



U.S. FOOD & DRUG
ADMINISTRATION

Human Foods Program





Toxicokinetic Chemical Simulator (ToCS): A Graphical User Interface for High- Throughput Chemical Analysis

Kristen Leonard

Contractor

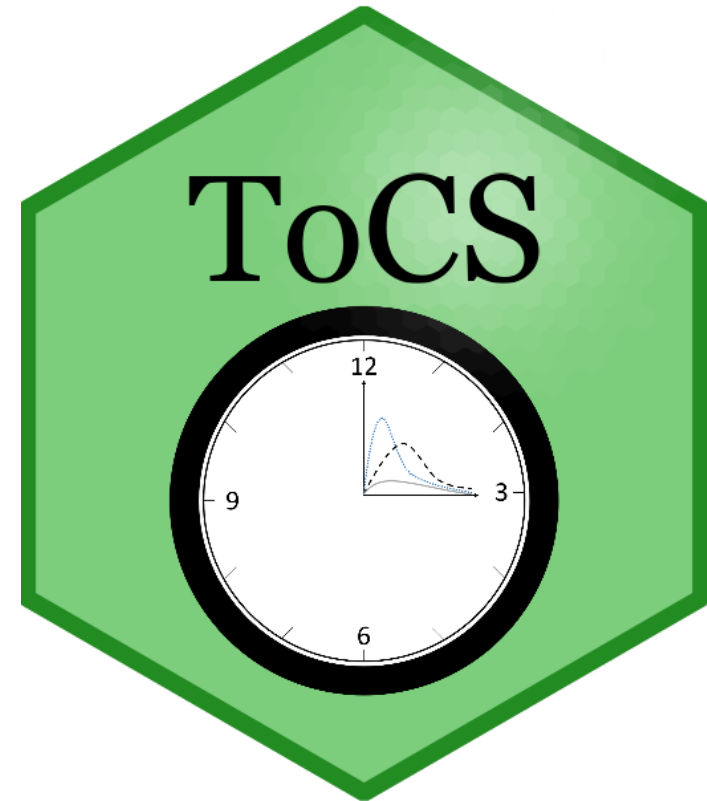
Office of Scientific Coordination and Computational Sciences (OSCCS)

October XX, 2025

Session I: Introduction to ToCS

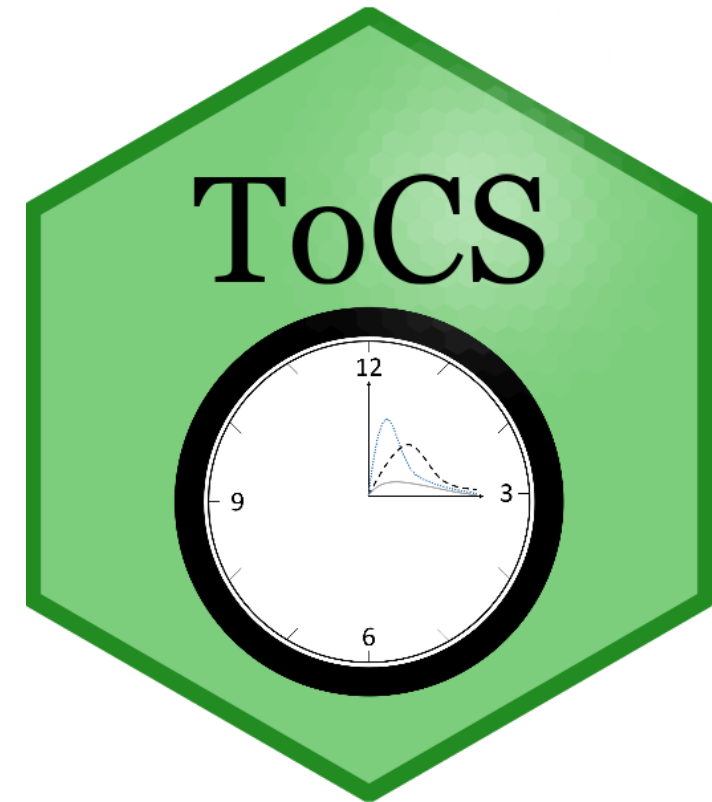
What is ToCS?

- An easy-to-use graphical user interface (GUI)
- Uses computational software to make high-throughput toxicokinetic (TK) chemical predictions
- No programming required
- Predict ADME profiles and characteristics, prioritize chemicals using in vitro to in vivo extrapolation, and generate TK parameters



Purpose of ToCS

- High throughput preliminary screening, prioritization, and characterization of chemicals at the beginning of studies
- Post market assessment of food relevant compounds
- Obtain parameters to use in other models
- Simulate ingredients used in dietary supplements



