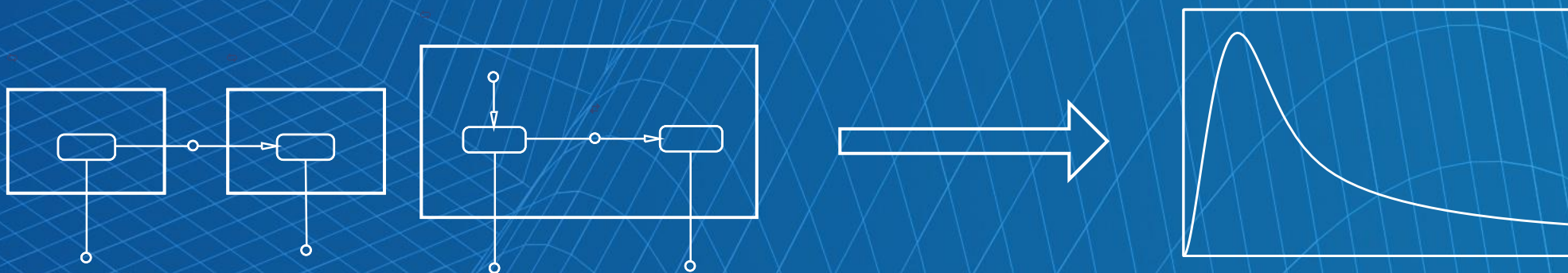
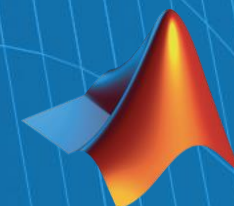


使用 MATLAB 进行新药发现及开发



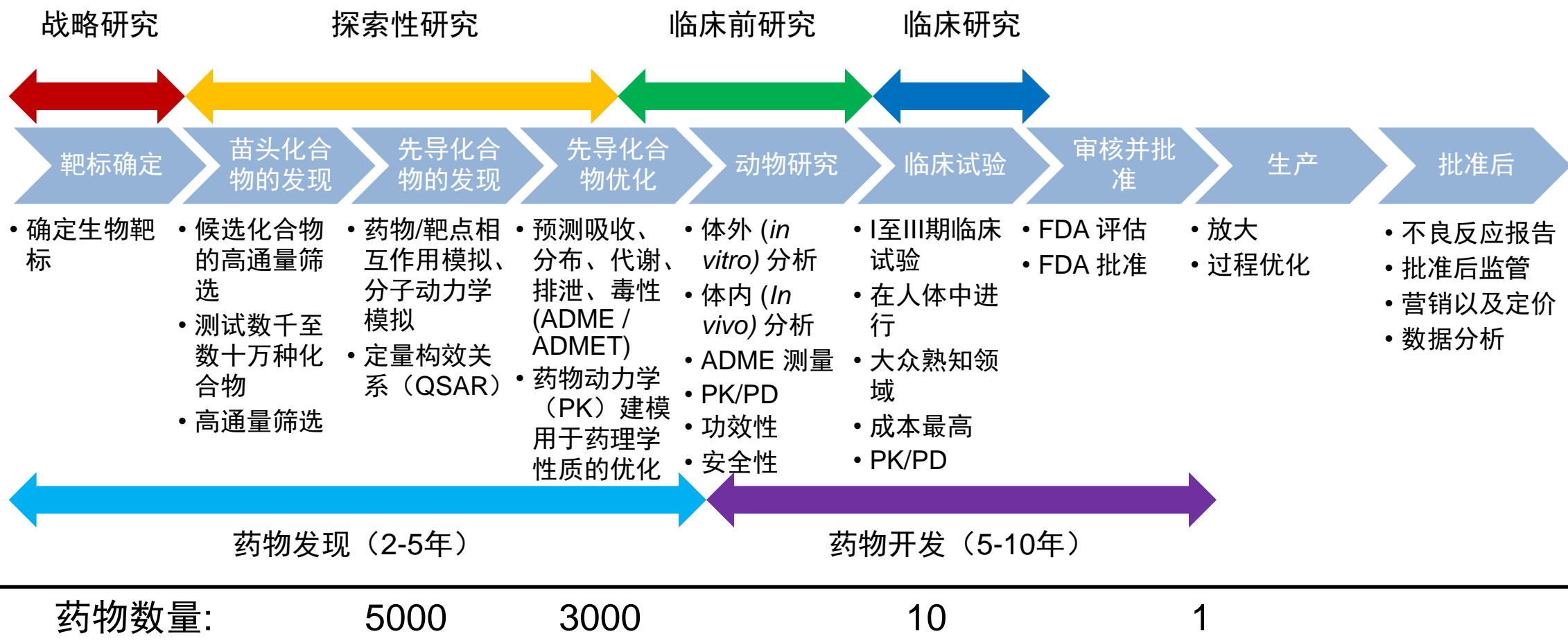
许悦伊
MathWorks 中国



日程

1. 新药发现及开发流程
2. SimBiology是什么？
3. 示例展示
4. 您可以使用 SimBiology 做什么？
5. 用户案例
6. 分享模型以及仿真结果
7. MathWorks 以及社区提供的支持

新药发现及开发流程



药物开发流程



目标：找到一个化合物，它可以：

- 适合人类食用（安全性）
- 可以与靶标结合
- 发挥治疗作用（有效性）
- 可以从人体中代谢

药物发现与开发

发现

临床前研究

临床研究

- 确定药物靶标
- 药物会达到靶标吗?
- 评估 ADME “吸收、分布、代谢和排泄”
- 为首次人体试验找到安全有效的剂量
- 定义目标人群

系统生物学

(PB)PK / PD

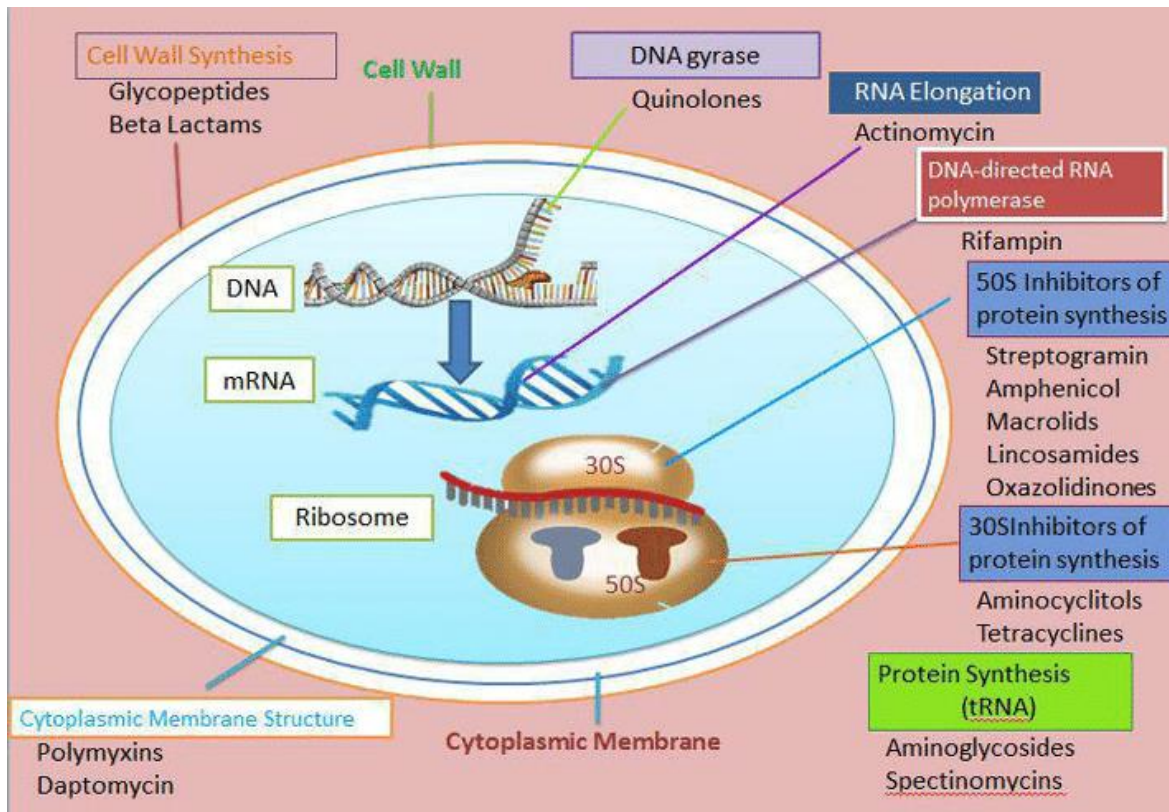
QSP

药物开发过程：靶标确定

发现

临床前研究

临床研究



不同类型的抗生素机理

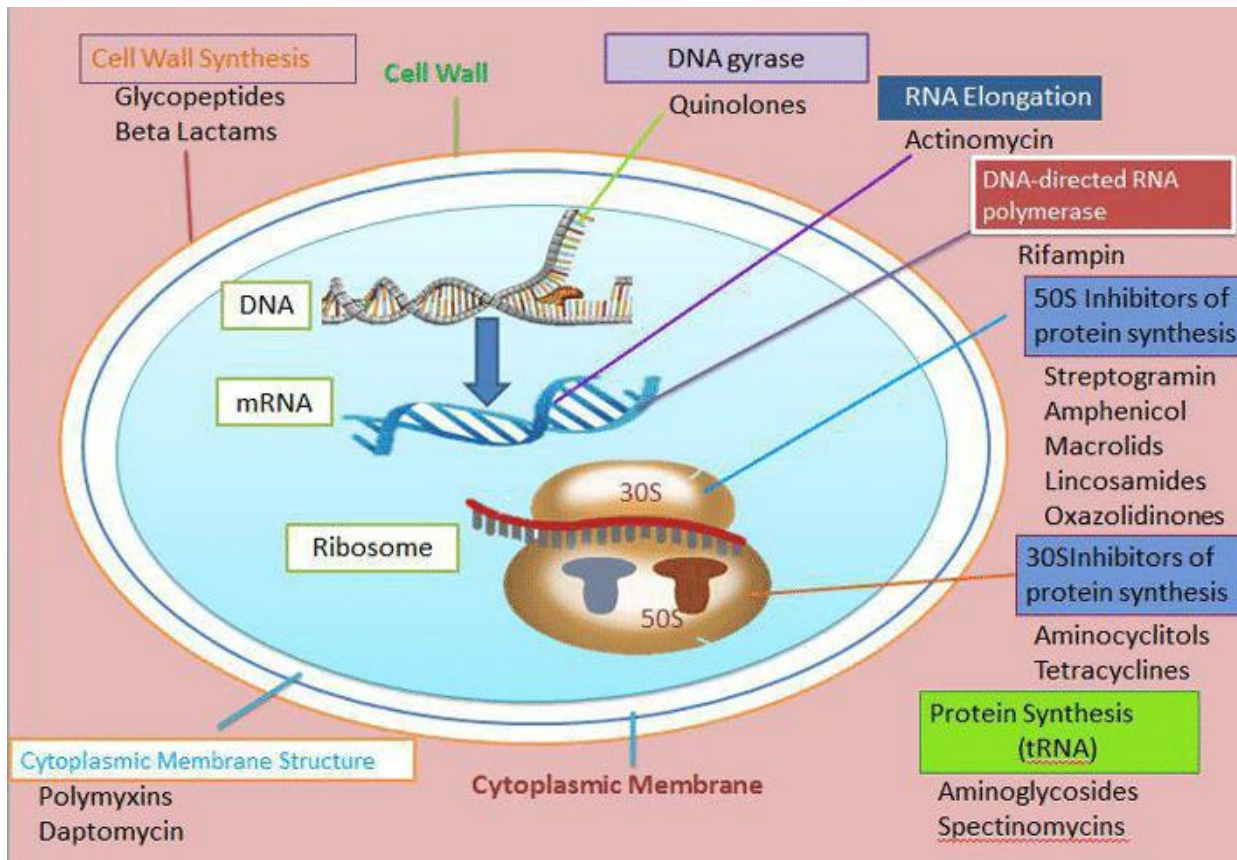
- 抑制或调节参与以下活动的酶 ——
 - 细胞膜生物合成
 - 核酸代谢与修复
 - 蛋白质合成
 - 膜结构的破坏

药物开发过程：靶标确定

发现

临床前研究

临床研究



你是否了解你的靶标:

- 为表型筛选启用基于靶点的药物发现
- 靶点的位置可能影响筛选实验或抑制剂设计
- 靶标的内源是什么

你是否了解你的化合物分子:

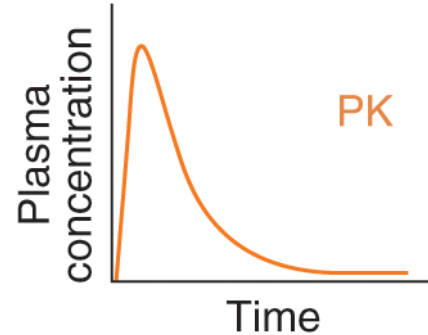
- 分子和哪些靶标和非靶标结合?
- 分子在哪里结合?
- 分子和靶标如何结合 (结合动力学)?

