHOLTZ Centre for Infection Research

Ascenion GmbH
Herzogstraße 64
D-80803 München
info@ascenion.de
www.ascenion.de

Licensing Contact
Dr. Petra Köhler
Technology Manager
T: +49 531 6181-2091
koehler@ascenion.de