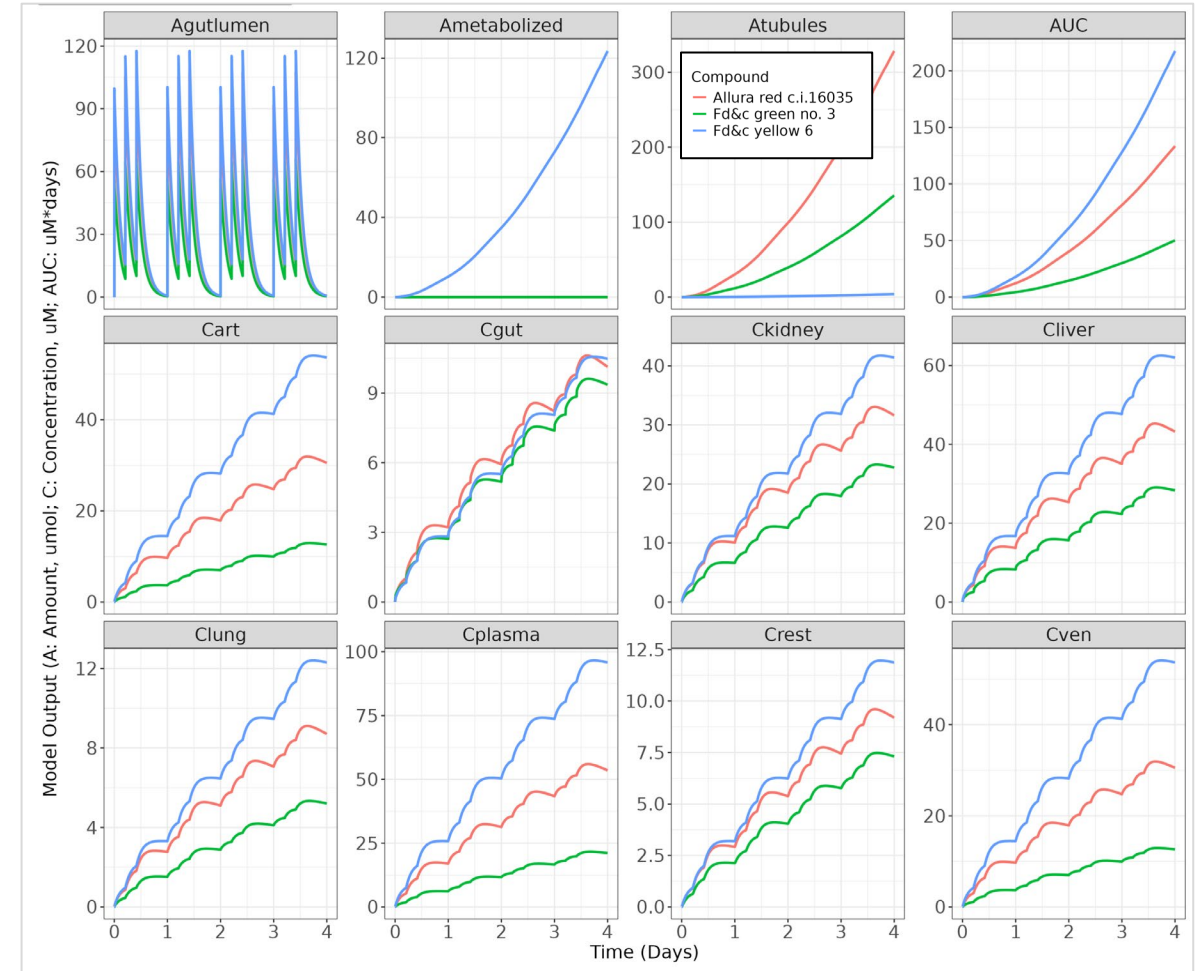
ToCS Outputs

Concentration-Time Profiles Module <ul style="list-style-type: none"> • ADME time course data (Amounts and concentrations over time) • Summary statistics (Tmax, Cmax, and AUC) 	Steady State Concentrations Module <ul style="list-style-type: none"> • Analytical steady state in desired concentration/tissue • Estimate of the time (days) it takes to reach steady state behavior following constant oral dosing
In Vitro to In Vivo Extrapolation (IVIVE) Module <ul style="list-style-type: none"> • OEDs (the external dose needed to produce the internal bioactive conc.) compared with exposure data (if provided by the user) • BERs if exposure data is provided by the user 	Parameter Calculations Module <ul style="list-style-type: none"> • Toxicokinetic parameters (half-life, total plasma clearance, elimination rate, volume of distribution) • Partition coefficients in different tissues

Abbreviations: ADME – absorption, distribution, metabolism, excretion; Cmax – maximal concentration; Tmax – time to Cmax; AUC – area under the curve; OED – oral equivalent dose; BER – bioactivity exposure ratio

Food Relevant Features

- Models with oral exposure route
- Ability to make a non-uniform exposure protocol (mimics food consumption at mealtimes)
- Customization of bioavailability settings
 - Use of in silico *Caco2.Pab* values
 - Ability to run simulations with 100% bioavailability - more conservative
- Contains explicit list of food chemicals available for simulation
 - 109-118 chemicals for human simulations (954-956 chemicals using in silico CL_{int} and F_{up})
 - 25-30 chemicals for rat simulations (no human data)



How does ToCS compare to other GUIs?



Feature	ToCS	ICE*
httk software version	2.7.0	2.2.2
Species	Human, rat, mouse, dog, rabbit	Human, rat
Food chemical subset	Yes	No
Loads in silico caco-2 permeability values	Yes	No
Customize parameter calculation methods	Yes	No
Dosing routes	Oral	Oral, iv, inhalation
ADME dosing	Single, evenly recurring, and non-uniform	Single, evenly recurring
Inclusion of full pregnancy model	Yes	No
AUC and Tmax calculated for plasma and all tissues	Yes	Plasma only

Feature	ToCS	ICE*
Analytical SS concentrations	Plasma and all tissues	Plasma only
Estimates days to plasma SS	Yes	No
OED calculation	Plasma and all tissues	Plasma only
Convert nominal in vitro bioactive conc to free conc	Yes	No
OED quantile returned	User's choice	5% and 50%
Option to view all OED samples	Yes	No
Built-in bioactivity data	No	Yes
Bioactivity exposure ratio (BER) calculation	Yes	No
Volume of distribution, elimination rate, total plasma clearance, and partition coefficient calculations	Yes	No

*Integrated Chemical Environment (<https://ice.ntp.niehs.nih.gov/>)

How to Access the ToCS Interface



1. Web Application

- pub-connect.foodsafetyrisk.org/tocs
- No programming needed →

```
Console Terminal x Background Jobs x
R 4.4.3 ~ /
> # --- LOAD OR INSTALL REMOTES PACKAGE
library(remotes) #or install.packages("remotes") if 'remotes'
package is not already installed

# --- INSTALL TOCS PACKAGE FROM GITHUB
remotes::install_github("KristenWindoloski/ToCS")

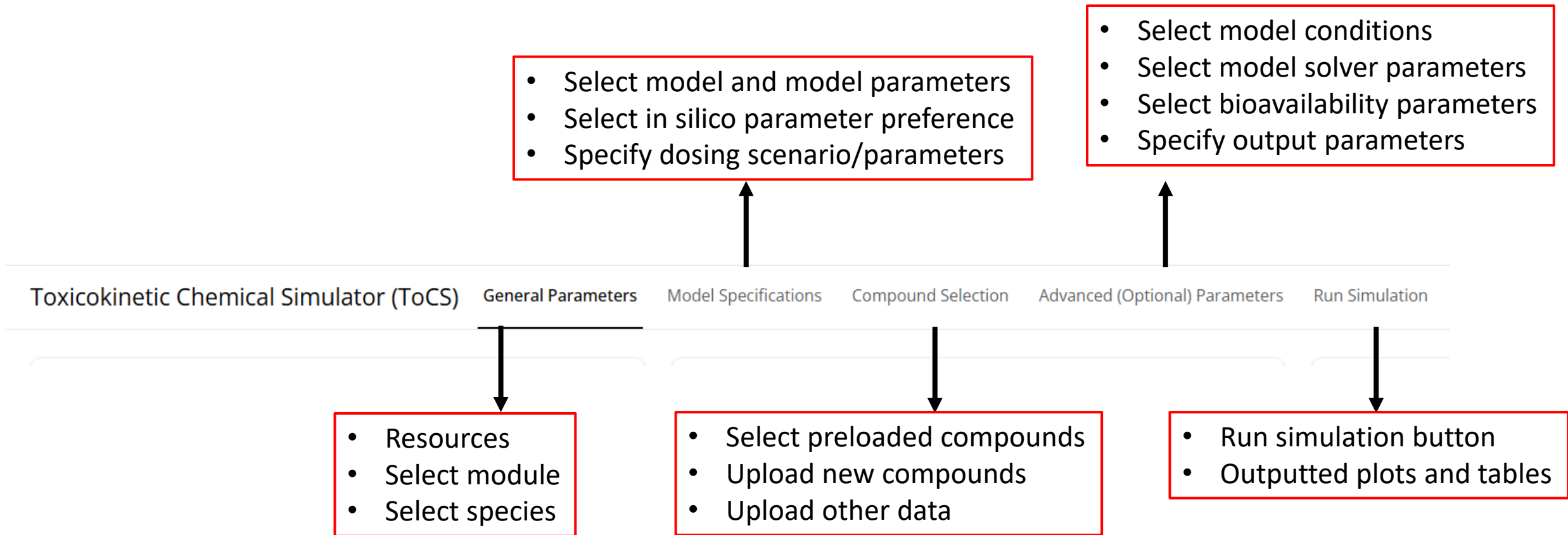
# --- LOAD TOCS LIBRARY
library(ToCS)

# --- OPEN TOCS APPLICATION INTERFACE
ToCS::run_ToCS()
```