药物开发流程：临床前研究和临床研究

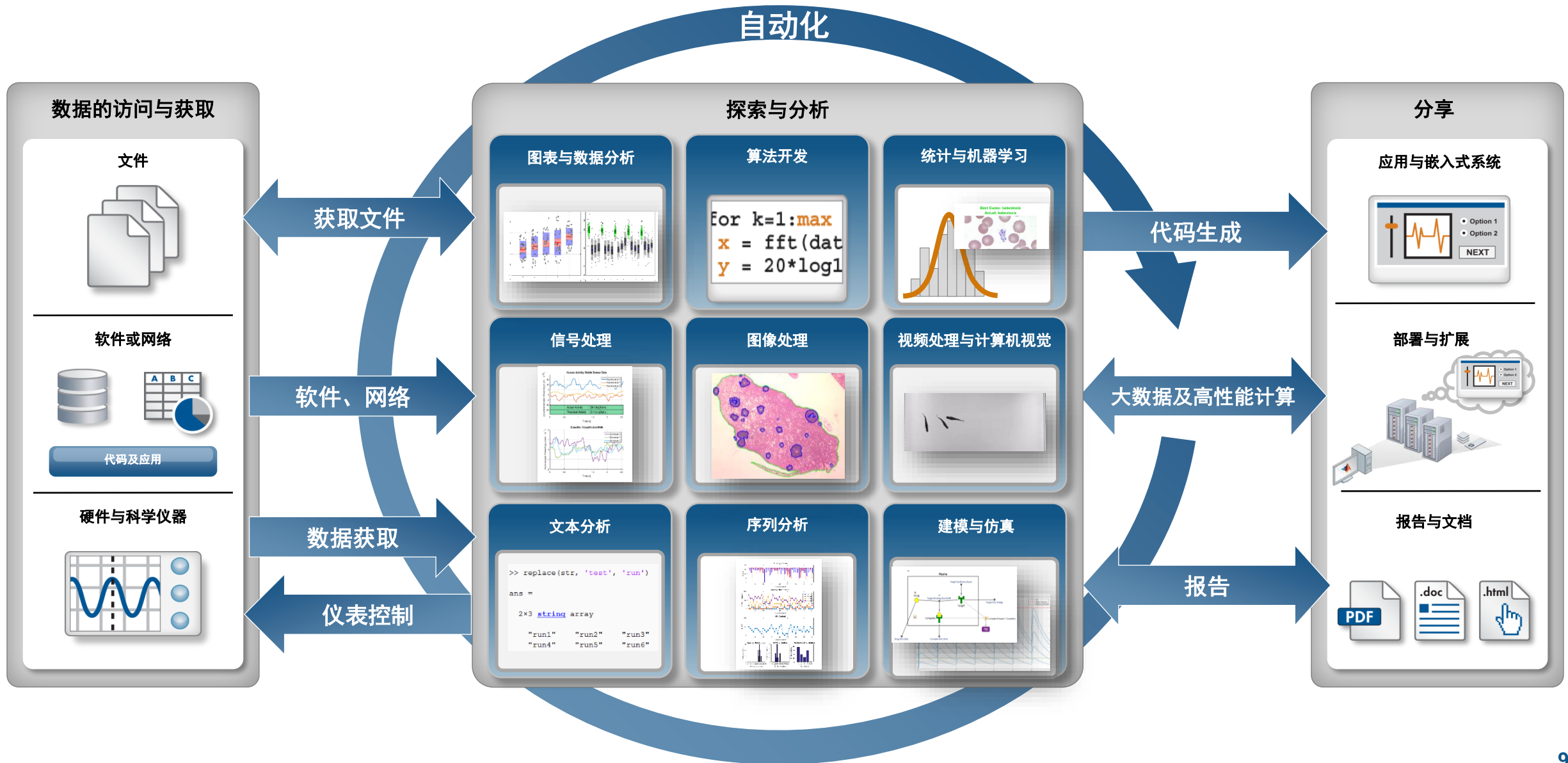
发现

临床前研究

临床研究



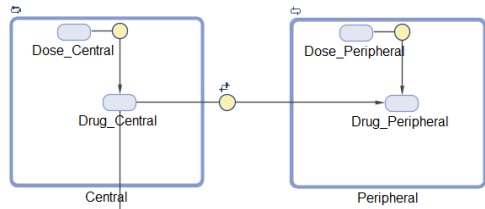
MATLAB: 一个可用于整个工作流的综合平台



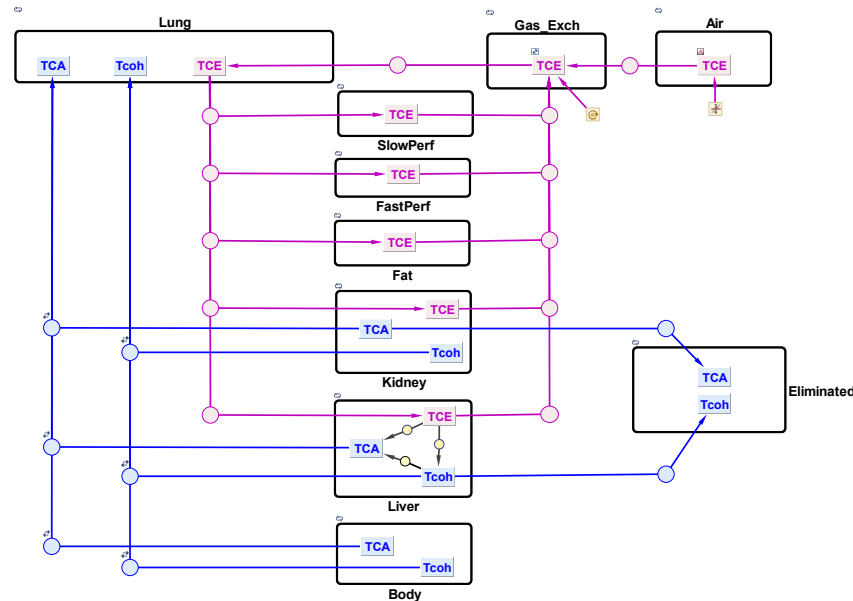
日程

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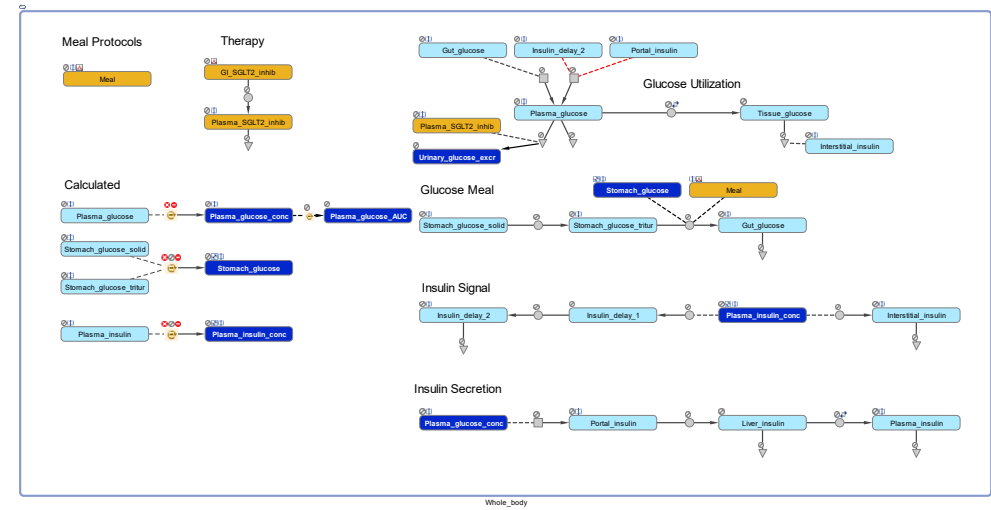
从 PK/PD 到定量系统药理学 (QSP)



PK/PD



PBPK

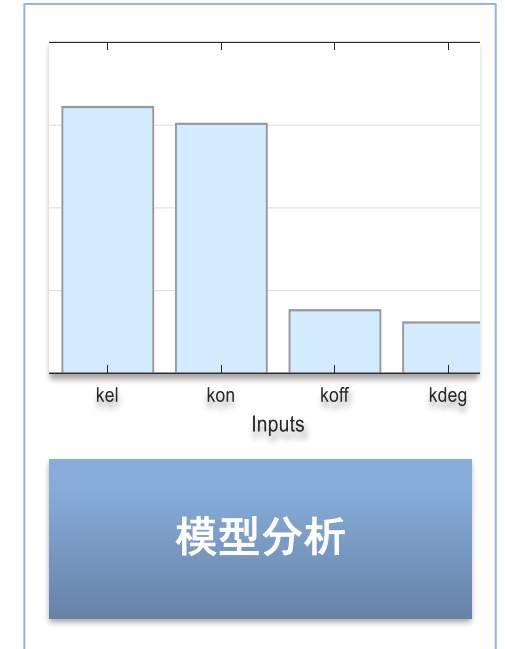
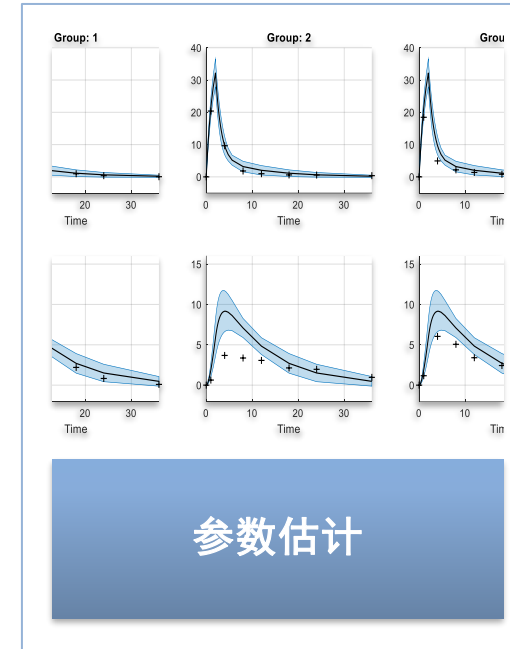
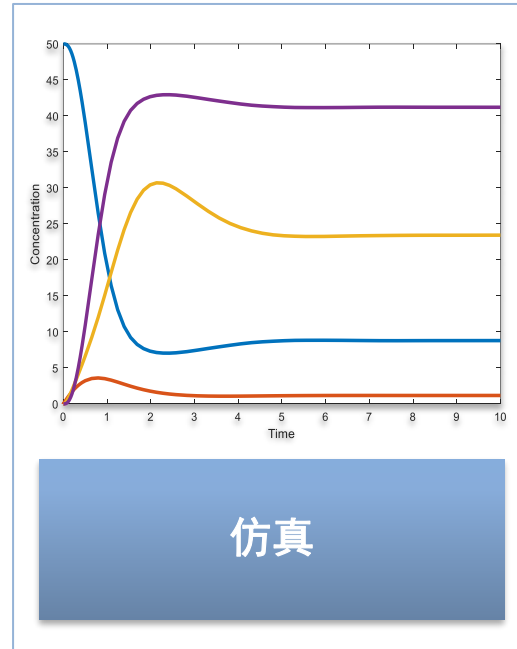
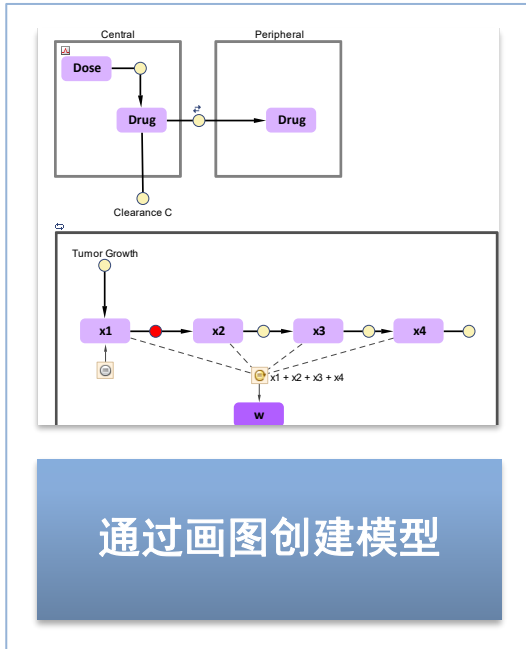


