

Parameter Calculations Examples

Kristen Leonard

May 30, 2025

If you have not already read the *Introduction to the ToCS App* vignette, it is highly recommended to do so to get a general idea of the app's layout and obtain a detailed description of common user inputs across all output modules. Users should also review the ToCS README file to setup ToCS if they have not accessed the app yet. This vignette assumes that you have access the ToCS app GUI already.

Introduction

This vignette provides two examples that use the ToCS app to generate parameter calculations, each example with different parameters selected. To begin, open the app by using any of the methods described in the README file. You have correctly accessed the app if your screen looks like the image below.

The screenshot displays the Toxicokinetic Chemical Simulator (ToCS) application interface. At the top, a navigation bar includes the title "Toxicokinetic Chemical Simulator (ToCS)" and five tabs: "General Parameters" (which is selected), "Model Specifications", "Compound Selection", "Advanced (Optional) Parameters", and "Run Simulation". The main content area is divided into three vertical panels. The leftmost panel, titled "INSTRUCTIONS", contains text about the app's purpose and provides links for more information. The middle panel, titled "OUTPUT", features a dropdown menu labeled "Select the desired output." with a "Select" option and a red error message below it: "Must not be equal to Select." The rightmost panel, titled "SPECIES", features a dropdown menu labeled "Select the species to analyze." with a "Select" option and a red error message below it: "Must not be equal to Select."

The opening interface to the ToCS app.

Example 1

Let's say that we want to calculate human TK parameters for eight sample chemicals:

- Acephate (CAS: 30560-19-1)
- Advantame (CAS: 714229-20-6)
- Caffeine (CAS: 58-08-2)
- Carboxin (CAS: 5234-68-4)
- Phenol (CAS: 108-95-2)
- Pirinixic acid (CAS: 50892-23-4)
- Titanium dioxide (CAS: 13463-67-7)
- Triadimenol (CAS: 55219-65-3)

without using httk's preloaded in silico parameters for hepatic clearance, fraction unbound in plasma, or caco-2 permeability.

General Parameters Tab

Since we want to calculate human TK parameters, we select *Parameter calculations* for the first drop down menu under the *Output* card and *Human* for the first drop down under the *Species* card. The completed *General Parameters* tab should look like the image below. The user should now move on to the *Model Specifications* tab.

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

INSTRUCTIONS

Fill out the prompts on each of the above tabs moving left to right. Then, click the 'Run Simulation' tab to run the simulation or reset all selections.

ToCS provides four toxicokinetic (TK) outputs: 1) Concentration-time profiles, which returns chemical concentrations in bodily compartments over time, 2) Steady state (SS) concentrations, which returns SS concentrations in bodily compartments from an oral infusion, 3) In vitro in vivo extrapolation (IVIVE), which returns oral equivalent doses to in vitro bioactive concentrations, 4) Parameter calculations, which returns elimination rates, volumes of distribution, tissue to unbound plasma partition coefficients, half-lives, and total plasma clearances.

This application uses the U.S. EPA's R package 'httk'. For more information on 'httk', refer to <https://doi.org/10.18637/jss.v079.i04> and/or <https://cran.r-project.org/web/packages/httk>

For additional guidance on ToCS, please refer to the vignettes (<https://github.com/KristenWindoloski/ToCS/tree/main/vignettes>). To report issues or suggestions for improvement, visit <https://github.com/KristenWindoloski/ToCS/issues>.

OUTPUT

Select the desired output.

Parameter calculations

SPECIES

Select the species to analyze.

Human

The completed general parameters tab for example 1.

Model Specifications Tab

As shown in the image below under the *Model* card, we select 'Schmitt' for the first drop down menu, which is the only option. Then, we select *No* under the second drop down menu since we do not want the program to simulate chemicals with in silico generated parameters for hepatic clearance, fraction unbound in plasma, and caco-2 permeability. There are no user selections under the *Dosing* card. The completed tab should look like the image below, and the user can proceed to the next tab.

MODEL

Select a model to simulate.