2. R Package

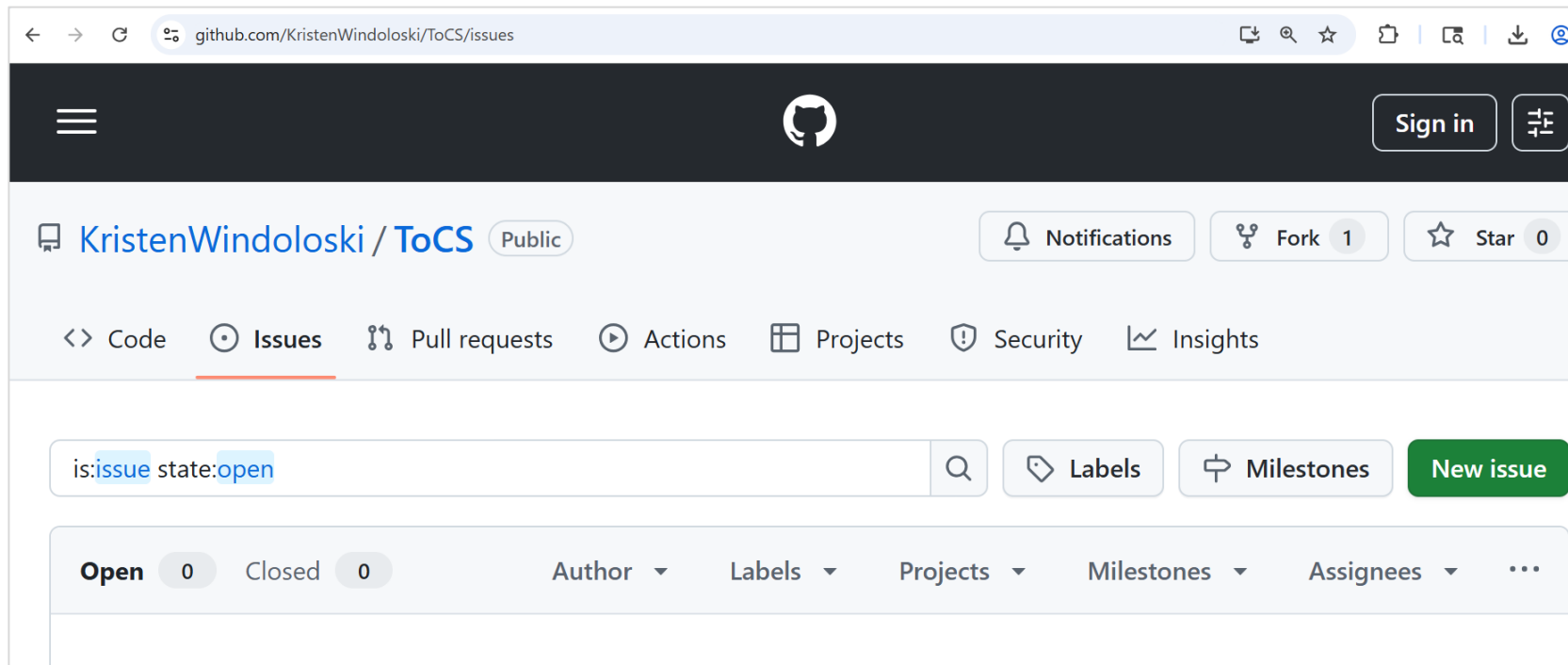
- Install in R from the ToCS GitHub
- Some programming needed ←

Interface Structure



Getting Help and Reporting Issues

- README file (<https://github.com/KristenWindoloski/ToCS>)
- Vignettes (<https://github.com/KristenWindoloski/ToCS/tree/main/vignettes>)



Click the “New Issue” button if any bugs or errors arise when using ToCS

Limitations & Challenges

- Generalized models - no chemical-specific physiological components, pathways, or compartments
 - More appropriate for reporting high-throughput preliminary toxicokinetics and risk estimation
 - Suggest ToCS be used as an earlier stage analytical software for screening and to guide further chemical studies
- Use caution when using the optional in silico parameters, as a different output would be achieved if the parameter data sets were loaded in another order
- Challenges users may face:
 - Uploading data
 - Entering non-uniform dosing schedule/long lists of numbers
 - Singular bioactivity data
 - Plotting customization

Future Work

- Include new htk models into ToCS (PFAS, time-dependent parameter version, and 1st trimester pregnancy models)
- Update non-uniform dosing input structure
- Estimation of additional parameters
- Incorporate user feedback (new analyses and methods, food relevant features, etc.)
- Fix programming bugs as needed

An overview of httk and its models

The httk R package



- Built by the U.S. EPA in 2015 and is continually maintained and updated
- Provides toxicokinetic analysis models and functions for chemical compounds
- Contains chemical data for over 17,000 compounds
- Newest version (2.7.0) contains time-varying parameter pbtk models, a three-trimester pregnancy model, and a PFAS model

httk: High-Throughput Toxicokinetics

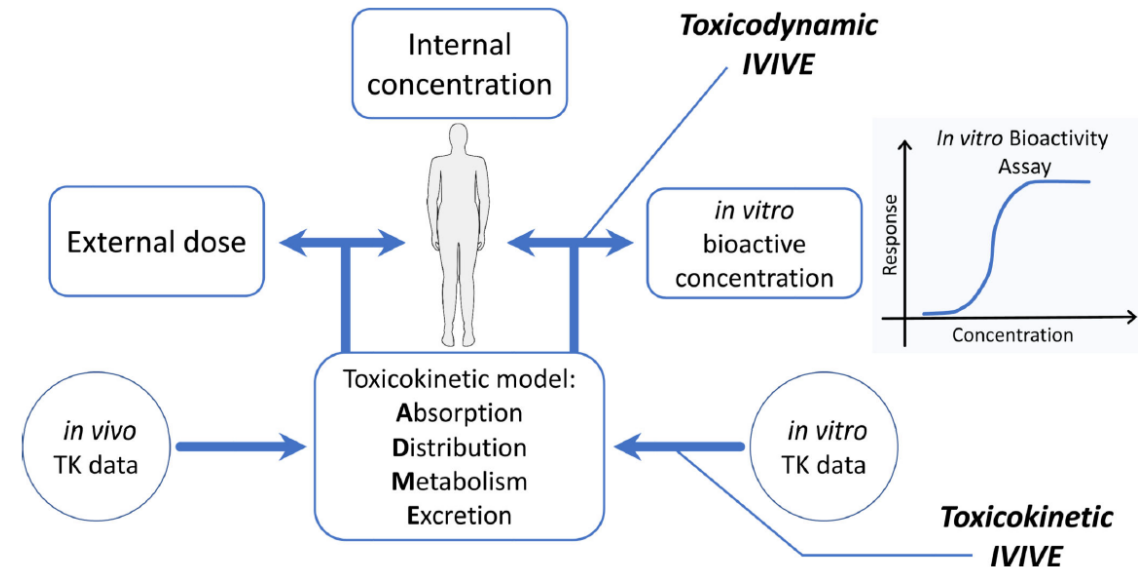
Pre-made models that can be rapidly tailored to various chemicals and species using chemical-specific in vitro data and physiological information. These tools allow incorporation of chemical toxicokinetics ("TK") and in vitro-in vivo extrapolation ("IVIVE") into bioinformatics, as described by Pearce et al. (2017) (<[doi:10.18637/jss.v079.i04](https://doi.org/10.18637/jss.v079.i04)>). Chemical-specific in vitro data characterizing toxicokinetics have been obtained from relatively high-throughput experiments. The chemical-independent ("generic") physiologically-based ("PBTK") and empirical (for example, one compartment) "TK" models included here can be parameterized with in vitro data or in silico predictions which are provided for thousands of chemicals, multiple exposure routes, and various species. High throughput toxicokinetics ("HTTK") is the combination of in vitro data and generic models. We establish the expected accuracy of HTTK for chemicals without in vivo data through statistical evaluation of HTTK predictions for chemicals where in vivo data do exist. The models are systems of ordinary differential equations that are developed in MCSim and solved using compiled (C-based) code for speed. A Monte Carlo sampler is included for simulating human biological variability (Ring et al., 2017 <[doi:10.1016/j.envint.2017.06.004](https://doi.org/10.1016/j.envint.2017.06.004)>) and propagating parameter uncertainty (Wambaugh et al., 2019 <[doi:10.1093/toxsci/kfz205](https://doi.org/10.1093/toxsci/kfz205)>). Empirically calibrated methods are included for predicting tissue:plasma partition coefficients and volume of distribution (Pearce et al., 2017 <[doi:10.1007/s10928-017-9548-7](https://doi.org/10.1007/s10928-017-9548-7)>). These functions and data provide a set of tools for using IVIVE to convert concentrations from high-throughput screening experiments (for example, Tox21, ToxCast) to real-world exposures via reverse dosimetry (also known as "RTK") (Wetmore et al., 2015 <[doi:10.1093/toxsci/kfv171](https://doi.org/10.1093/toxsci/kfv171)>).