QSP

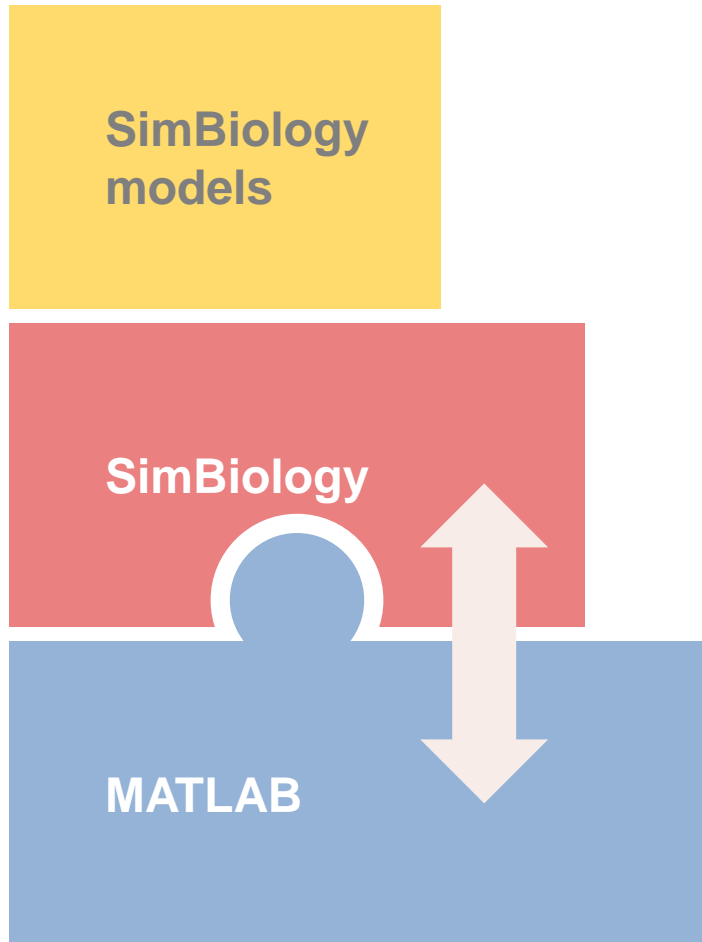
模型复杂性

SimBiology 是什么？

SimBiology® 为用户提供可操作 App 和编程工具，用于：

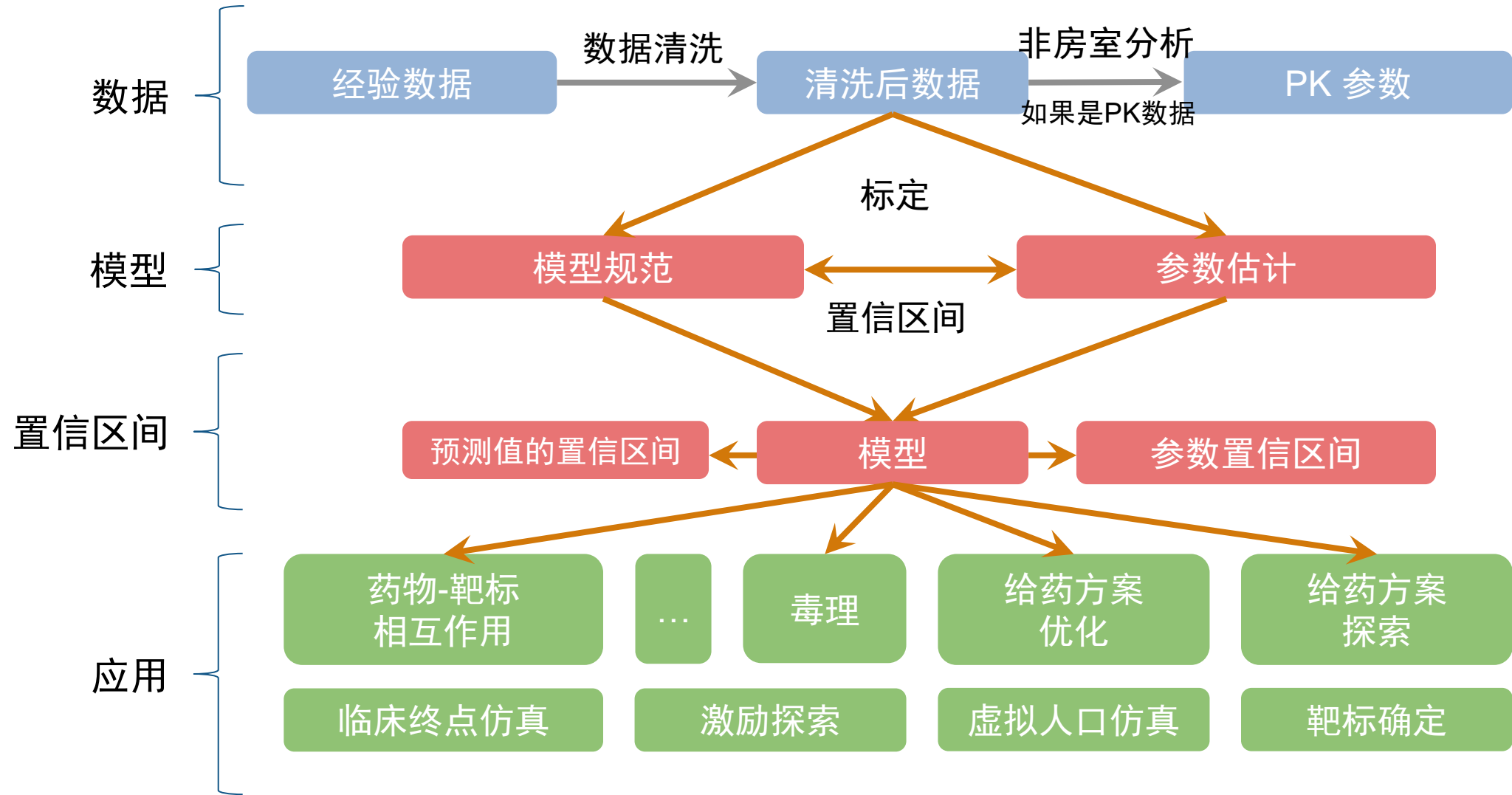


SimBiology 和它所在的 MATLAB 生态系统



- 由终端用户开发
 - 项目促进结果的连续性和可追溯性
 - 图形化模型
 - MATLAB 与 SimBiology 框架确保可重复性
-
- MATLAB 工具箱
 - 基于图形或者代码的工作流
 - 全面的内置分析工具集
 - 通过编译成C代码实现模型加速
-
- 编程语言
 - 多功能平台
 - 专人维护并更新
 - 严格的测试框架，确保平台质量

建模过程工作流示例



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靶向介导药物处置 (TMDD) 模型

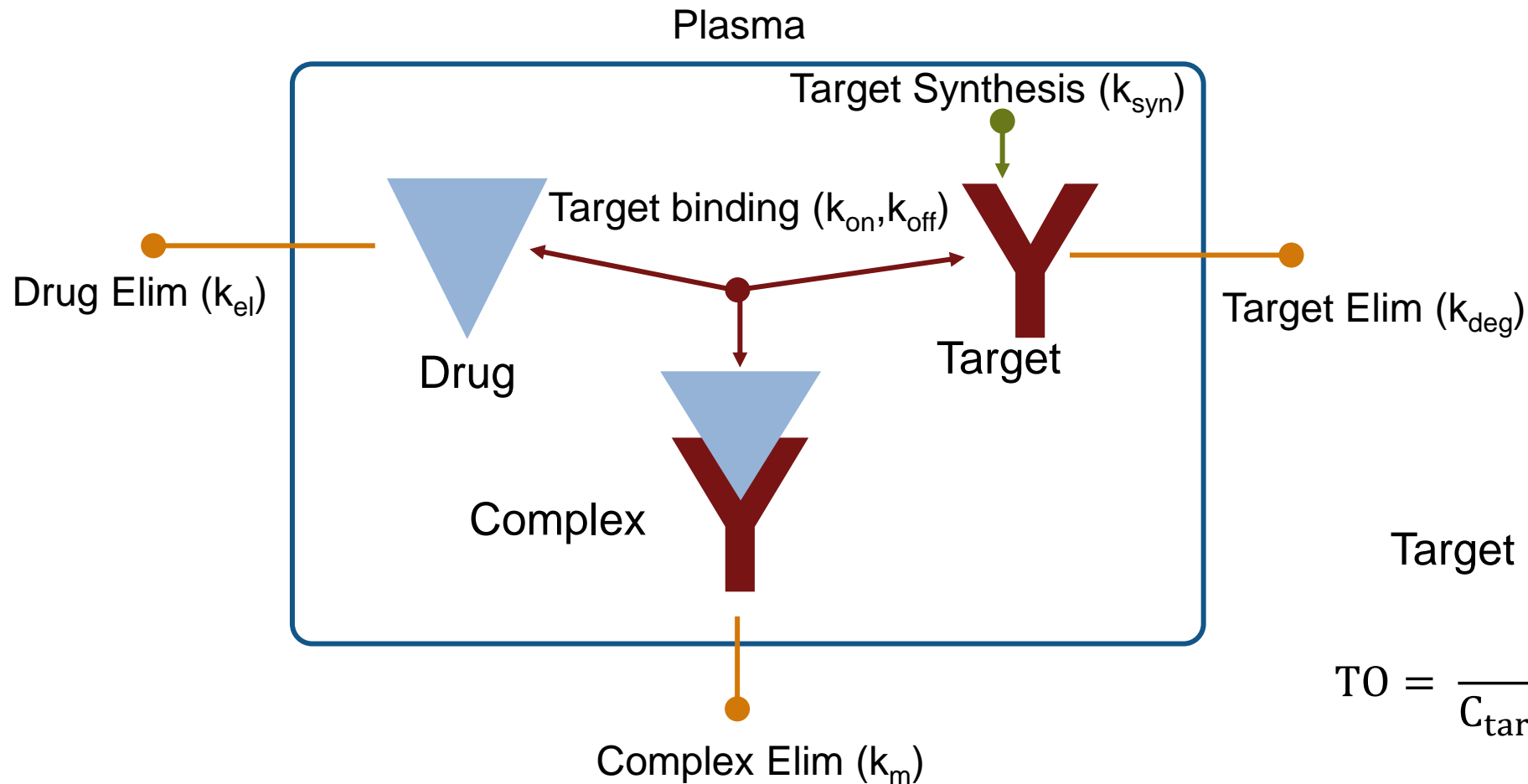
General Pharmacokinetic Model for Drugs Exhibiting Target-Mediated Drug Disposition

Donald E. Mager, William J. Jusko

Journal of Pharmacokinetics and Pharmacodynamics 2001; 28(6): 507–532

- 机械 PK 模型
- 适用于对药理靶点具有高结合亲和力的药物
- 结合靶向介导药物消除
- 目标：描述药物与药理靶点的非线性 PK 行为

TMDD 模型

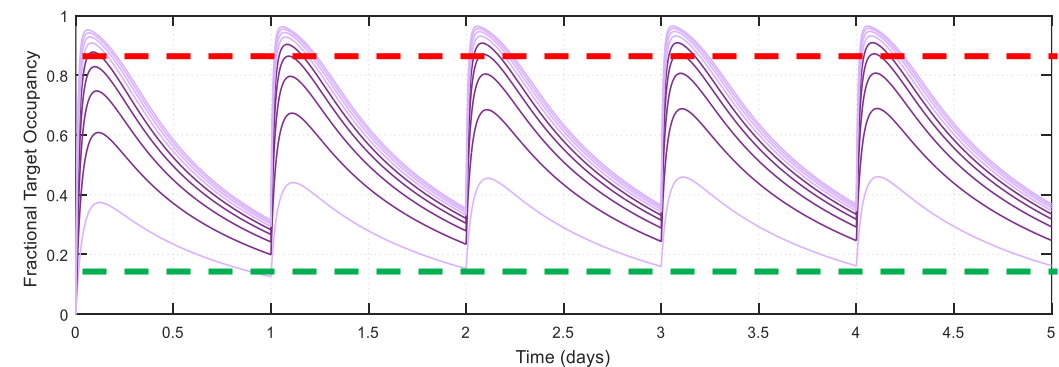
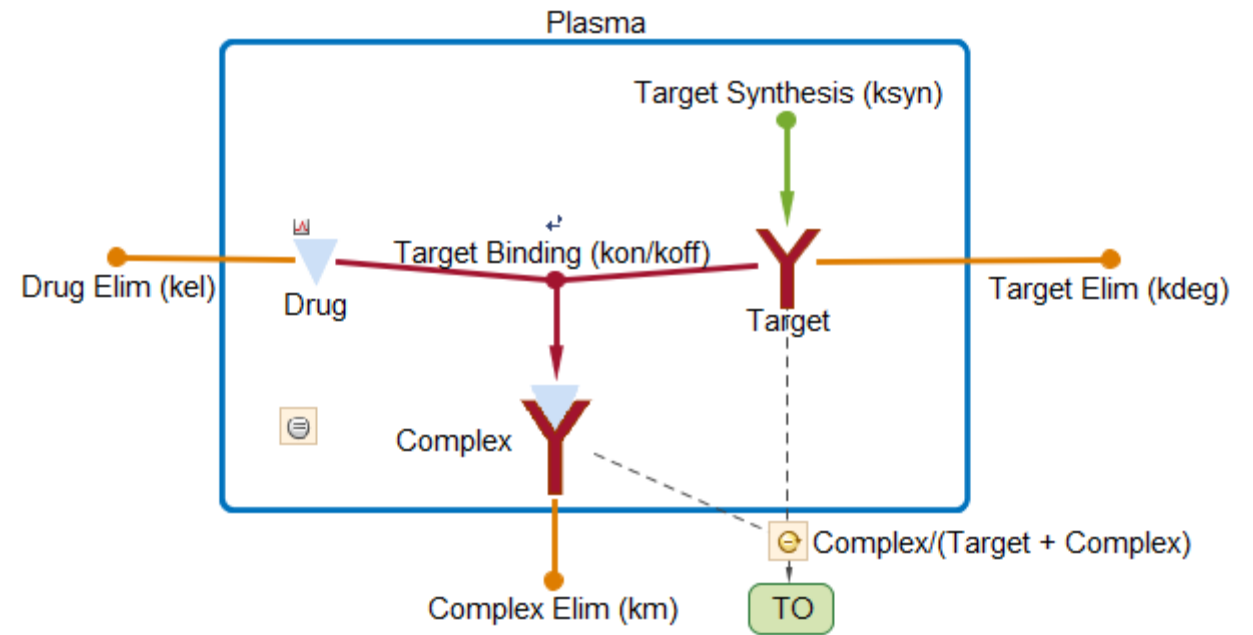


