Getting more out of your (eco)toxicity data by applying mechanistic interpretation with open source models

Toxicokinetic-toxicodynamic modelling – examples to use and available tools

Thomas G. Preuss, Vanessa Roeben, David Heckmann, Andre Gergs

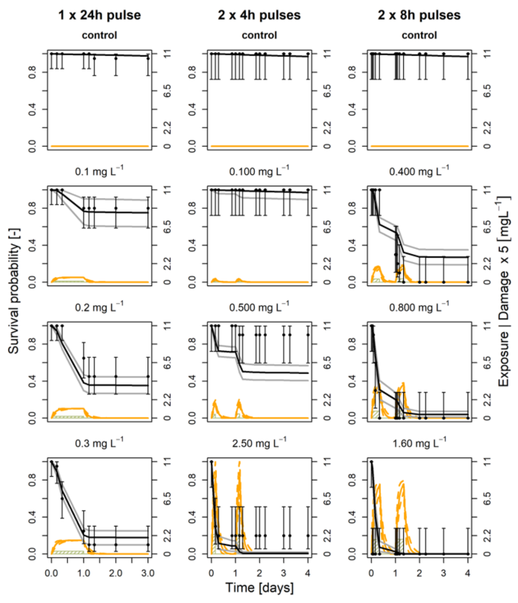
GUTS

Simulating survival over time at constant or variable exposure.

Species: generic (all species)

Data need: survival over time

➔ GUTS model analyse and predict survival under constant and time variable exposure using the whole data package resulting in higher statistical and predictive power



Paper

Book

OpenGUTS

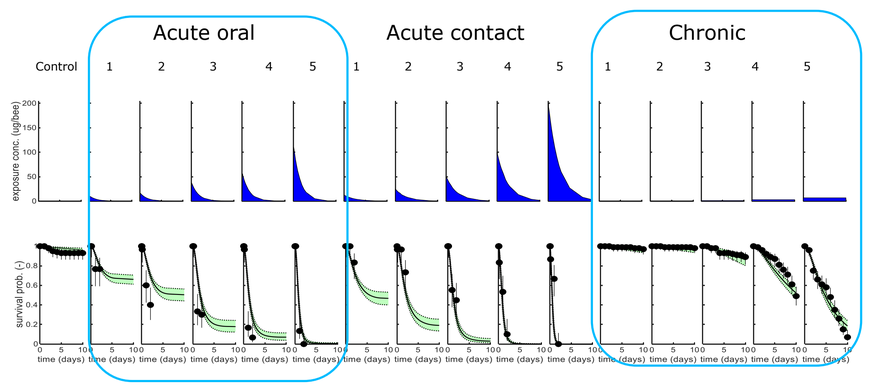
Mosaic

BeeGUTS

Simulating survival over time for different exposure routes.

Species: honey bee, bumble bee, solitary bees

Data need: survival over time



Paper

BeeGUTS

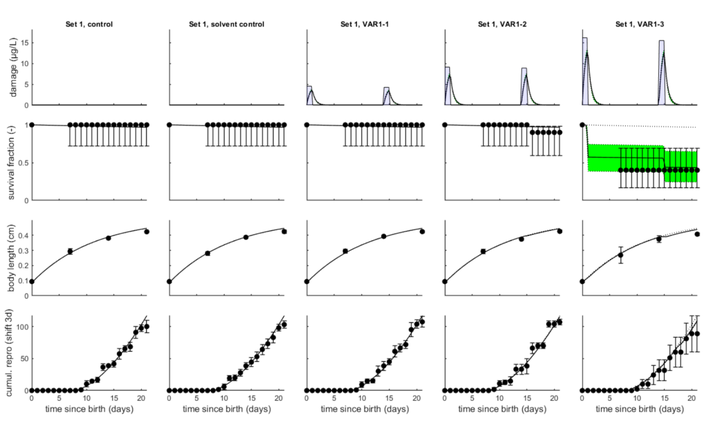
➔ With the BeeGUTS model we are able to analyse all laboratory tests together and extrapolate to real world exposure patterns