Version: 2.7.3
Depends: R (≥ 2.10)
Imports: deSolve, msm, data.table, survey, mvtnorm, truncnorm, stats, graphics, utils, magrittr, purrr, methods, Rdpack (≥ 2.3), ggplot2, dplyr
Suggests: knitr, rmarkdown, eplots, scales, EnvStats, MASS, RColorBrewer, stringr, reshape, viridis, gmodels, colorspace, cowplot, ggrepel, forcats, smatr, gridExtra, readxl, ks, testthat, ggpubr, tidyverse
Published: 2025-09-12
DOI: [10.32614/CRAN.package.httk](https://doi.org/10.32614/CRAN.package.httk)
Author: John Wambaugh [aut, cre], Sarah Davidson-Fritz [aut], Robert Pearce [aut], Caroline Ring [aut], Greg Honda [aut], Mark Sfeir [aut], Matt Linakis [aut], Dustin Kapraun [aut], Kimberly Truong [aut], Colin Thomson [aut], Meredith Scherer [aut], Annabel Meade [aut], Celia Schacht [aut], Leonie Lautz [aut], Todor Antonijevic [ctb], Miyuki Breen [ctb], Shannon Bell [ctb], Xiaqing Chang [ctb], Jimena Davis [ctb], Elaina Kenyon [ctb], Gilberto Padilla Mercado [ctb], Katie Paul Friedman [ctb], Nathan Pollesch [ctb], Noelle Sinski [ctb], Nisha Sipes [ctb], James Sluka [ctb], Caroline Stevens [ctb], Barbara Wetmore [ctb], Lily Whipple [ctb], Woodrow Setzer [ctb]
Maintainer: John Wambaugh <wambaugh.research@gmail.com>
BugReports: <https://github.com/USEPA/CompTox-ExpoCast-httk/issues>
License: MIT + file LICENSE
Copyright: This package is primarily developed by employees of the U.S. Federal government as part of their official duties and is therefore public domain.
URL: <https://www.epa.gov/chemical-research/rapid-chemical-exposure-and-dose-research>
NeedsCompilation: yes
Citation: [httk citation info](#)
Materials: [README, NEWS](#)
CRAN checks: [httk results](#)
Documentation:
Reference manual: [httk.html](#), [httk.pdf](#)
Vignettes: [1\) Introduction to HTTK \(source, R code\)](#), [2\) Introduction to IVIVE \(source, R code\)](#), [a\) Pearce \(2017\): HTTK Basics \(source, R code\)](#), [b\) Ring \(2017\) HTTK-Pop: Generating subpopulations \(source, R code\)](#), [c\) Pearce \(2017\): Evaluation of Tissue Partitioning \(source, R code\)](#), [d\) Frank \(2018\): Neuronal Network IVIVE \(source, R code\)](#), [e\) Truong \(2025\): Full Human Gestational IVIVE \(source, R code\)](#), [f\) Wambaugh \(Submitted\): HTTK for PFAS \(source, R code\)](#), [g\) Meade \(Submitted\): High Throughput Dermal Exposure Model \(source, R code\)](#), [h\) Scherer \(Submitted\): In Vitro Distribution \(source, R code\)](#)

The httk R package

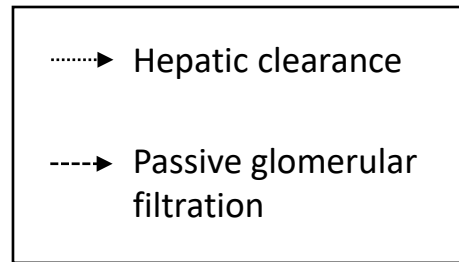
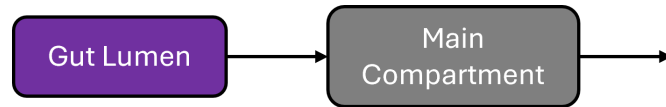


- Contains generalized mathematical models (same structure for each chemical, but use of chemical-specific parameters)
- Chemical specific parameters include:
 - In vitro intrinsic hepatic clearance
 - In vitro fraction unbound in plasma
 - Molecular weight
 - Octanol water partition coefficient
 - Many others...

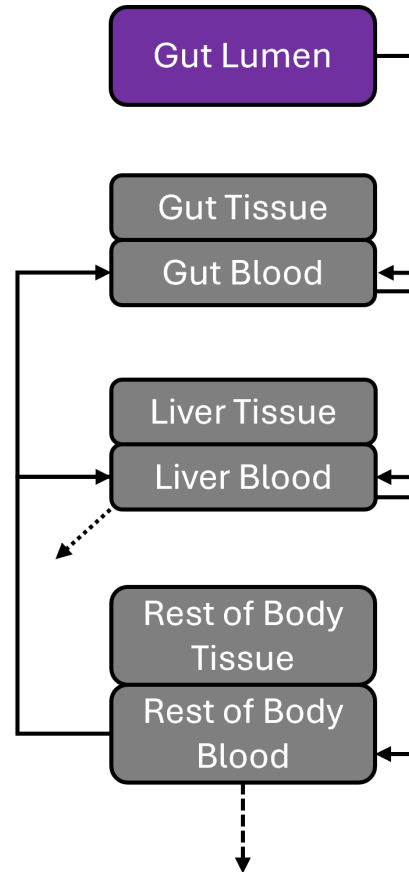


Breen, M., Ring, C.L., Kreutz, A., Goldsmith, M.R. and Wambaugh, J.F. (2021). High-throughput PBTK models for in vitro to in vivo extrapolation. *Expert opinion on drug metabolism & toxicology*

