PhysPK

Disruptive software for simulation of physiologically based pharmacokinetic models in individuals and populations

https://www.physpk.com/

Physiologically based pharmacokinetic (PBPK)/Pharmacokinetics (PK)/Pharmacodynamics (PD)

version: May-2021 contact: info@physpk.com

Analysis & Models (Unlimited compartments)	
Noncompartmental analysis	✓
Compartmental analysis	✓
Single-compartment model	✓
Multi-compartmental models	✓
M&S individual & population	✓
Standard PD empirical models	✓
Physiological models	✓
Population estimation module	✓
Population validation module	✓
Re-use & export of models & experiments	✓
Physiological mechanisms	
Mass conservation - Continuity	✓
Non-linear elimination	✓
Phase partition of compounds	✓
Net generation - Reactants	✓
Volumetric capacitance	✓
Macromolecule and transporter vesicle trafficking	✓
Quasi-static binding to macromolecules	✓
3D/2D/1D spatial region	✓
Membranes and barriers/passive and transporter	✓
Multilevel physiological tissues	✓
Flow limited tissues	✓
External devices	✓
Biological activity	
Transit absorption and liberation structures	✓
Intrinsic clearances or direct Michaelis – Menten	✓
Metabolism and for carrier-mediated transport	✓
In Vitro In Vivo Correlation (IVIVC)	✓
Virtual bioequivalence	✓
Direct effect PD elements	✓
Pathology/Tissues - oriented WB-PBPK models	✓
Customized macromolecules database	✓
Customized metabolic network	✓
General law of mass action kinetics	✓

Preclinical ADME and Human Studies	
First-time-in-human	✓
Single ascending dose	✓
Multiple ascending dose	✓
Drug-drug interaction	✓
Thorough QT	✓
Hepatic impaired	✓
Renal impaired	✓
Site of absorption	✓
Radiolabeled mass balance	✓
Exposure-response	
Characterize drug exposure	✓
Predict dosage requirements	✓
Assess changes in dosage requirements	✓
Estimate rate of elimination and rate of absorption	✓
Assess relative bioavailability / bioequivalence	✓
Characterize intra- and inter-subject variability	✓
Understand concentration-effect relationships	✓
Establish safety margins and efficacy characteristics	✓
Dosing simulations (Route administration)	
Intra-venous (IV)	✓
Extra-basal (EB)	✓
Oral	✓
Inhaled	✓
Drug reservoir	✓
Simulation scenarios and studies	
Computing calculator elements	✓
PBPK/PK/PD indices	✓
Interaction with other external software	✓
User-centered design approach	✓
Graphical user-friendly interface	✓
Integrated PK study reports	✓
Standalone PK reports	✓
Data collection and interrogation	✓
Dataset generation	✓

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Pharmacokinetics (PK)	
Complete set of categorized PK components	✓
Combination of ADME mechanisms and functions	✓
Non-compartmental analysis (NCA) integrated	✓
Standard PK models parameterized	✓
Pharmacodynamics (PD)	
Direct effect PD elements: Hill, Emax, Linear,etc.	✓
Cell proliferation – kill models with phases	✓
N-compart. delay with different transduction signals	✓
Indirect response models: Models I, II, III and IV	✓
Drag-and-drop PBPK/PK components using ports	✓
Physiologically based PK (PBPK)	
ADME mechanisms for region given by a set of DAEs	✓
Standard PBPK tissues (membranes, barriers, etc.)	✓
Drug administration elements	✓
Physicochemical in-vivo and vitro properties	✓
Liberation and absorption	✓
Passive and transporter flow mass	✓
Quasi-static binding to macromolecules	✓
Non-linear metabolism equations	✓
Customized metabolic networks	✓
Physical laws for continuity of drugs and metabolites	✓
Pressure – vascular flow rates, capacitive laws	✓
Absorption, transit and liberation coefficients	✓
User friendly environment	
Highly intuitive graphics environment	✓
Drag-and-drop components into a canvas	✓
Connection ports to facilitate connections	✓
Easy to learn OO language to create new components	✓
Monitor for plotting graphs, histograms, etc.	✓
Easy to model with differential equations	✓
Use 1D, 2D and 3D tables for interpolation	✓

Applications	
Connect biological system with pharmacokinetics	✓
Models of diabetes mellitus & end-stage renal disease	✓
Absorption and transit gastrointestinal models	✓
Tissue PBPK models: kidney, liver, gut and lung	✓
Population validation module with Montecarlo	✓
Predictive population validation functions	✓
Goodness of Fit (GoF) plots, Bootstrap & Virtual data	✓
Validation of scientific publications	✓
Users can define new PBPK components	✓
Population Estimation (FO, FOCE, FOCEI, ITS, SAEM)	✓
Covariates with variation and real nature	✓
Inter-subject variability with covariance matrix	✓
Validation of the model by epsilon- and eta-shrink.	✓
PK/PD/PBPK models as a standalone black box.	✓
Connectivity	
Export the model to Excel	✓
Reuse the model from other sotfware (using APIs)	✓
Define public and private variables for another users	✓
C++ code generation	✓
Export the model to be executed from the web	✓
Execute the model remotely using web services	✓
Use of csv, xml formats for input/output data	✓
Use of binary HDF5 format for post-process analysis	✓
Connection to C, C++ and FORTRAN libraries	✓
Automatic customization of R Scripts	✓
Target users	
Pharma industry	✓
Academia	✓
Healthcare and e-health industry	✓
Nutrition industry	✓
Chemical risk analysis companies	✓