Target Occupancy:

$$TO = \frac{C_{complex}}{C_{target} + C_{complex}}$$

在 SimBiology 中实现

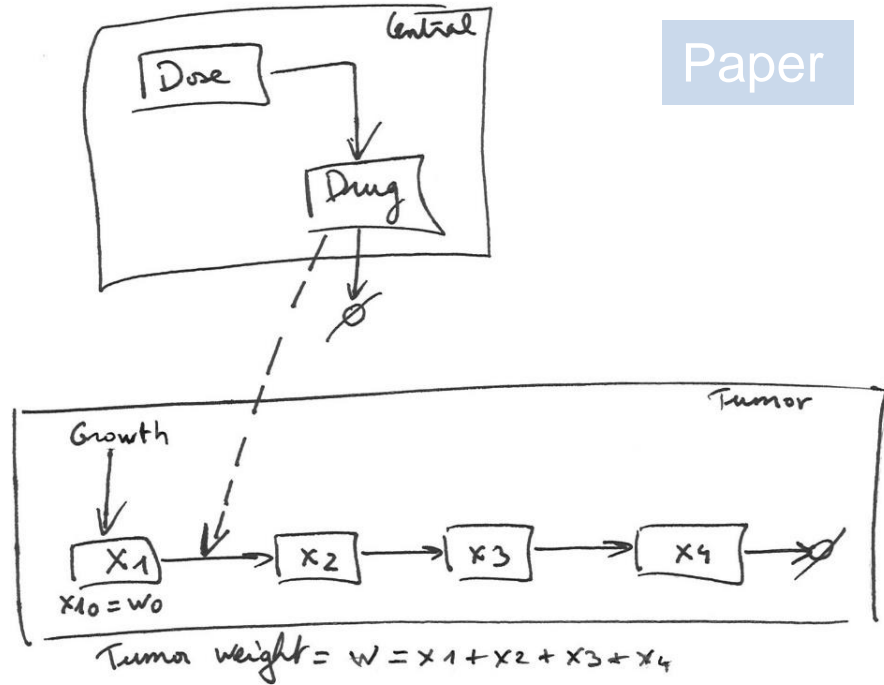
- 图形化模型展示
- 模型可执行：
 - 仿真
 - 非房室分析 (NCA)
 - 数据拟合
 - 给药方案优化
 - 等等等等
- 交互式分析模型表现
- 可以和 MATLAB 以及它的其他工具箱整合



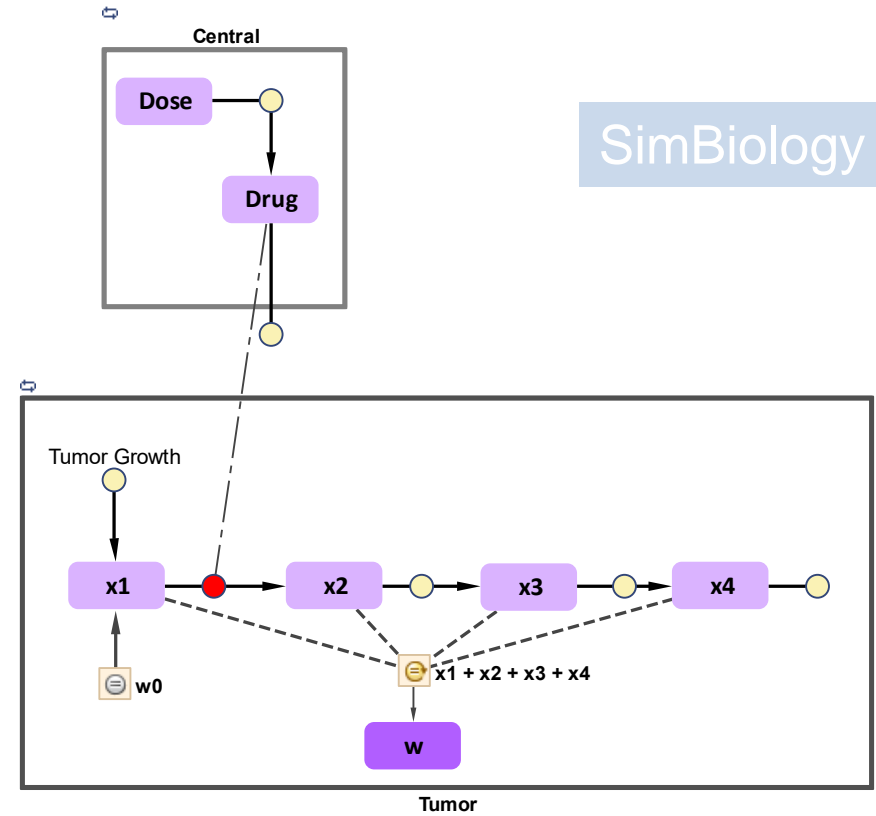
日程

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6. 分享模型以及仿真结果
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SimBiology 使您可以通过画图创建任何模型