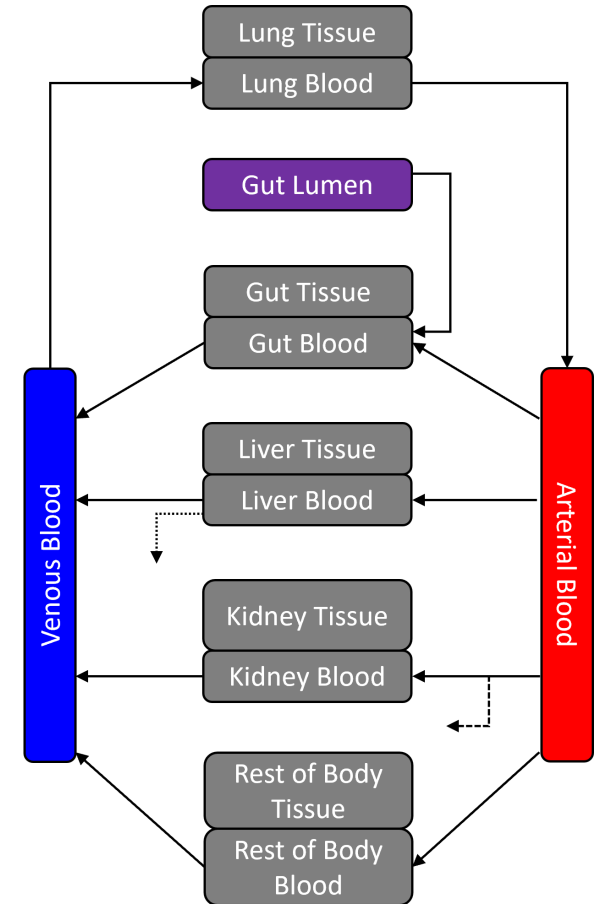
1compartment



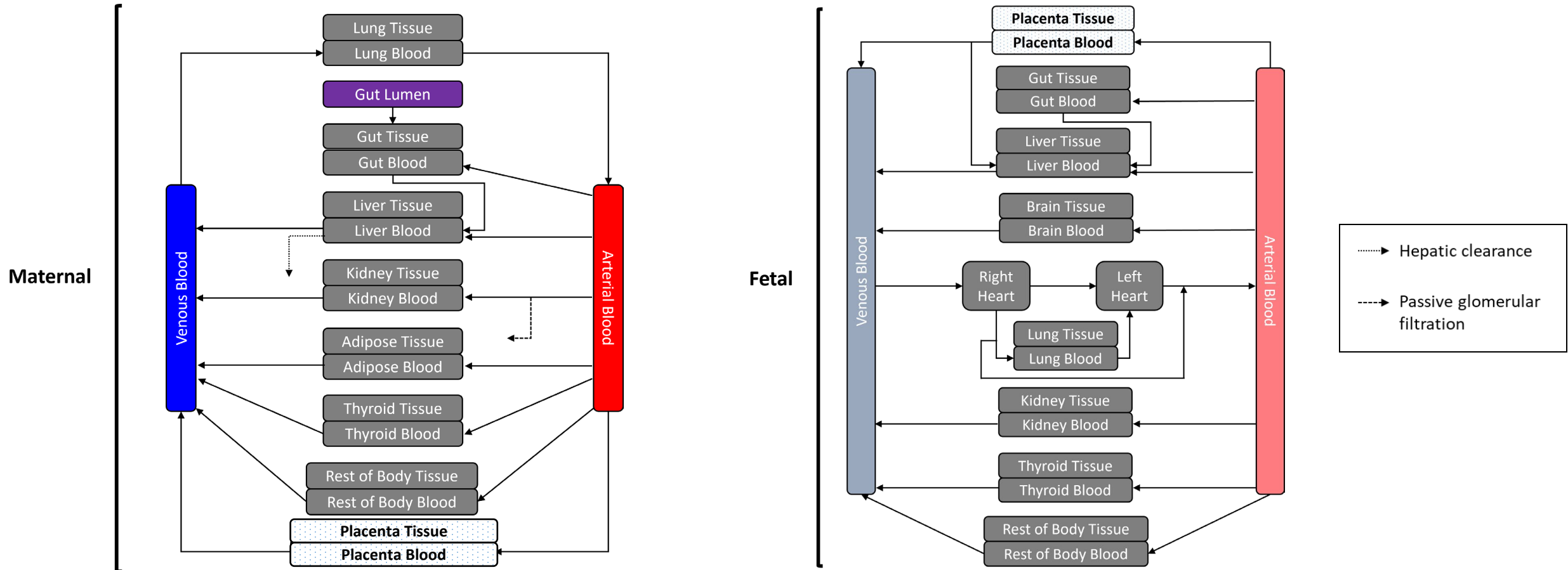
3compartment



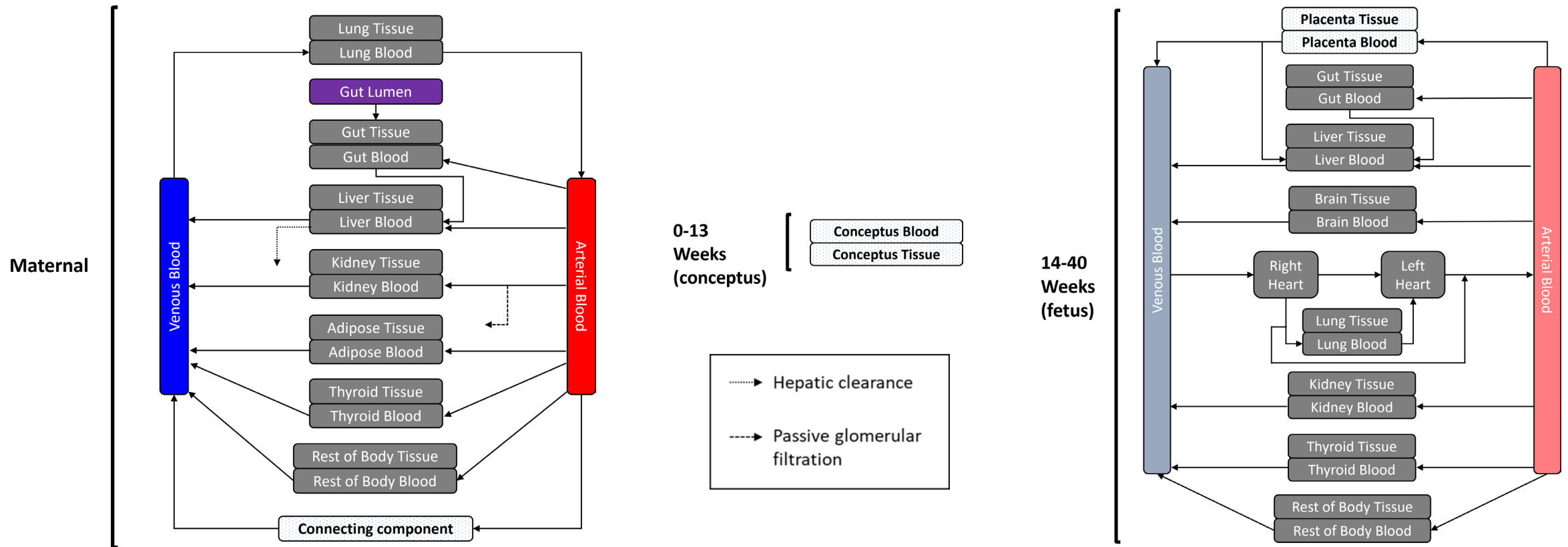
pbtk



fetal_pbtk model (2nd and 3rd trimesters)