Dynamic Energy Budget (DEB)

Simulating sublethal effect over time

Species: generic (all animal species)

Data need: effects on reproduction, growth and development



Paper:

DEBTox

Add my Pet collection

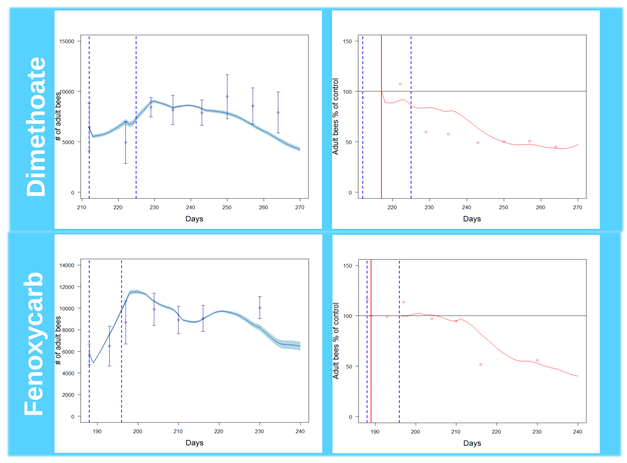
➔ With the DEB model effects are analysed in combination and extrapolation to untested exposure scenarios is possible

BEEHAVE

Simulating colony over time

Species: honey bee

Data need: standard ecotox dataset (OECD 214, 213, 245, 239)



BEEHAVE:

BEEHAVE Ecotox:

BEEHAVE Ecotox:

➔ Extrapolation from individual (lab) to colony at (semi)field

PBTK

Simulating uptake, distribution and elimination over time

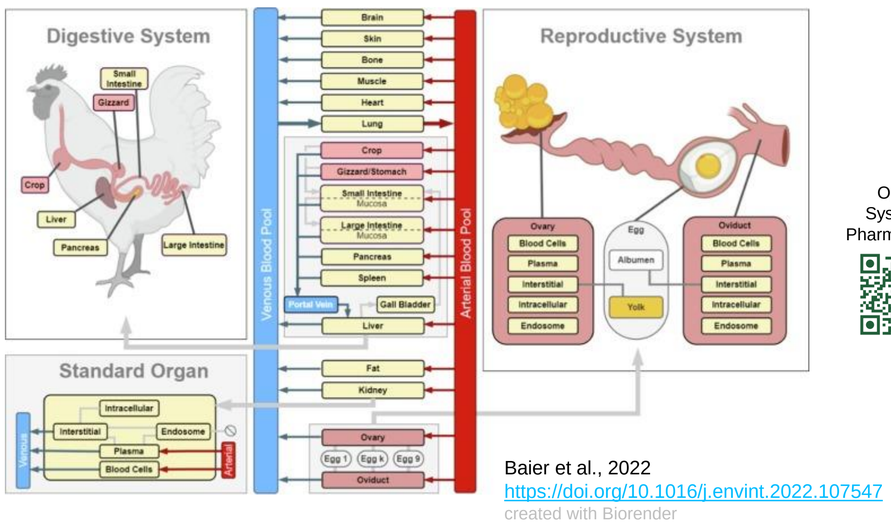
Species: rat, mouse, dog, human, rabbit, quail, duck

Data need: phys-chem, residues in at least one organ over time

Bird:

Rabbit:

Fish:



Baier et al., 2022
https://doi.org/10.1016/j.envint.2022.107547
created with Biorender

Open Systems Pharmacology

Why should I use these models?

Standardized TKTD modelling offers a new way of interpreting standard toxicity data. This allows a scientifically sound extrapolation from the constant laboratory condition to the local situation.

This approach allows to extrapolate to different environmental conditions and maybe even to untested species.