Schmitt

Select whether to use in silico generated parameters for compounds with missing in vitro data. These parameters will not overwrite existing in vitro data, and it will expand the number of compounds available.

No, do not load in silico parameters

DOSING

No options for this category.

The completed model specifications tab for example 1.

Compound Selection Tab

We keep the first drop menu in the *Preloaded Compounds* card on *Choose from all available chemicals* and then under the second drop down, we search by either compound name or CAS for all eight compounds. All but two compounds (advantame and titanium dioxide) are available, so we select the six available compounds under the *Preloaded Compounds* tab. Thus, we have to upload the chemical data for advantame and titanium dioxide. So, we copy the SampleCSV file in the *Uploaded Compound File Folder* under the *Instructions* card and enter the appropriate chemical information for each compound, as shown in the table below. See the *Introduction to ToCS* vignette for more information on upload instructions. For the purpose of this example, we use fake chemical data and upload the following csv file (CSV_PCvignette.csv) by clicking *Browse* under the *Uploaded Data* card.

A csv file with chemical information for advantame and titanium dioxide. Data other than the chemical identifiers are

Compound	CAS	CAS.Checksum	DTXSID	Formula	All.Compound.Names	logHenry
Titanium Dioxide	13463-67-7	NA	DTXSID3021352	NA	NA	NA

Compound	CAS	CAS.Checksum	DTXSID	Formula	All.Compound.Names	logHenry
Advantame	714229-20-6	NA	DTXSID00991787	NA	NA	NA

Now that all simulation chemicals are uploaded, the final *Compound Selection* tab should look like the image below.

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.

30560-19-1, Acephate
58-08-2, Caffeine
5234-68-4, Carboxin
108-95-2, Phenol
50892-23-4, Pirinixic acid
55219-65-3, Triadimenol

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...
CSV_PCvignette.csv

Upload complete

The completed compound selection tab for example 1.

Advanced (Optional) Parameters Tab

In the *Advanced Parameters* tab, we are not going to customize any additional parameters for this example and so we leave all inputs as is. The *Advanced Parameters* tab should look like the image below.

MODEL CONDITIONS	MODEL SOLVER	BIOAVAILABILITY	OUTPUT SPECIFICATION
<p>Enter the Ratio of Distribution coefficient D of totally charged species and that of the neutral form.</p> <input type="text" value="0.001"/>	No options for this category.	<p>Enter a default value for the Caco-2 apical-to-basal membrane permeability (denoted Caco2.Pab, 10⁻⁶ cm/s).</p> <input type="text" value="1.6"/>	No options for this category.
<p>Select whether protein binding is taken into account in liver clearance.</p> <div>Yes, include protein binding (default) ▾</div>		<p>Select whether to use the Caco2.Pab value set above to estimate F_{abs} (the in vivo measured fraction of an oral dose absorbed from the gut lumen into the gut) if bioavailability data is unavailable.</p> <div>Use the Caco2.Pab value selected above (default) ▾</div>	
<p>Select whether to adjust the chemical fraction unbound in presence of plasma proteins for lipid binding.</p> <div>Yes, adjust the fraction of unbound plasma (default) ▾</div>		<p>Select whether to use the Caco2.Pab value set above to calculate F_{gut} (the in vivo measured fraction of an oral dose that passes gut metabolism and clearance) if bioavailability data is unavailable.</p> <div>Use the Caco2.Pab value selected above (default) ▾</div>	
<p>Select whether to use regressions when calculating partition coefficients.</p> <div>Use regressions (default) ▾</div>		<p>Select whether to overwrite in vivo F_{abs} and F_{gut} data (if available).</p> <div>Do not overwrite in vivo values (default) ▾</div>	
<p>Enter the p-value threshold for the in vitro intrinsic hepatic clearance rate where clearance assay results with p-values above this threshold are set to zero.</p> <input type="text" value="0.05"/>		<p>Select whether to keep F_{abs} and F_{gut} at 100% availability (which overwrites all other bioavailability parameter settings above).</p> <div>Do not keep Fabs and Fgut at 100% availability (default) ▾</div>	
<p>Enter the minimum acceptable chemical fraction unbound in presence of plasma proteins. All values below this will be set to this value.</p> <input type="text" value="0.0001"/>			

The completed advanced parameters tab for example 1.