Full_pregnancy model



Additional Information on htk



Websites

<https://github.com/USEPA/CompTox-ExpoCast-htk>

<https://cran.r-project.org/web/packages/htk/index.html>

Select Publications

1. Breen, M., Ring, C.L., Kreutz, A., Goldsmith, M., and Wambaugh, J.F. (2021). High-throughput PBTK models for in vitro to in vivo extrapolation. *Expert Opin. Drug Metab. Toxicol.* 17(8), 903–921. doi: 10.1080/17425255.2021.1935867.
2. Breen, M., Wambaugh, J.F., Bernstein, A., Sfeir, M., and Ring, C.L. (2022). Simulating toxicokinetic variability to identify susceptible and highly exposed populations. *J. Expo. Sci. Environ. Epidemiol.* 32(6), 855-863. doi: 10.1038/s41370-022-00491-0.
3. Kapraun, D.F., Sfeir, M., Pearce, R.G., Davidson-Fritz, S.E., Lumen, A., Dallmann, A., et al. (2022). Evaluation of a rapid, generic human gestational dose model. *Reprod. Toxicol.* 113, 172-188. doi: 10.1016/j.reprotox.2022.09.004.
4. Pearce, R.G., Setzer, R.W., Strobe, C.L., Wambaugh, J.F., and Sipes, N.S. (2017). htk: R package for high-throughput toxicokinetics. *J. Stat. Softw.* 79(4), 1-26. doi: 10.18637/jss.v079.i04.
5. Truong, K.T., Wambaugh, J.F., Kapraun, D.F., Davidson-Fritz, S.E., Eytcheson, S., Judson, R.S., et al. (2025). Interpretation of thyroid-relevant bioactivity data for comparison to in vivo exposures: A prioritization approach for putative chemical inhibitors of in vitro deiodinase activity. *Toxicology* 515, 154157. doi: 10.1016/j.tox.2025.154157.
6. Wambaugh, J.F., Wetmore, B.A., Ring, C.L., Nicolas, C.I., Pearce, R.G., Honda, G.S., et al. (2019). Assessing toxicokinetic uncertainty and variability in risk prioritization. *Toxicol. Sci.* 172(2), 235-251. doi: 10.1093/toxsci/kfz205.

Chemical Selection

Compound Selection Interface



Toxicokinetic Chemical Simulator (ToCS) General Parameters Model Specifications **Compound Selection** Advanced (Optional) Parameters Run Simulation

INSTRUCTIONS

You must choose at least one compound from the preloaded compounds, upload a CSV file with data for at least one compound not included in the preloaded compounds, or both.

Click on the appropriate link(s) below to download guidance on how to upload data under the 'Uploaded Data' card. Follow the 'Instructions' document in the downloaded folder to correctly format the file you want to upload.

[Uploaded Physical-Chemical Data File Folder](#)

PRELOADED COMPOUNDS

Select the types of compounds you want to simulate.

Choose from all available chemicals ▼

Select any preloaded compounds. Search through the list by clicking on the box and scrolling or typing in a name. The list may not show all available compounds. Click on a compound to select it. You may select multiple.

At least one compound must be selected or uploaded

UPLOADED DATA

Upload a CSV file of physical and chemical data for compounds not in the preloaded list (if desired). Download the 'Uploaded Physical-Chemical Data File Folder' under the 'Instructions' card for file formatting instructions.

Browse... No file selected

Downloadable folder detailing how to upload physicochemical data to simulate new compounds

Drop-down list of chemicals with data already preloaded into httk, contains only compounds with adequate data for simulation

Click here to upload a CSV file of physicochemical data for chemicals not available in the preloaded drop-down list

Compound Selection: Preloaded Drop-Down List

- Contains compounds with data already in htk
- Search the drop-down list by:
 - Typing in the CAS number (recommended)
 - Typing in the compound name
 - Scrolling the list (all compounds are not visible)

The screenshot shows a web interface with three tabs: "Model Specifications", "Compound Selection" (which is active), and "Advanced (Optional) Parameters". Under the "Compound Selection" tab, there is a section titled "PRELOADED COMPOUNDS". It contains a dropdown menu with the text "Choose from only food relevant chemicals". Below this is a text box with instructions: "Select any preloaded compounds. Search through the list by clicking on the box and scrolling or typing in a name. The list may not show all available compounds. Click on a compound to select it. You may select multiple." Below the text box is a scrollable list of compounds with their CAS numbers and names: 94-13-3, Propylparaben; 94-26-8, Butylparaben; 95-48-7, 2-methylphenol; 97-53-0, Eugenol; 98-54-4, 4-tert-butylphenol; 99-76-3, Methylparaben; and 84-66-2, Diethylphthalate.

Model Specifications **Compound Selection** Advanced (Optional) Parameters

PRELOADED COMPOUNDS

Select the types of compounds you want to simulate.

Choose from only food relevant chemicals ▼

Select any preloaded compounds. Search through the list by clicking on the box and scrolling or typing in a name. The list may not show all available compounds. Click on a compound to select it. You may select multiple.

|

94-13-3, Propylparaben
94-26-8, Butylparaben
95-48-7, 2-methylphenol
97-53-0, Eugenol
98-54-4, 4-tert-butylphenol
99-76-3, Methylparaben
84-66-2, Diethylphthalate

Compound Selection: Upload Your Own Compounds

Toxicokinetic Chemical Simulator (ToCS) General

INSTRUCTIONS

You must choose at least one compound from the preloaded compounds, upload a CSV file with data for at least one compound not included in the preloaded compounds, or both.

Click on the appropriate link(s) below to download guidance on how to upload data under the 'Uploaded Data' card. Follow the 'Instructions' document in the downloaded folder to correctly format the file you want to upload.

[Uploaded Physical-Chemical Data File Folder](#)

Variable Name	Description	Units
Compound	Name of chemical compound	
CAS	Chemical Abstracts Service Registry Number	
CAS.Checksum	Is CAS valid?	
DTXSID	DSTox Structure ID	
Formula	The proportions of atoms within the chemical compound	
All.Compound.Names	All names of chemical as they occur in the data	
logHenry	The log10 Henry's law constant	log10(atmospheres*m^3/mole)
logHenry.Reference	Reference for logHenry	
logMA	The log10 phospholipid water partition coefficient (PC) or "Membrane affinity"	log10 unitless ratio
logMA.Reference	Reference for logMA	
logP	The log10 octanol:water PC	log10 unitless ratio
logP.Reference	Reference for logP	
logPwa	The log10 water:air PC	log10 unitless ratio
logPwa.Reference	Reference for logPwa	
logWSol	The log10 water solubility	log10 (mole/L)
logWSol.Reference	Reference for logWSol	
MP	The chemical compound melting point	Degrees celcius
MP.Reference	Reference for MP	

DataDescriptions
Type: Adobe Acrobat Document

Instructions
Type: Adobe Acrobat Document

RequiredData
Type: Adobe Acrobat Document

SampleCSV
Type: Microsoft Excel Comma Separated Values File

AutoSave Off SampleCSV - Read-Only

File Home Insert Draw Page Layout Formulas Data Review View Automate Help Acrobat