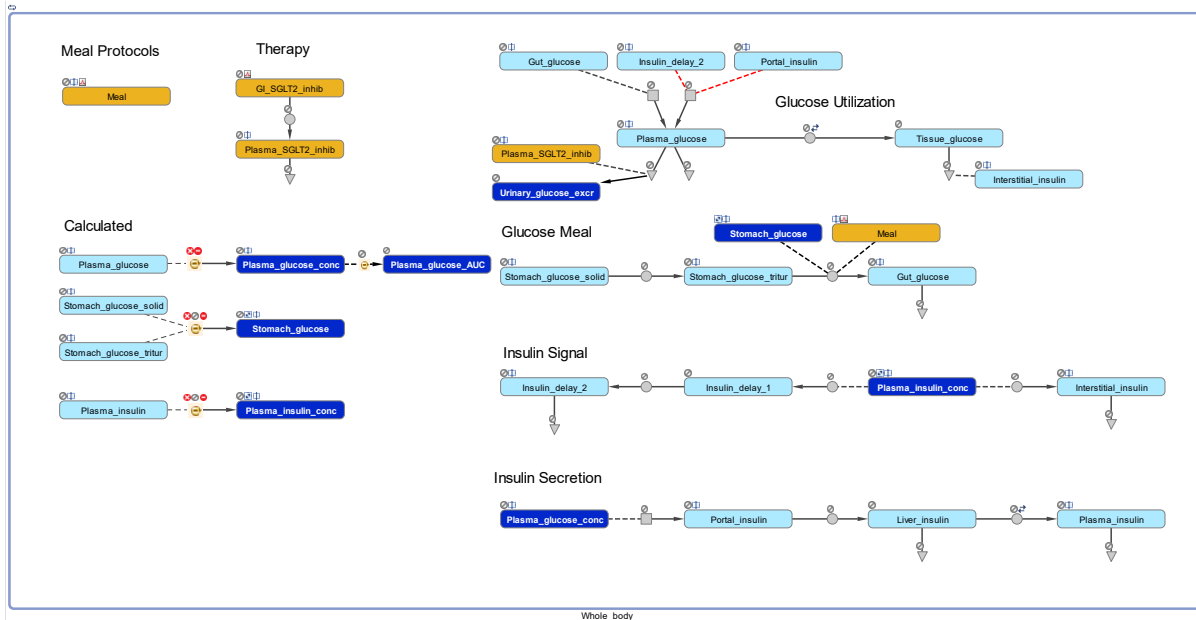


Paper



SimBiology

SimBiology 使您可以通过画图创建任何模型



```

Equations
  Repeated Assignments
    plasma_glucose_AUC_24hr = Plasma_glucose_AUC*body_weight/(time+10080)*1440
    urinary_glucose_excr_24hr = Urinary_glucose_excr/1e3*body_weight/(time+10080)*1440
    renal_threshold = basal_renal_threshold*(1-compound_lmax*Whole_body.Plasma_SGLT2_inhib^2/(compound_IC50^2+Whole_body.Plasma_SGLT2_inhib^2))
    Plasma_insulin_conc = Plasma_insulin/plasma_vol_insulin
    insulin_secr = k_liver_portal*Portal_insulin
    hepatic_extract = -hepatic_extract_dep*insulin_secr+hepatic_extract_basal
    k_insulin_deg_liver = hepatic_extract*k_insulin_plasma_liver/(1-hepatic_extract)
    glucose_excretion = (Plasma_glucose>renal_threshold)*GFR*(Plasma_glucose-renal_threshold)
    Vmax_glucose_util = Vmax_basal_glucose_util+Vmax_dep_glucose_util*Interstitial_insulin
    insulin_dep_glucose_util = Vmax_glucose_util*Tissue_glucose/(Km_glucose_util+Tissue_glucose)
    glucose_utilization = insulin_indep_glucose_util+insulin_dep_glucose_util
    glucose_appearance_rate = fraction_abs*k_glucose_abs*Gut_glucose*(basis/body_weight)
    glucose_prod = EGP_max-LGE*Plasma_glucose-IAL*Insulin_delay_2-PIAL*Portal_insulin
    insulin_prod =
      (glucose_prod+glucose_appearance_rate-insulin_indep_glucose_util-glucose_excretion-k_tissue_plasma*Plasma_glucose+k_plasma_tissue*Tissue_glucose)/plasma_vol_glucose
    delayed_glucose_signal=basal_insulin_secr+(plasma_glucose_conc_rate>0*plasma_glucose_conc_rate&&Plasma_glucose_conc>basal_plasma_glucose_conc)*K_insulin_prod*plasma_glu...
    Stomach_glucose = Stomach_glucose_solid+Stomach_glucose_tritur
    k_emptying = gastric_emptying_kmin+0.5*(gastric_emptying_kmax-gastric_emptying_kmin)/(tanh(gastric_emptying_a*(Stomach_glucose-gastric_emptying_b)*Stomach_Glucose_After_Dosing))-tanh(gastric_emptying_c*(Stomach_glucose-gastric_emptying_d*(Stomach_Glucose_After_Dosing)))+2

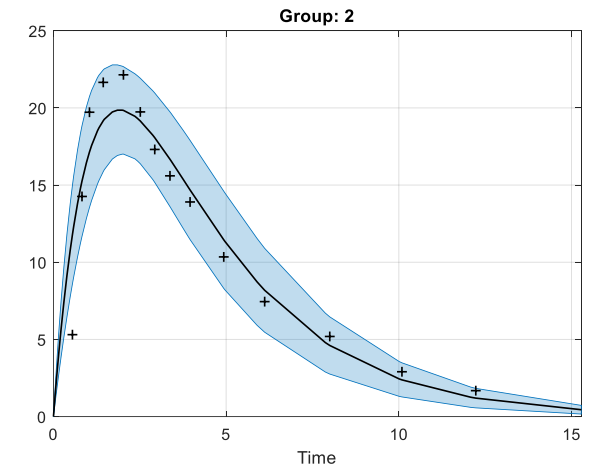
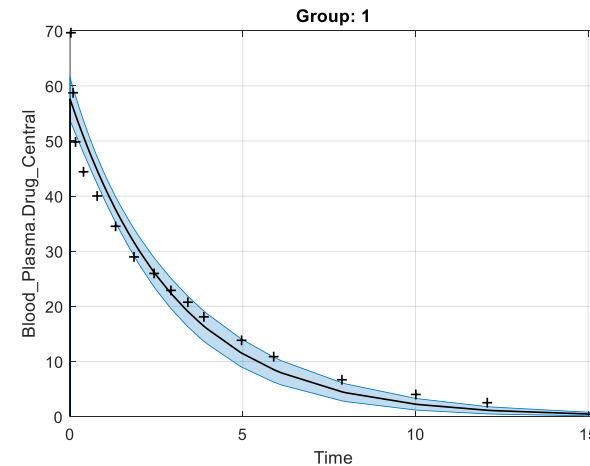
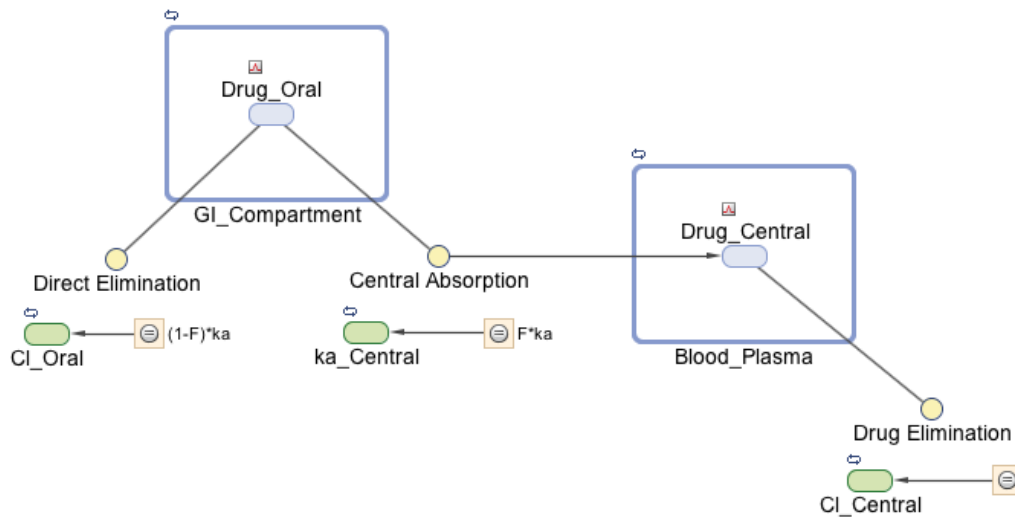
  ODEs
    d(Stomach_glucose_solid)/dt = -(k_grinding*Stomach_glucose_solid)
    d(Stomach_glucose_tritur)/dt = (k_grinding*Stomach_glucose_solid) - (k_emptying*Stomach_glucose_tritur)
    d(Gut_glucose)/dt = (k_emptying*Stomach_glucose_tritur) - (k_glucose_abs*Gut_glucose)
    d(Plasma_glucose)/dt = (glucose_appearance_rate) - (k_tissue_plasma*Plasma_glucose-k_plasma_tissue*Tissue_glucose) + (glucose_prod) - (insulin_indep_glucose_util) - (glucose_excretion)
    d(Tissue_glucose)/dt = (k_tissue_plasma*Plasma_glucose-k_plasma_tissue*Tissue_glucose) - (insulin_dep_glucose_util)
    d(GI_SGLT2_inhib)/dt = -(k_compound_absorption*GI_SGLT2_inhib)
    d(Plasma_SGLT2_inhib)/dt = (k_compound_absorption*GI_SGLT2_inhib) - (CL/Vd*Plasma_SGLT2_inhib)
    d(Insulin_delay_2)/dt = 1/Whole_body*(((k_insulin_delay*Insulin_delay_1)*Whole_body) - ((k_insulin_delay*Insulin_delay_2)*Whole_body))
    d(Insulin_delay_1)/dt = 1/Whole_body*(((k_insulin_delay*Plasma_insulin_conc)*Whole_body) - ((k_insulin_delay*Insulin_delay_1)*Whole_body))
    d(Interstitial_insulin)/dt = 1/Whole_body*(((Plasma_insulin_conc>basal_plasma_insulin_conc)*IAGU*(Plasma_insulin_conc-basal_plasma_insulin_conc))*Whole_body) - ((IAGU*Interstitial_insulin)*Whole_body))
    d(Plasma_insulin)/dt = (k_insulin_plasma_liver*Liver_insulin-k_insulin_liver_plasma*Plasma_insulin) - (k_insulin_deg_plasma*Plasma_insulin)
    d(Liver_insulin)/dt = (insulin_secr) - (k_insulin_plasma_liver*Liver_insulin-k_insulin_liver_plasma*Plasma_insulin) - (k_insulin_deg_liver*Liver_insulin)
    d(Portal_insulin)/dt = (insulin_prod) - (insulin_secr)
    d(Urinary_glucose_excr)/dt = (glucose_excretion)
    d(Plasma_glucose_AUC)/dt = 1/Whole_body*(((Plasma_glucose_conc*AUC_rate)*Whole_body))
  
```

优点:

- 充分的灵活性
- 图表 = 可以进行仿真的模型
- 方便与实验人员交流

参数估计并计算置信区间

- 使用非线性回归和非线性混合效应技术
- 示例：估计药物昂丹司琼（ondansetron）的生物利用度：



	Group	Name	Estimate	ConfidenceInterval		Type	Alpha	Status
1	pooled	'ka'	0.78292	0.41447	1.1514	Gaussian	0.05	success
2	pooled	'clearance'	45.007	39.145	50.869	Gaussian	0.05	success
3	pooled	'Blood_Pla...	138.9	129.6	148.19	Gaussian	0.05	success
4	pooled	'F'	0.64302	0.50814	0.77789	Gaussian	0.05	success

示例链接：<https://ww2.mathworks.cn/help/releases/R2022b/simbio/ug/estimating-the-bioavailability-of-a-drug.html>

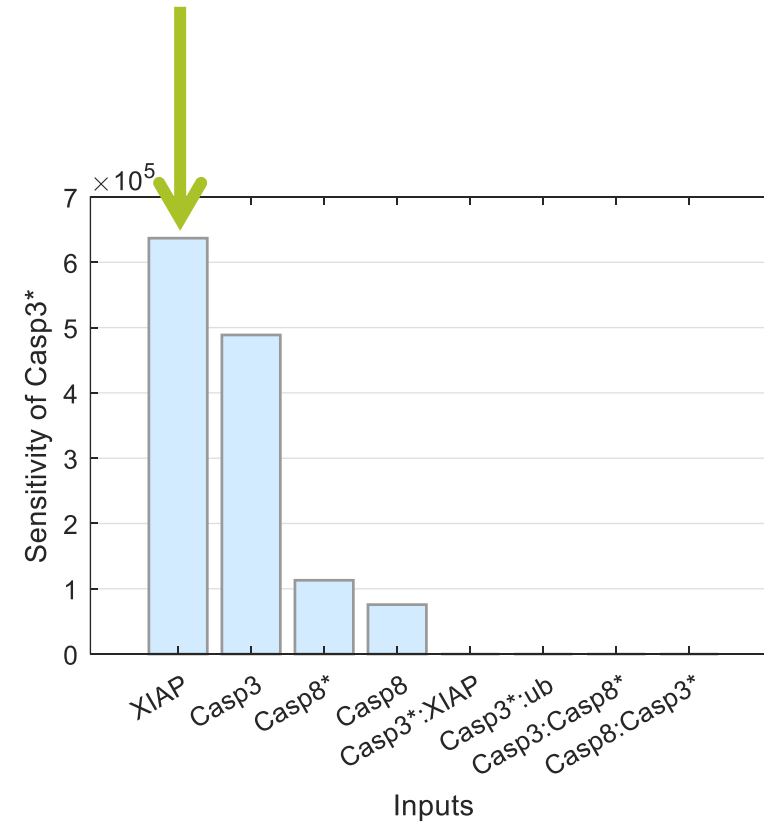
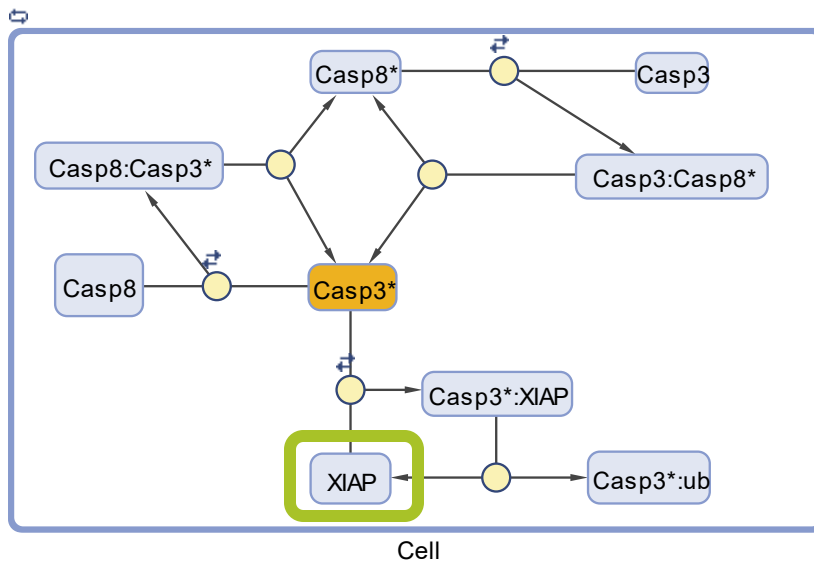
SimBiology中参数估计的支持方法

Method	Additional Toolbox Required	Supports Parameter Bounds	Uses Parameter Sensitivities [†]	Response-specific Error Models	Fixed or Mixed Effects	Supports Stochastic EM Algorithm	SimBiology Function to Use
<code>fminsearch</code>	—	Yes*	No	Yes	Fixed	No	<code>sbiofit</code> or <code>fitproblem</code>
<code>scattersearch</code>	—	Yes	Depends on the selected local solver.	Depends on the selected local solver.	Fixed	No	
<code>nlinfit</code> (Statistics and Machine Learning Toolbox)	Statistics and Machine Learning Toolbox™	Yes*	No	No	Fixed	No	
<code>fminunc</code> (Optimization Toolbox)	Optimization Toolbox™	Yes*	Yes	Yes	Fixed	No	
<code>fmincon</code> (Optimization Toolbox)	Optimization Toolbox	Yes	Yes	Yes	Fixed	No	
<code>lsqcurvefit</code> (Optimization Toolbox)	Optimization Toolbox	Yes	Yes	Yes	Fixed	No	
<code>lsqnonlin</code> (Optimization Toolbox)	Optimization Toolbox	Yes	Yes	Yes	Fixed	No	
<code>patternsearch</code> (Global Optimization Toolbox)	Global Optimization Toolbox	Yes	No	Yes	Fixed	No	
<code>ga</code> (Global Optimization Toolbox)	Global Optimization Toolbox	Yes	No	Yes	Fixed	No	
<code>particleswarm</code> (Global Optimization Toolbox)	Global Optimization Toolbox	Yes	No	Yes	Fixed	No	
<code>nlmefit</code> (Statistics and Machine Learning Toolbox)	Statistics and Machine Learning Toolbox	No	No	No	Mixed	No	<code>sbiofitmixed</code> or <code>fitproblem</code>
<code>nlmefitsa</code> (Statistics and Machine Learning Toolbox)	Statistics and Machine Learning Toolbox	No	No	No	Mixed	Yes	

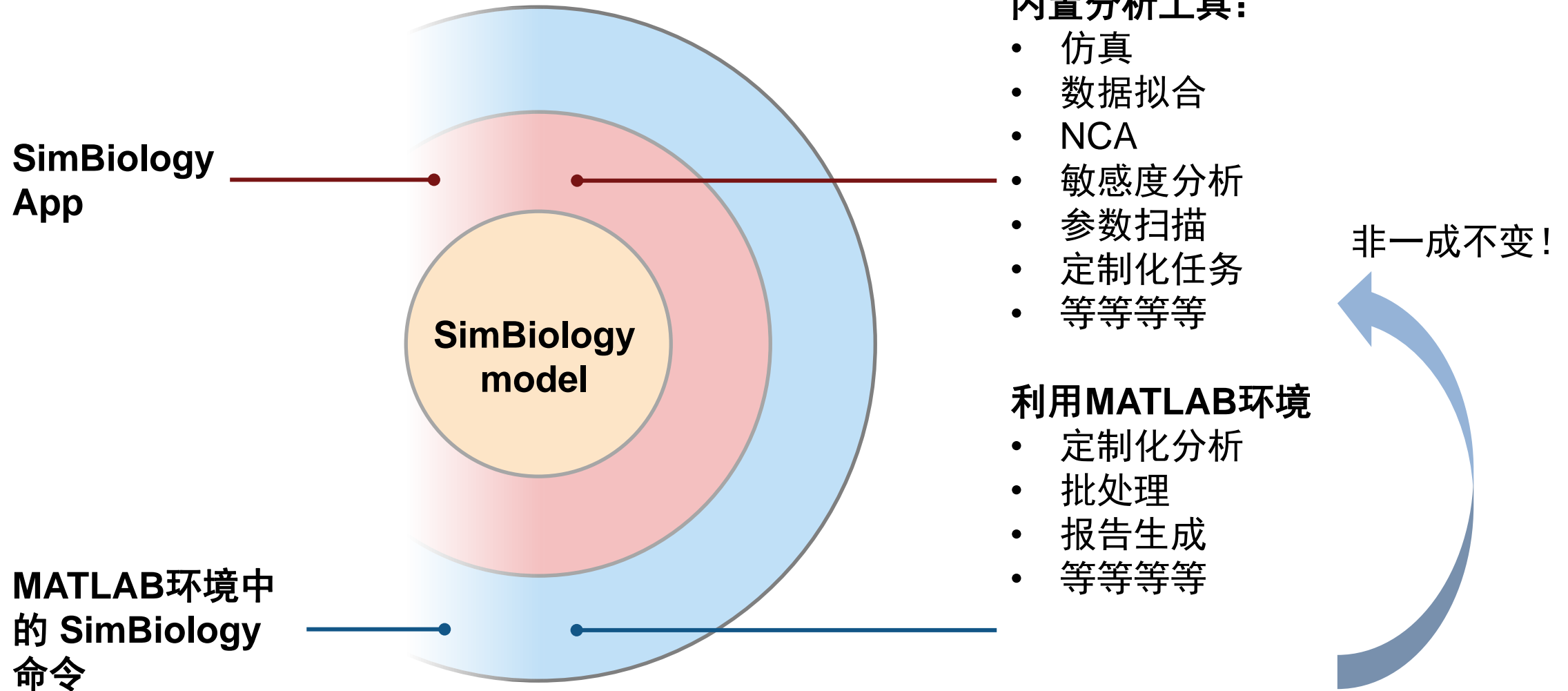
<https://ww2.mathworks.cn/help/simbio/ug/supported-methods-for-parameter-estimation.html>