Run Simulation Tab

Now that all user selections have been made and all of the desired simulation compounds appear under the *Selected Compounds* card, we hit the *Run Simulation* button under the *Actions* card. The page prior to simulation completion should look like the image below, with five drop downs where results will appear under the *Results* card.

ACTIONS

Click on the 'Run Simulation' button when all information has been entered.

Run Simulation

Click on the button below to reset your session. This will clear all selections and any uploaded data, and is recommended to be done every time a new simulation is run.

Reset Session

☐ Check the box to display plots with a log10 scale y-axis.

SELECTED COMPOUNDS

Selected Compounds

Acephate

Advantame

Caffeine

Carboxin

Phenol

Pirinixic acid

Titanium Dioxide

Triadimenol

RESULTS

Parameter Plots

Parameter Table

Partition Coefficient Plots

Partition Coefficient Table

Simulation Parameters

The run simulation tab prior to simulation completion for example 1.

Once the simulation is complete, users will see a group of four plots appear under the *Parameter Plots* tab in the *Results* card. The plots show each compound's elimination rate (1/h, top left), volume of distribution (L/kg BW, top right), half life (h, bottom left), and total plasma clearance (L/h/kg BW, bottom right). The users have the option to download this figure as is using the *Download Figure 1* button. The user's interface should look like the image below.