Clipboard Font Alignment Number Styles Cells Editing Sensitivity Add-ins Analyze Data Create and Share Adobe PDF

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	Compound	CAS	CAS.Checksum	DTXSID	Formula	All.Compound.Names	logHenry	logHenry.Reference	logMA	logMA.Reference	logP	logP.Reference	logPwa	logPwa.Reference	logWSol	logWSol.Reference	MP	MP.Reference	MW	MP
2	Chem1	111-11-2		DTX1					3.8		3.73								206.3	
3	Chem2	222-22-0		DTX2					NA		4.19								293.3	
4	Chem3	333-33-5		DTX3					3.46		2.7								308.3	

Compound Selection: Uploaded Data

Required Data

- Compound name
- CAS number
- DTXSID
- Molecular weight
- Log10 octanol:water partition coefficient
- In vitro intrinsic hepatic clearance
- In vitro fraction unbound in presence of plasma proteins

Optional Data

- Log10 Henry's law constant
- Log10 phospholipid water partition coefficient
- Log10 water air partition coefficient
- Log10 water solubility
- Melting point
- Hydrogen acceptor equilibria concentration
- Hydrogen donor equilibria concentration
- In vivo measured fractional systemic bioavailability of an oral dose
- Caco-2 apical-to-basal membrane permeability
- Probability that there is no clearance observed
- In vivo fraction of oral dose absorbed and entering gut lumen
- In vivo fraction of oral dose surviving first pass metabolism in the gut
- In vivo fraction of oral dose surviving first pass hepatic clearance
- Ratio of blood to plasma chemical concentration

Where Can I Find the Chemical Data?

NTP's Integrated Chemical Environment (ICE)
(<https://ice.ntp.niehs.nih.gov/>) →

EPA United States Environmental Protection Agency

Environmental Topics Laws & Regulations About EPA

CompTox Chemicals Dashboard v2.5.3 Home Search Lists About Tools Submit Comments

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Approved Name.

Properties: Summary

Summary Search Chemical Properties

EXPORT

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range
Polarizability	-	27.0 (1)	-	27.0	-	27.0
Henry's Law	-	1.26e-7 (1)	-	1.26e-7	-	1.26e-7
Boiling Point	200 (1)	367 (4)	200	362	200	343 to 401
Flash Point	-	190 (2)	-	190	-	188 to 192
Melting Point	155 (7)	137 (3)	156	132	153 to 156	125 to 153
Molar Refractivity	-	68.2 (1)	-	68.2	-	68.2
Molar Volume	-	200 (1)	-	200	-	200
Viscosity	-	9.66 (1)	-	9.66	-	9.66
Index of Refraction	-	1.60 (1)	-	1.60	-	1.60
Surface Tension	-	46.0 (1)	-	46.0	-	46.0

Integrated Chemical Environment

Home Search Tools

Chemical Quest **Chemical Characterization** Curve Surfer PBPK IVIVE

Input **Results**

Chemical Characterization Results

Click on the arrows to show results

Chemical Properties Summary

Values displayed are Open Structure Activity/Property Relationship App (OPERA) predictions:

Lists A Demo List of Chemicals

Send filtered results to: Select tool...

Chemical List (OPERA) Predictions by Input List, CASRN

List	Substance Name	CASRN (CEBS Link)	DTXSID (Dashboard Link)	Molecular Weight, g/mol	OPERA, Boiling Point, C	OPERA, Henry's Law Constant, atm-m ³ /mol	OPERA, Melting Point, C	OPERA, Negative Log of Acid Dissociation Constant, pKa, Acid	OPERA, Octanol-Air Partition Coefficient, K _{OA} log10	OPERA, Octanol-Water Distribution Coefficient, logD log10	OPERA, Octanol-Water Partition Coefficient, logP log10
A Demo List of Chemicals	Perfluorooctanoic acid	335-67-1	DTXSID8031865	413.974	189.0	-9.72	54.0	0.34	4.16	-2.05	3.11
A Demo List of Chemicals	17beta-Estradiol	50-28-2	DTXSID0020573	272.178	373.0	-5.43	200.0	11.66	9.15	3.91	3.91
A Demo List of Chemicals	Caffeine	58-08-2	DTXSID0020232	194.08	286.0	-5.81	238.0	NaN	8.52	-0.07	-0.07
A Demo List of Chemicals	Bifenthrin	82657-04-3	DTXSID9020160	422.126	371.0	-7.31	69.0	NaN	10.47	6.19	6.19

← EPA's CompTox Chemicals Dashboard
(<https://comptox.epa.gov/dashboard>)

Demo: Uploading Chemical Data

Calcium Benzoate

A direct food additive used as an antimicrobial agent

Demo: Uploading Chemical Data

1. Download physicochemical data folder
2. Copy SampleCSV file to a new file to edit
3. Search for chemical data within EPA's CompTox Dashboard
4. Update appropriate fields in new CSV file
5. Save CSV file and upload within ToCS interface

Demo: Uploading Chemical Data

1. Download physicochemical data folder

Toxicokinetic Chemical Simulator (ToCS)
General Parameters
Model Specifications
Compound Selection
Advanced (Optional) Parameters
Run Simulation

INSTRUCTIONS

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UPLOADED DATA

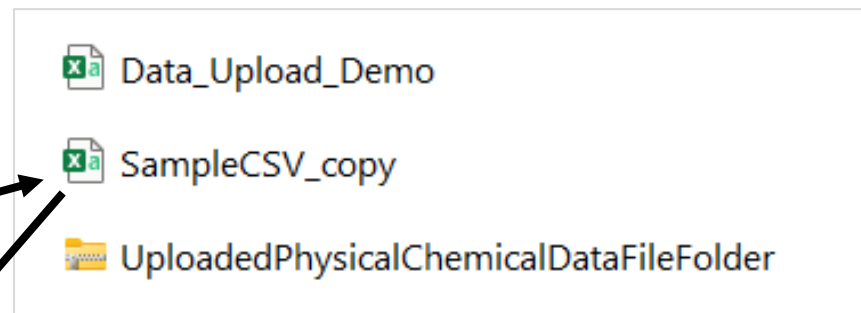
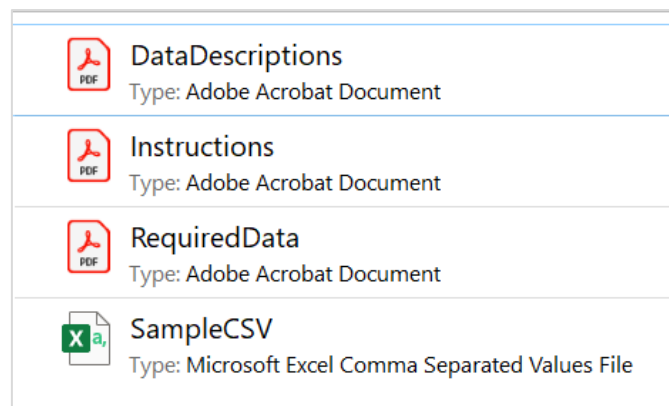
Upload a CSV file of physical and chemical data for compounds not in the preloaded list (if desired). Download the 'Uploaded Physical-Chemical Data File Folder' under the 'Instructions' card for file formatting instructions.