敏感度分析

- 寻找影响模型结果的重要参数
 - 寻找需要仔细估计的参数
 - 寻找潜在的药物靶点
- 示例：凋亡通路模型



MATLAB 中的 SimBiology 生态系统



SimBiology App *vs.* script

```

% model
proj = sbioloadproject('TMDD_training.sbproj','m1');
model = proj.m1;
    
```

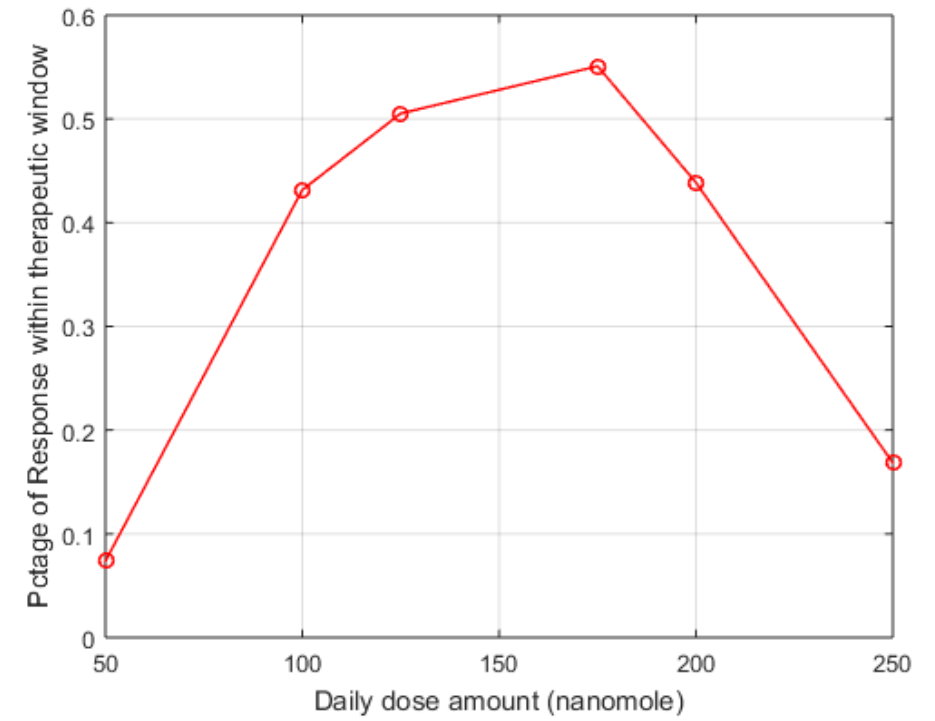
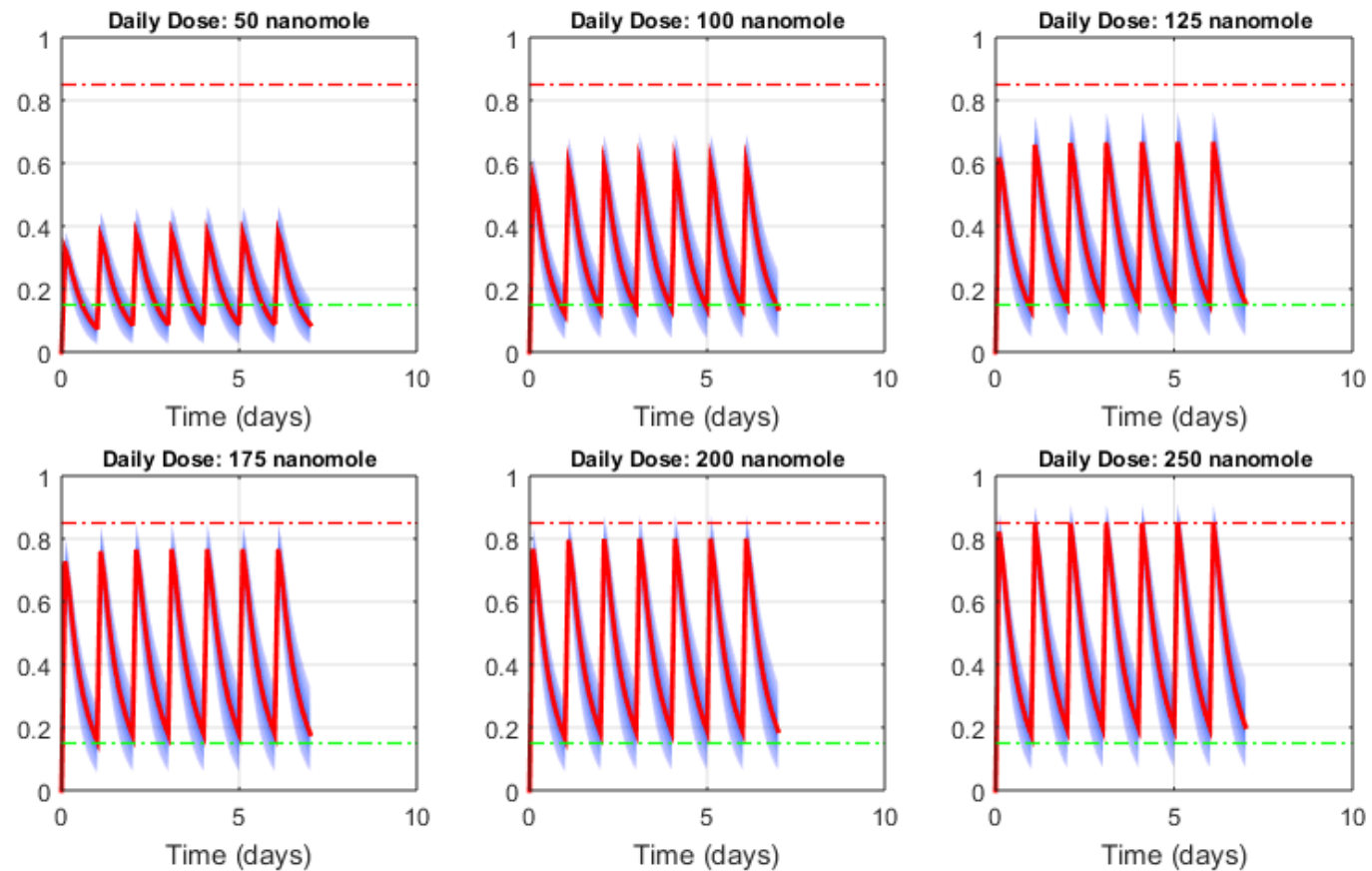
The screenshot shows the SimBiology Task Editor interface for a simulation named "Simulation Multiple Doses (Simulation)". The interface includes a toolbar with a "Run" button highlighted in orange. Below the toolbar, the "Description" section is expanded, showing several configuration options:

- Model:** TMDD
- Task StopTime:** StopTime: 3 day (task specific)
- Task StatesToLog:** Using Simulation Settings StatesToLog
- Variants to Apply:** No variants are being applied to the model
- Doses to Apply:** 100 nanomole every d...
- Variants to Generate:** No variants are being created after the task complet...
- Plots to Generate:** No plots are being generated when the task comple...
- Explorer Tools:** Explorer values are used only when the Explorer is [open](#)

On the right side of the interface, a plot shows the variable R0 over time. The plot displays a series of pulses, with R0 values ranging from 0 to 9. The plot area is also highlighted with an orange border.

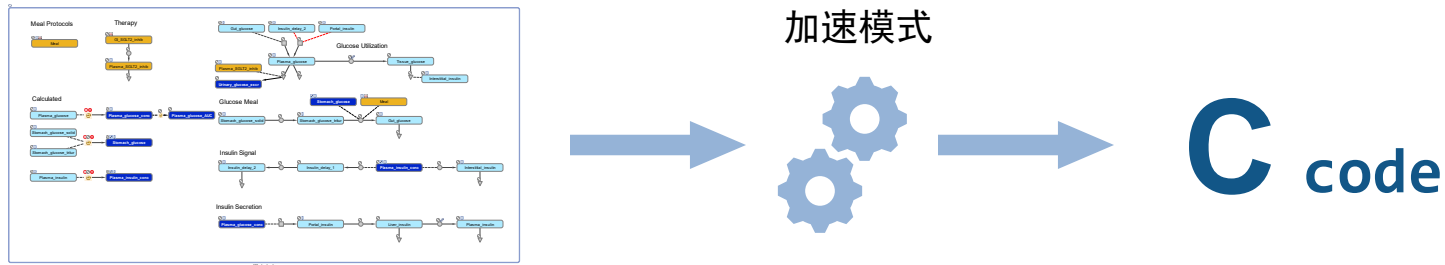
模拟虚拟人群，假设场景

- 示例：使用TMMD模型优化给药方案

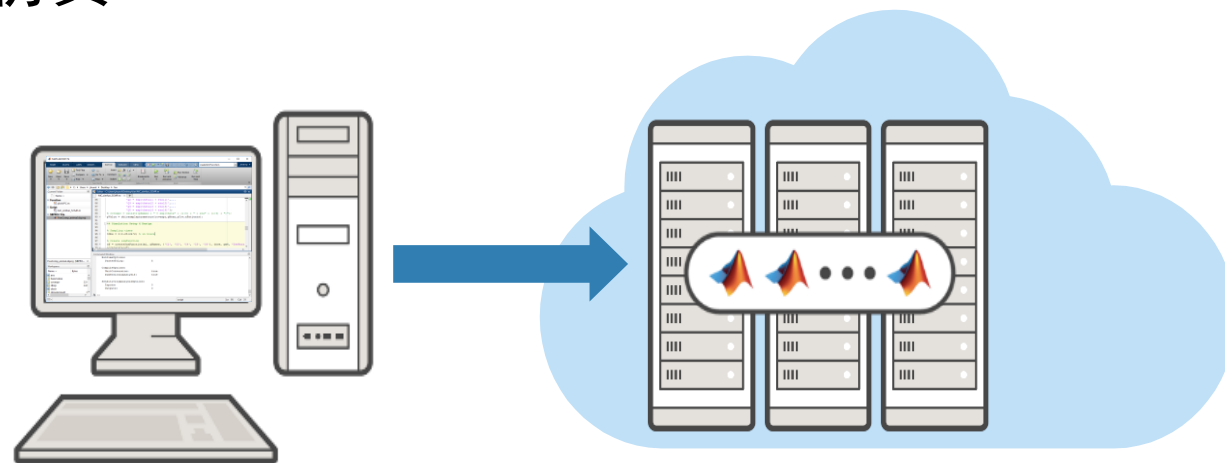


在各种设备上快速仿真

- 快速地进行单次仿真



- 并行运行多个仿真



扩展至集群或者云端

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7. MathWorks 以及社区提供的支持

ORIGINAL ARTICLE

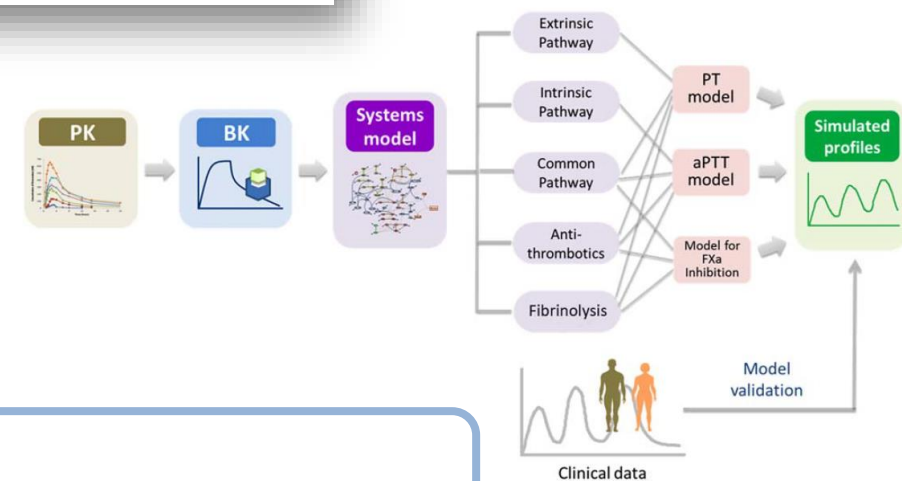
A Systems Pharmacology Model for Predicting Effects of Factor Xa Inhibitors in Healthy Subjects: Assessment of Pharmacokinetics and Binding KineticsX Zhou^{1*}, DRH Huntjens² and RAHJ Gilissen¹■ **背景:**

- Xa 因子 (FXa) = 有效抗凝预防静脉血栓栓塞的有希望的靶点
- 没有模型可以预测 FXa 抑制剂的临床凝血行为
- Zhou *et al.* 开发了一个详细的 QSP 模型来回答以下问题

我们能否通过药物发现阶段的动力学数据来预测 FXa 抑制剂的药物作用?
药物靶点结合动力学是药物作用的重要决定因素吗?