RESULTS

Parameter Plots

Download Figure 1

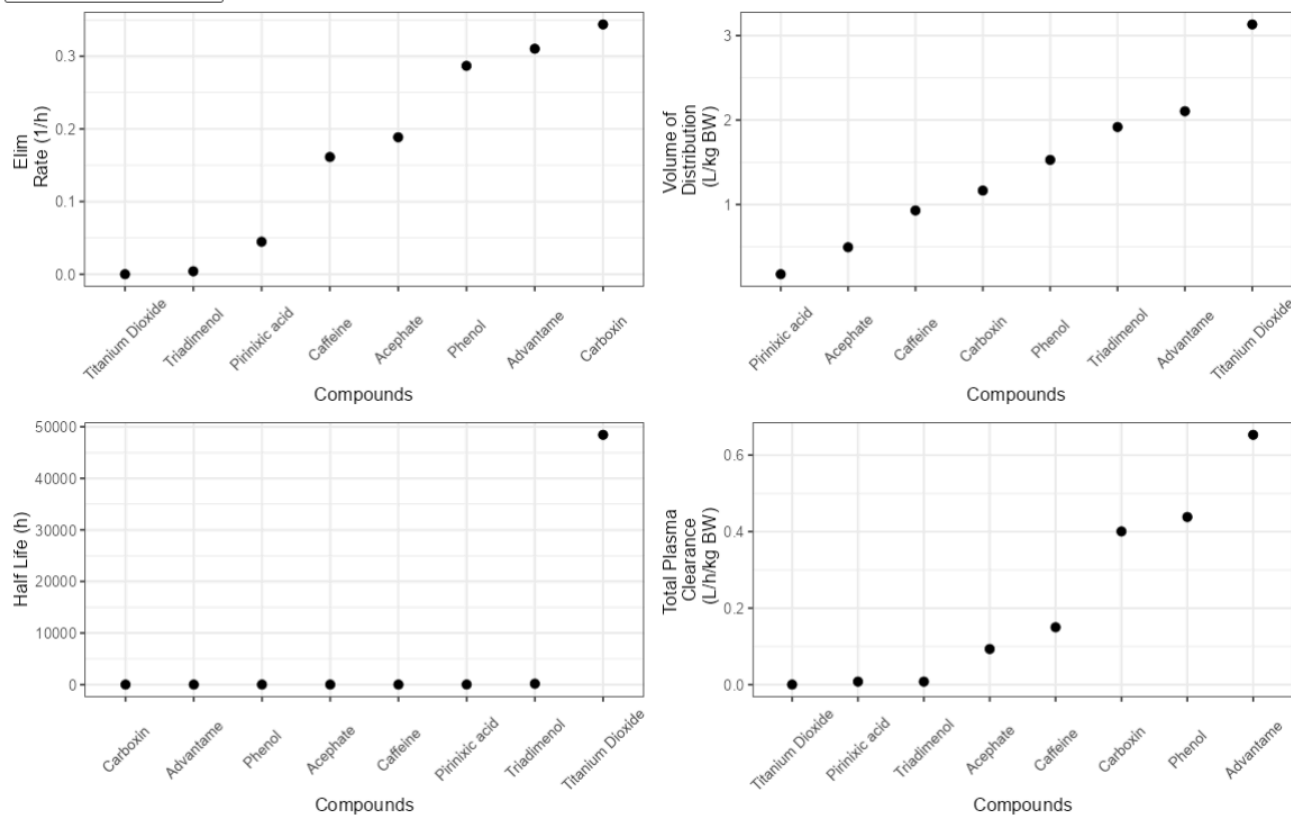


Figure 1: Plots of the estimated elimination rate (1/h), volume of distribution (L/kg BW), half life (h), and total plasma clearance (L/h/kg BW) for all selected compounds.

The parameter plots with linear y-axis drop down under the run simulation tab for example 1.

If we wanted to view the plots under this tab using a log10 y-axis, we would check the bottom box under the *Actions* card, and then the user would see the plots in the image shown below which makes it clearer to distinguish the parameter values of smaller magnitudes.