Browse...
No file selected

Click here to download the folder

Demo: Uploading Chemical Data

2. Copy SampleCSV file to a new file to edit

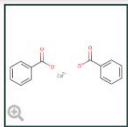


	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	
1	Compound	CAS	CAS.Chec	DTXSID	Formula	All.Compo	logHenry	logHenry.F	logMA	logMA.Refer	logP	logP.Refer	logPwa	logPwa.Re	logWSol	logWSol.R	MP	MP.Refer	MW	MW.Refer	pKa_Accep	pKa_Accep	pKa_Donor	pKa
2																								
3																								

Demo: Uploading Chemical Data

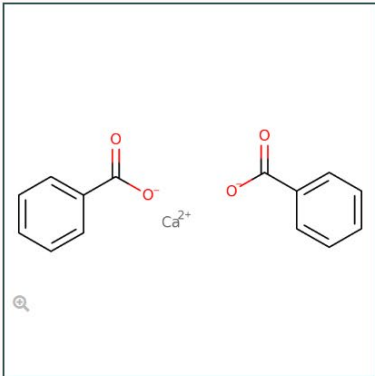
3. Search for chemical data within EPA's CompTox Dashboard

CompTox Chemicals Dashboard v2.6.0 Home Search Lists About Tools Submit Comments Search all data



Calcium dibenzoate
 2090-05-3 | DTXSID4044612
 Searched by CASRN

Chemical Details



Wikipedia

Calcium benzoate refers to the calcium salt of benzoic acid. When used in the food industry as a preservative, its E number is E213 (INS number 213); it is approved for use as a food additive in the EU, USA and Australia and New Zealand.

The formulas and structures of calcium carboxylate derivatives of calcium and related metals are complex. Generally the coordination number is eight and the carboxylates form Ca-O bonds. Another variable is the degree of hydration.

[Read more](#)

Quality Control Notes

Intrinsic Properties

Molecular Formula: $C_{14}H_{10}CaO_4$
 MOL FILE
 FIND ALL CHEMICALS

Average Mass: 282.308 g/mol
 ISOTOPE MASS DISTRIBUTION

Monoisotopic Mass: 282.0205 g/mol

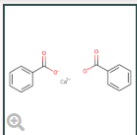
Structural Identifiers

Demo: Uploading Chemical Data



3. Search for chemical data within EPA's CompTox Dashboard

CompTox Chemicals Dashboard v2.6.0 Home Search Lists About Tools Submit Comments Search all data

 **Calcium dibenzoate**
2090-05-3 | DTXSID4044612
Searched by CASRN

Chemical Details
Executive Summary
Physchem Prop.
Env. Fate/Transport
Hazard Data
Safety > GHS Data
ADME > IVIVE
Exposure
Bioactivity
GenRA
ACToR
Literature
Links
Comments

Properties: Summary

Summary Search Chemical Properties

EXPORT

Summary

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Henry's Law	-	2.69e-7 (1)	-	2.69e-7	-	2.69e-7	atm-m3/mole
Boiling Point	-	249 (1)	-	249	-	249	°C
Melting Point	-	184 (1)	-	184	-	184	°C
LogD5.5	-	-2.27 (1)	-	-2.27	-	-2.27	Log10 unitless
LogD7.4	-	-4.15 (1)	-	-4.15	-	-4.15	Log10 unitless
Vapor Pressure	-	7.08e-4 (1)	-	7.08e-4	-	7.08e-4	mmHg
Water Solubility	-	0.331 (1)	-	0.331	-	0.331	mol/L
LogKoa: Octanol-Air	-	5.91 (1)	-	5.91	-	5.91	Log10 unitless
LogKow: Octanol-Water	-	-0.950 (1)	-	-0.950	-	-0.950	Log10 unitless
pKa Acidic Apparent	-	4.20 (1)	-	4.20	-	4.20	Log10 unitless

Demo: Uploading Chemical Data



4. Update appropriate fields in new CSV file

No real data available, so we set the clint and Funbound.plasma as 0.2 and 0.95 in this example

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Compound	CAS	CAS.Checksum	DTXSID	Formula	All.Compound.Names	logHenry	logHenry.Reference	logMA	logMA.Reference	logP	logP.Reference	logPwa	logPwa.Reference	logWSol	logWSol.Reference
2	Calcium Benzoate	2090-05-3		DTXSID4044612			2.69E-07	EPA CompTox v2.6.0			-0.95	EPA CompTox v2.6.0			-0.480172006	EPA CompTox v2.6.0

	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	
1	MP	MP.Reference	MW	MW.Reference	pKa_Accept	pKa_Accept.Reference	pKa_Donor	pKa_Donor.Reference	All.Species	Dog.Foral	Dog.Foral.Reference	DTXSID.Reference	Formula.Reference	Human.Caco2.Pab	Human.
2	184	EPA CompTox v2.6.0	282.308	EPA CompTox v2.6.0	4.2	EPA CompTox v2.6.0						EPA CompTox v2.6.0			

	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO
1	Human.Caco2.Pab.Reference	Human.Clint	Human.Clint.pValue	Human.Clint.pValue.Reference	Human.Clint.Reference	Human.Fabs	Human.Fabs.Reference	Human.Fgut	Human.Fgut.Reference	Human.Fhpe	Human.Fhpe.Reference
2		0.2			NA						

	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY
1	Human.Foral	Human.Foral.Reference	Human.Funbound.plasma	Human.Funbound.plasma.Reference	Human.Rblood2plasma	Human.Rblood2plasma.Reference	Monkey.Foral	Monkey.Foral.Reference	Mouse.Foral	Mouse.Foral.Reference
2			0.95	NA						

	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG
1	Mouse.Foral	Mouse.Foral.Reference	Mouse.Funbound.plasma	Mouse.Funbound.plasma.Reference	Rabbit.Funbound.plasma	Rabbit.Funbound.plasma.Reference	Rat.Clint	Rat.Clint.pValue	Rat.Clint.pValue.Reference	Rat.Clint.Reference
2										

	3D	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN
1	Clint	Rat.Clint.pValue	Rat.Clint.pValue.Reference	Rat.Clint.Reference	Rat.Foral	Rat.Foral.Reference	Rat.Funbound.plasma	Rat.Funbound.plasma.Reference	Rat.Rblood2plasma	Rat.Rblood2plasma.Reference	Chemical.Class
2											
3											

Demo: Uploading Chemical Data

5. Save CSV file and upload within ToCS interface

Toxicokinetic Chemical Simulator (ToCS)

General Parameters

Model Specifications

Compound Selection

Advanced (Optional) Parameters

Run Simulation

INSTRUCTIONS

Click on the appropriate link(s) below to download guidance on how to upload data under the 'Uploaded Data' card. Follow the 'Instructions' document in the downloaded folder to correctly format the file you want to upload.

[Uploaded Physical-Chemical Data File Folder](#)

PRELOADED COMPOUNDS

Select the types of compounds you want to simulate.

Choose from all available chemicals

Select any preloaded compounds. Search through the list by clicking on the box and scrolling or typing in a name. The list may not show all available compounds. Click on a compound to select it. You may select multiple.

UPLOADED DATA

Upload a CSV file of physical and chemical data for compounds not in the preloaded list (if desired). Download the 'Uploaded Physical-Chemical Data File Folder' under the 'Instructions' card for file formatting instructions.

Browse...

Data_Upload_Demo.csv

Upload complete

Questions?

10–Minute Break