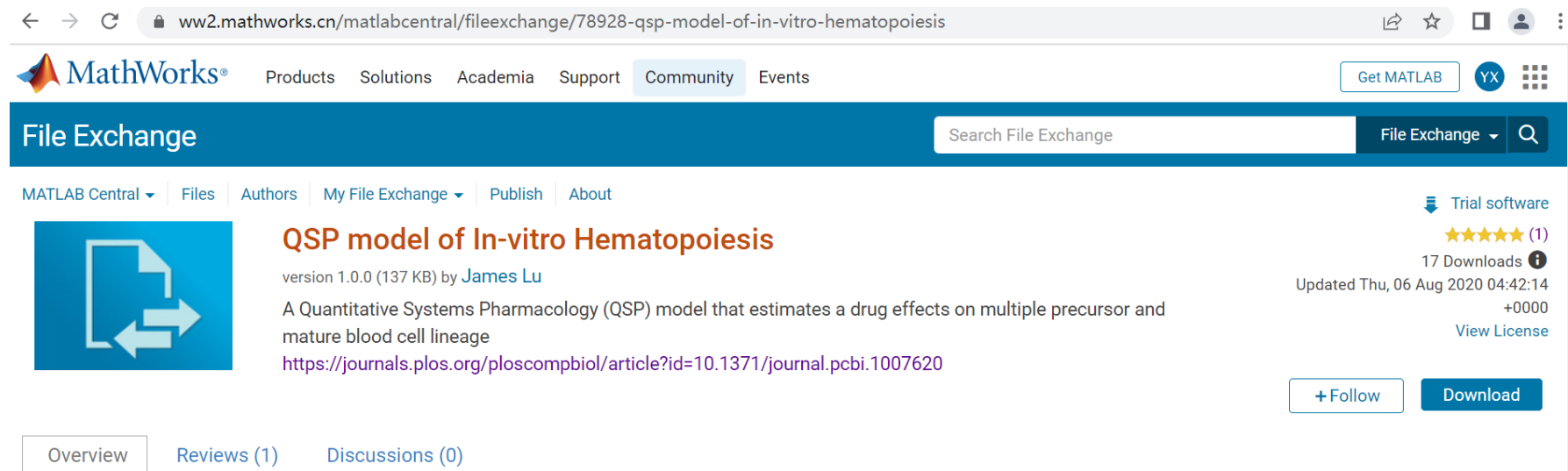
■ **结论:**

- 不仅与药物和靶点相关的特性, 而且与生物系统相关的参数和物种都是药物作用的重要决定因素。
- 系统药理学模型可用于识别和验证凝血级联中的目标。



Genentech: 体外造血 QSP 模型

- 骨髓抑制是与抗癌治疗相关的最常见和最严重的不良反应之一，并且可能是药物损耗的来源。
- 本文开发了体外造血的定量系统药理学 (QSP) 模型用于量化抗癌剂对多种造血细胞谱系的影响。
- 源代码可以在 MathWorks 官网访问：
<https://ww2.mathworks.cn/matlabcentral/fileexchange/78928-qsp-model-of-in-vitro-hematopoiesis>、



The screenshot shows the MathWorks File Exchange page for the "QSP model of In-vitro Hematopoiesis". The page includes the MathWorks logo, navigation links (Products, Solutions, Academia, Support, Community, Events), and a search bar. The main content area displays the file details: "QSP model of In-vitro Hematopoiesis" by James Lu, version 1.0.0 (137 KB). The description states: "A Quantitative Systems Pharmacology (QSP) model that estimates a drug effects on multiple precursor and mature blood cell lineage". A link to the PLOS article is provided: <https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1007620>. The page also shows a star rating of 5 stars (1 review), 17 downloads, and a "Download" button.



哈佛医学院使用 SimBiology 教学

改进定量药理学课程

“Basing the course on graphical programming offer the course a more intuitive programming environment.”

With SimBiology, students can focus on graphically modeling biological processes, rather than estimation, validation, and optimization.”

This aspect alleviates the challenges of programming and helps the students to focus on the modeling aspects.”

Dr. Jagesh Shah
Harvard Medical School

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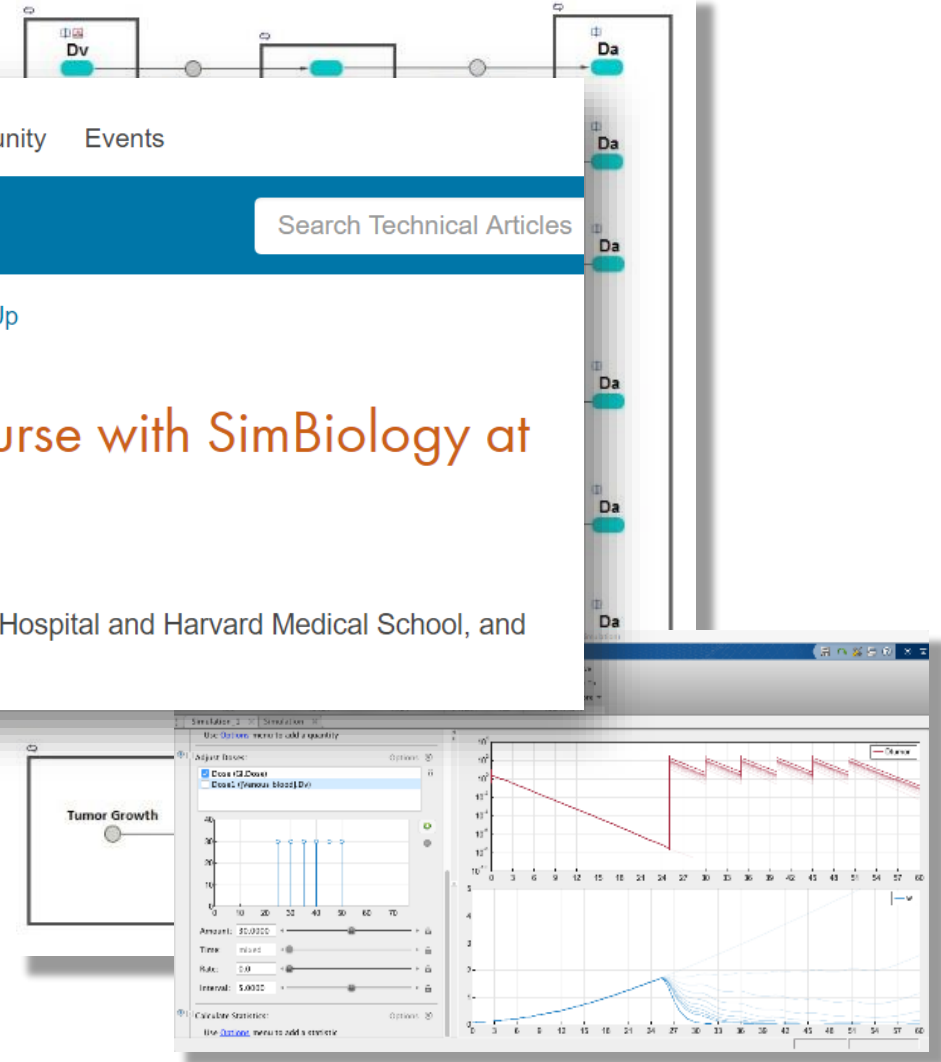
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Improving a Quantitative Pharmacology Course with SimBiology at Harvard Medical School

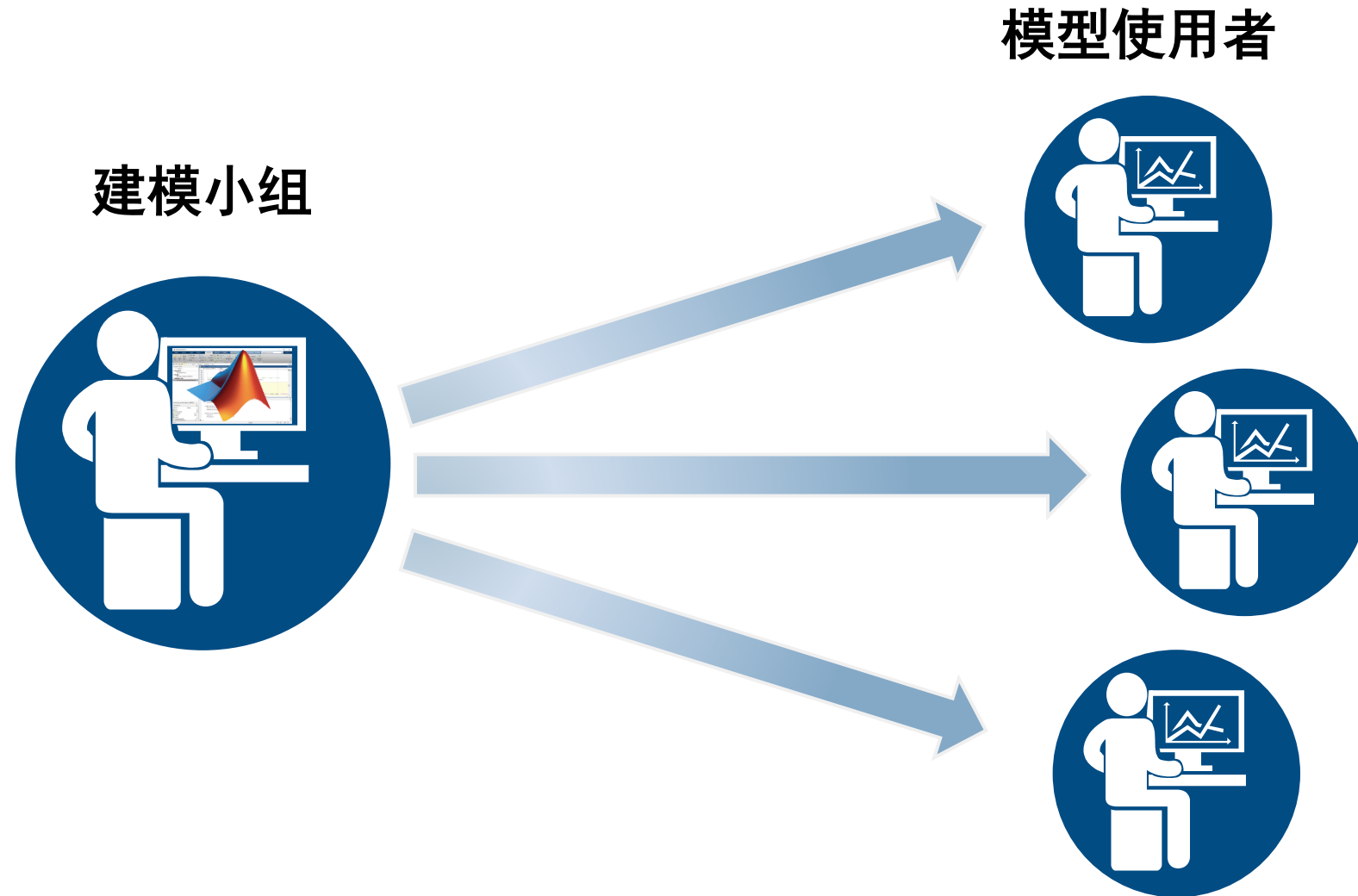
By Jagesh Shah, Harvard Medical School, Lorette Noiret, Massachusetts General Hospital and Harvard Medical School, and Fulden Buyukozturk, MathWorks