RESULTS

Parameter Plots

Download Figure 1

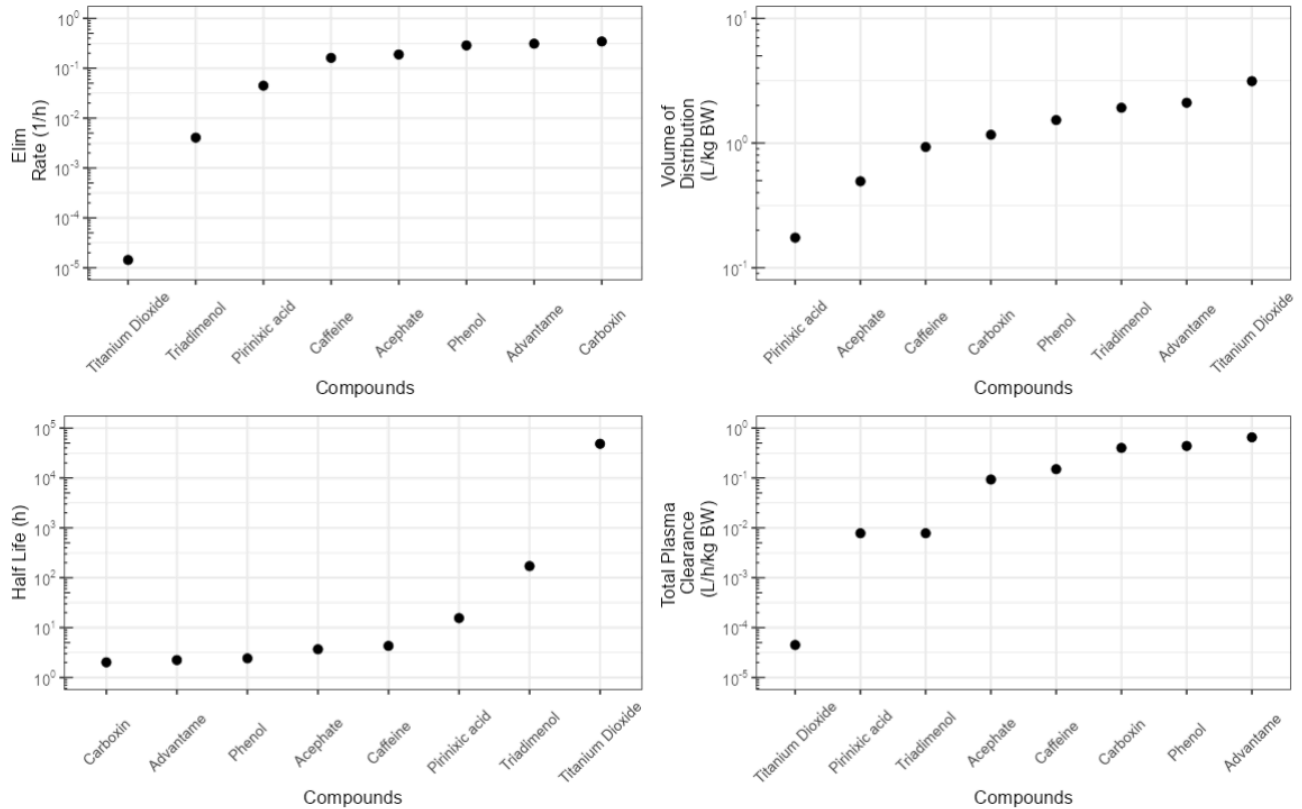


Figure 1: Plots of the estimated elimination rate (1/h), volume of distribution (L/kg BW), half life (h), and total plasma clearance (L/h/kg BW) for all selected compounds.

The parameter plots with log10 y-axis drop down under the run simulation tab for example 1.

Under the next drop down tab, there is a table of the parameter values from the previous tab. The user has the option to download the table by clicking the *Download Table 1* button. The drop down tab should look like the image below.

RESULTS

Parameter Plots

Parameter Table

Download Table 1

Show 10 entries

Search:

	CompoundName	EliminationRate	VolumeOfDistribution	HalfLife	TotalClearance
1	Acephate	0.1885	0.4934	3.677	0.09303
2	Advantame	0.3103	2.105	2.234	0.6531
3	Caffeine	0.1613	0.9294	4.297	0.1499
4	Carboxin	0.3438	1.165	2.016	0.4005
5	Phenol	0.2868	1.528	2.417	0.4382
6	Pirinixic acid	0.04467	0.1742	15.52	0.007782
7	Titanium Dioxide	0.00001431	3.133	48440	0.00004483
8	Triadimenol	0.004059	1.918	170.8	0.007785

Showing 1 to 8 of 8 entries

Previous1Next

Table 1: Table of estimated elimination rates (1/h), volumes of distribution (L/kg BW), half lifes (h), and total plasma clearances (L/h/kg BW) for all selected compounds. Compounds are listed in ascending order of the elimination rate.

Partition Coefficient Plots

Partition Coefficient Table

Simulation Parameters

The parameter table drop down under the run simulation tab for example 1.

Under the third drop down tab, the user should see 13 plots, one per partition coefficient. This compilation of plots is available for download by clicking the *Download Figure 2* button at the top of the tab. The user's plots should look like the image below.

RESULTS

Partition Coefficient Plots

Download Figure 2

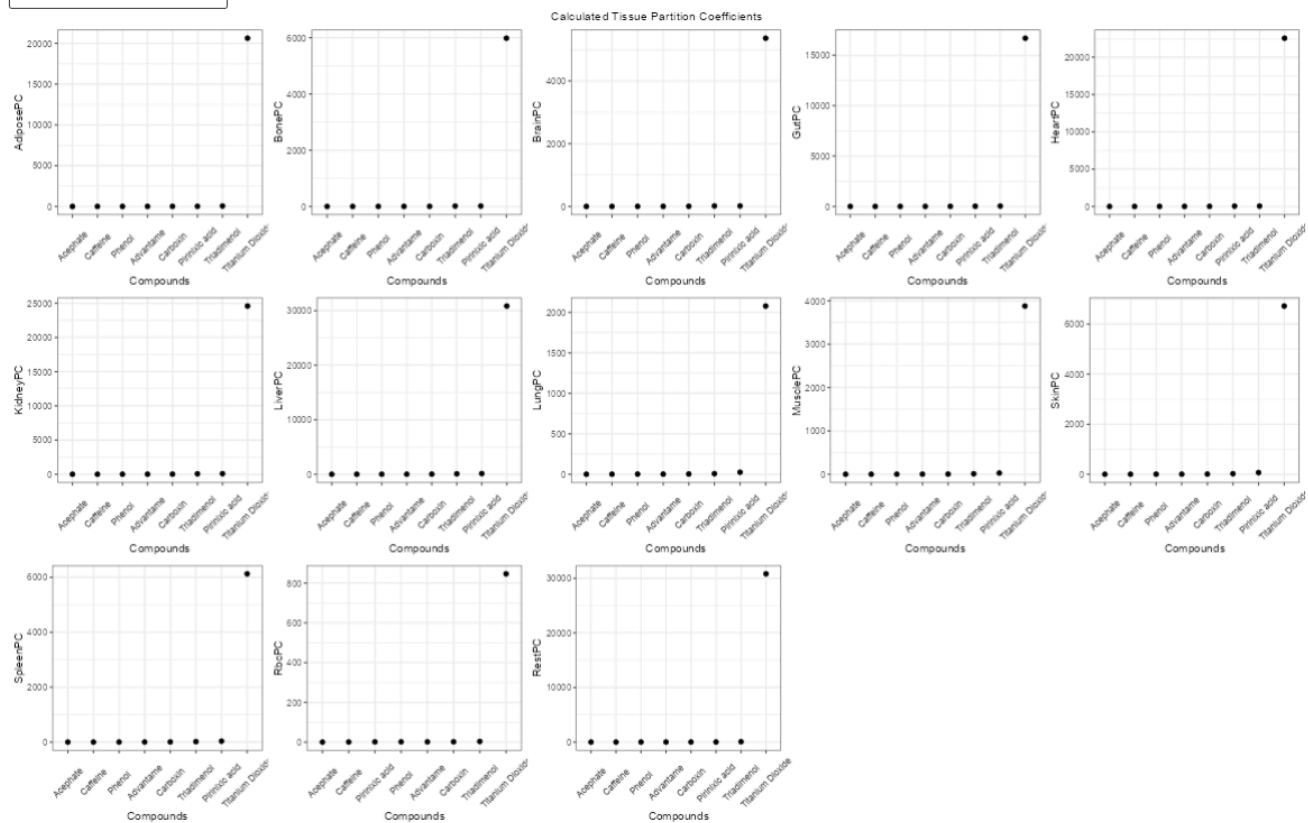


Figure 2: Plots of the estimated partition coefficients (no units) using Schmitt's method for all tissues available (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, spleen, skin, rbc, rest).

The partition coefficients plots with linear y-axis under the run simulation tab for example 1.

Now as with the first drop down tab, the user can change the scale on the y-axis of the partition coefficient plots to be a log10 y-axis scale in order to easier distinguish the smaller magnitudes. The user can download the partition coefficient plot by clicking the *Download Figure 2* button. The log10 y-axis scale plots should look like the image below.