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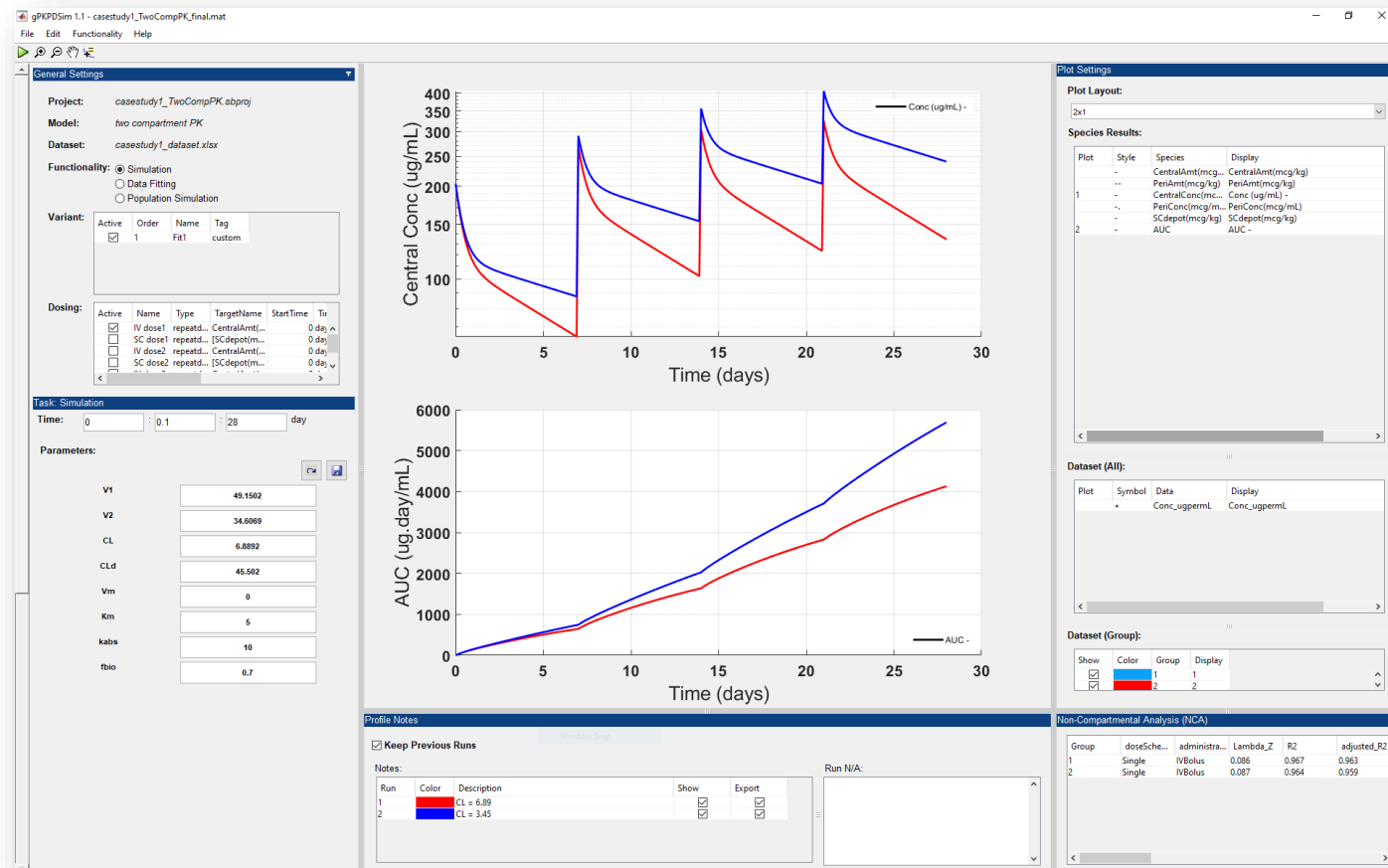
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gPKPDSim: 一个基于 SimBiology® 的 GUI 应用程序，用于药物开发中的 PKPD 建模

- Genentech 希望能够轻松使用复杂模型来执行各种常见的 PKPD 分析，即使是非建模人员也可以操作
- 该项目为 MathWorks 咨询项目



gPKPDSim: 一个基于 SimBiology® 的 GUI 应用程序，用于药物开发中的 PKPD 建模

Journal of Pharmacokinetics and Pharmacodynamics (2018) 45:259–275
<https://doi.org/10.1007/s10928-017-9562-9>

ORIGINAL PAPER



gPKPDSim: a SimBiology®-based GUI application for PKPD modeling in drug development

Iraj Hosseini¹ · Anita Gajjala² · Daniela Bumbaca Yadav¹ · Siddharth Sukumaran¹ · Saroja Ramanujan¹ · Ricardo Paxson³ · Kapil Gadkar¹

Received: 1 August 2017 / Accepted: 16 December 2017 / Published online: 4 January 2018
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Abstract

Modeling and simulation (M&S) is increasingly used in drug development to characterize pharmacokinetic-pharmacodynamic (PKPD) relationships and support various efforts such as target feasibility assessment, molecule selection, human PK projection, and preclinical and clinical dose and schedule determination. While model development typically require mathematical modeling expertise, model exploration and simulations could in many cases be performed by scientists in various disciplines to support the design, analysis and interpretation of experimental studies. To this end, we have developed a versatile graphical user interface (GUI) application to enable easy use of any model constructed in SimBiology® to execute various common PKPD analyses. The MATLAB®-based GUI application, called gPKPDSim, has a single screen interface and provides functionalities including simulation, data fitting (parameter estimation), population

Add-On Explorer

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gPKPDSim Toolbox
 version 1.1 (14.2 MB) by Iraj Hosseini
 The app is used for PKPD Modeling and Simulation.
 0 Ratings
 18 Downloads
 Updated 19 Apr 2018
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Overview

The source code and case studies are included in this toolbox. The description of gPKPDSim and case studies are in the publication titled "gPKPDSim: A SimBiology®-based GUI application for PKPD modeling in drug development."

Requires

- SimBiology
- Statistics and Machine Learning Toolbox

- SimBiologyNCA toolbox - GUI Layout Toolbox - If the Optimization or Global Optimization Toolbox is installed, gPKPDSim can also use the parameter estimation methods from either of those toolboxes.

MATLAB Release
 MATLAB 9.0 (R2016a)

Comments and Ratings (2)

Rate this submission ★★★★★ (Rating not required)

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yichen yang good
 13 Jun 2018

为仿真生成可部署 App

Task Editor - Create App (Simulation)

EDITOR EXPLORER VIEW

TASK LAYOUT SETTINGS RUN TASK RESULTS

Create App

Adjust Quantities:

Options

kel: 0.5230

kon: 0.049322

km: 0.0458

kdeg: 0.0934

Adjust Doses:

Options

Daily Dose (Plasma Drug)

Amount: 150.0

Time: mixed

Rate: 0.0

Interval: 1.0000

Calculate Statistics:

Options

isFeasible: 1.00000000

Explore Model

Explore Model Plot Setup

Simulation Time (in hours):

Stop time: 120

Output times: []

Explore Parameter Values:

kel 1/hour: 0.523

kon liter/nanomole/hour: 0.049322

km 1/hour: 0.0458

kdeg 1/hour: 0.0934

Explore Dose Schedules:

Daily Dose (Plasma Drug)

Amount: nanomole: 150

Rate: nanomole/hour: 0

StartTime: 0 day

Interval: 1

RepeatCount: 10

Statistics:

isFeasible: 1

Target occupancy

在您的局域网中通过 URL 分享您的仿真 App

The screenshot shows a MATLAB Web App interface for a simulation. The browser address bar shows the URL: `muc-teslab:9988/webapps/home/session.html?app=TMDDsim`. The page title is "MATLAB Web Apps".

Simulation setup:

- Dosing amount: 150 nanomole
- Dosing interval: 24 hours
- Duration of simulation: 120 hours

Adjust parameters:

- Binding constant (k_{on}): 0.1
- Drug elimination (k_{el}): 0.5

Simulation controls: Simulate (blue button), Reset (grey button), Target occupancy between thresholds (green indicator).

Graph: Receptor occupancy (%) vs Time (hours). The graph shows a periodic oscillating curve between approximately 25% and 75% occupancy. Two horizontal red dashed lines are drawn at 20% and 80% occupancy.

NCA parameters for bound target ('Complex'):

doseSchedule	administrationRoute	Lambda_Z	R2	adjusted_R2	Num_points	AUC_0_last	Tlast	C_max	C_max_Dose	T_max	MRT	T_half	AUC_infinity	AUC_infinity_dose
Multiple	IVBolus	0.0530	0.9999	0.9999	69	775.5569	120	7.6757	51.1712	3.2474	149.0303	13.0900	844.2600	5.6284e+03

[show log](#)

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- Automate workflow elements

"Researchers are typically interested in results, not programming. MATLAB enables us to think at a higher level of abstraction and spend less time developing, debugging, testing, and creating graphs. As a result, we get research results faster."

[Computational Biology Solutions Page](#)

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MATLAB® and Simulink® enable engineers to speed up medical device software and hardware development by efficiently integrating and automating the various phases of design, implementation, and verification.

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[Medical Devices Solutions Page](#)

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- Implement pharmacokinetic and pharmacodynamics (PKPD) models and fit model parameters to drug data
- Optimize and control biochemical manufacturing processes

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SimBiology Tutorials for QSP, PBPK, and PK/PD Modeling and Analysis

SimBiology provides apps and programmatic tools to model, simulate, and analyze dynamic systems, focusing on quantitative systems pharmacology (QSP), physiologically-based pharmacokinetics (PBPK), and pharmacokinetics/pharmacodynamics (PK/PD) applications. The videos in this series walk you through how to use SimBiology and perform common tasks.

- SimBiology Tutorials: Getting Started with SimBiology**
Get an overview of the SimBiology app layout and navigation. 9:06
- SimBiology Tutorials: Building a Model in SimBiology**
Build and simulate a model using the SimBiology desktop. 12:56
- SimBiology Tutorials: Simulating a Model in SimBiology**
This video demonstrates how to simulate a model in SimBiology in the SimBiology Model Analyzer App. 7:17

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New project

Central repository for SimBiology demos and related code. [Read more](#)

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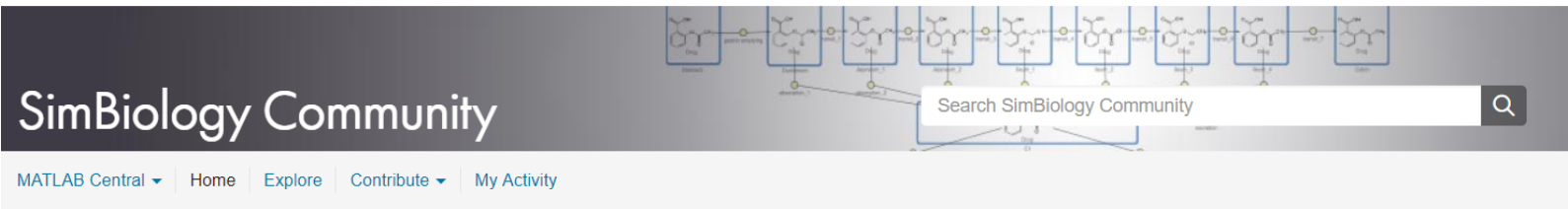
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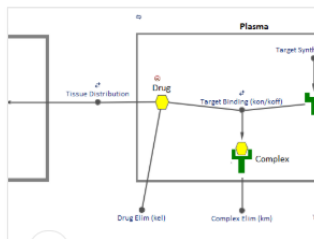
<https://ww2.mathworks.cn/videos/series/simbiology-tutorials-for-qsp-pbpbk-and-pk-pd-modeling-and-analysis.html>

<https://github.com/mathworks-simbiology>

支持：SimBiology 专属社区

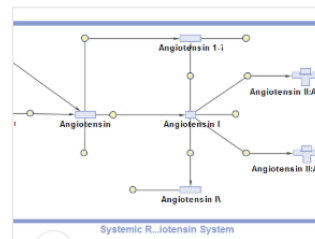


Projects



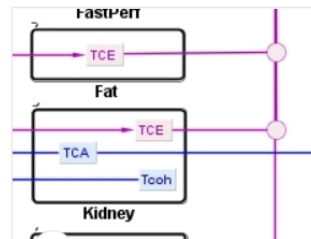
Target-Mediated Drug Disposition

Generic Target-Mediated Drug Disposition (TMDD) model that accounts for saturable drug-target binding, as well as target mediated elimination.



Systemic Renin-Angiotensin-System

Model of the systemic Renin-Angiotensin-System (RAS) to investigate the effects of different RAS-modulating therapies.



Physiologically-based pharmacokinetics of trichloroethylene

Physiologically based: Human PBPK model for trichloroethylene (TCE) and its metabolites to assess human health risks associated with low level exposure

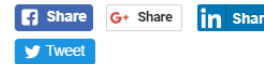


Welcome to the SimBiology Community

Moderator:
Fulden Buyukozturk

A gathering place for scientists working in QSP, PBPK, and PK/PD modeling using SimBiology and MATLAB. Features discussions, shared models and code, and other resources from our global community of users.

Unfollow the community



- 问答
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- 代码
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<https://www.mathworks.com/matlabcentral/simbiology.html>

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