Partition Coefficient Plots

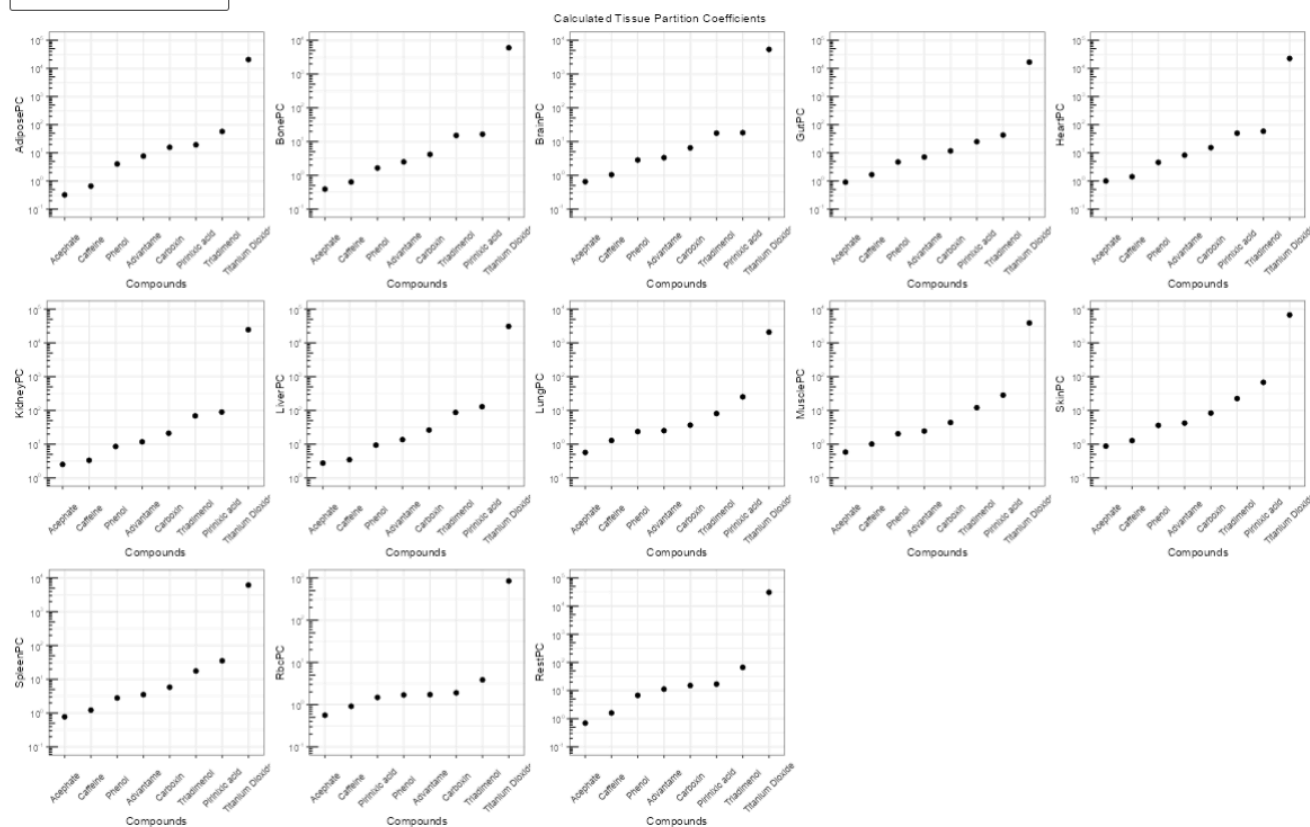
[Download Figure 2](#)


Figure 2: Plots of the estimated partition coefficients (no units) using Schmitt's method for all tissues available (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, skin, spleen, and blood cells (rbc), testis, collectively representing various tissues). Compounds are ordered in ascending order based on the median partition coefficient for

The partition coefficients plots with log₁₀ y-axis drop down under the run simulation tab for example 1.

Under the fourth drop down tab is a table of partition coefficients from the plots under the previous tab. Users can download the table of partition coefficients by clicking the *Download Table 2* button. The user's table should look like the image below.

RESULTS

Partition Coefficient Plots

Partition Coefficient Table

Download Table 2

Show 10 entries

Search:

	CompoundName	AdiposePC	BonePC	BrainPC	GutPC	HeartPC	KidneyPC	LiverPC	LungPC	MusclePC	S
1	Acephate	0.3215	0.3908	0.6517	0.9064	0.9987	2.518	2.753	0.5698	0.583	
2	Advantame	7.639	2.504	3.341	7.08	8.235	11.74	13.66	2.515	2.451	
3	Caffeine	0.6593	0.6355	1.047	1.68	1.417	3.335	3.471	1.286	1.011	
4	Carboxin	15.72	4.178	6.522	11.71	15.34	21.14	26.3	3.669	4.382	
5	Phenol	4.016	1.652	2.849	4.724	4.589	8.555	9.381	2.363	2.04	
6	Pirinixic acid	19.25	16.5	18.28	24.91	49.98	89.58	128.9	25.23	28.38	
7	Titanium Dioxide	20630	5984	5360	16690	22540	24590	30850	2079	3880	
8	Triadimenol	57.25	15.19	17.79	42.74	58.35	68.95	87.26	8.083	12.06	

Showing 1 to 8 of 8 entries

Previous

1

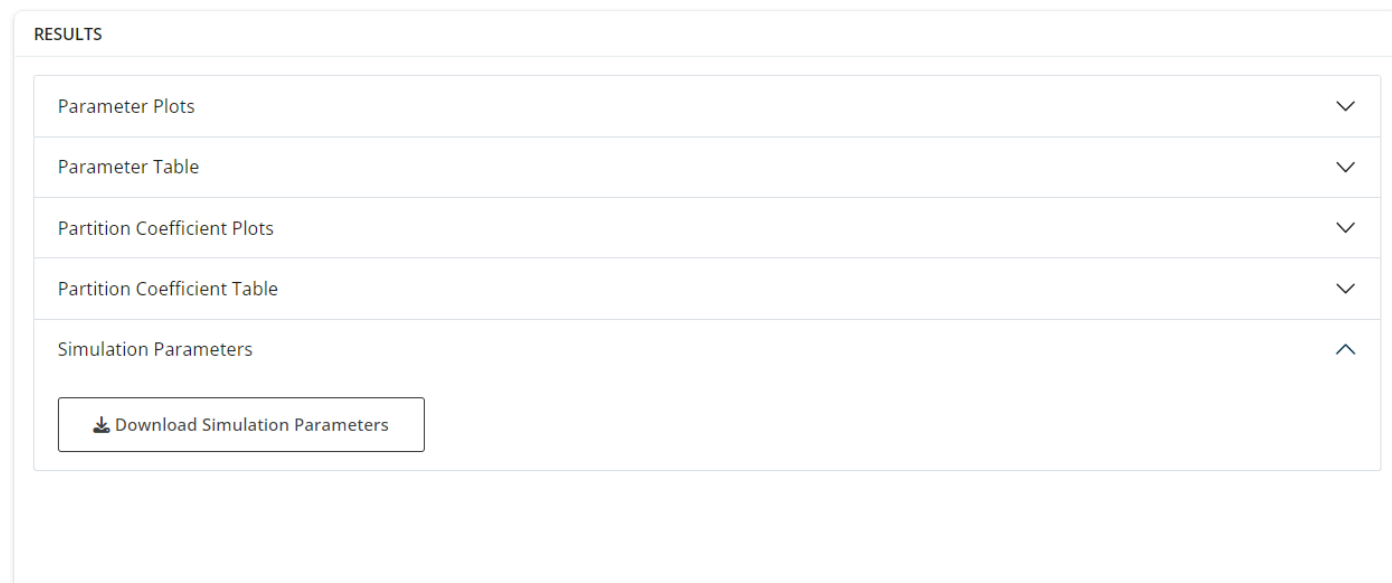
Next

Table 2: Table of partition coefficients for all selected compounds in each of the available tissues (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, skin, spleen, red blood cells (rbc), rest - collective term for remaining tissues). The compounds are listed in ascending order based on the median partition coefficient of each compound across all tissues. The median partition coefficient for each compound is shown in the last column of the table.

Simulation Parameters

The partition coefficients table drop down under the run simulation tab for example 1.

The fifth and final tab offers the user the option to download all of the user parameter selection and chemical information used to generate the simulation. The user can download this information by clicking the *Download Simulation Parameters* button. The user's screen should look like the image below.



The simulation parameters drop down under the run simulation tab for example 1.

As with other vignettes, we suggest that the user clicks the *Reset Session* button if they want to run another simulation.

Example 2

For this example, let's say that we want to calculate rat TK parameters for five unknown sample chemicals, where we will not allow chemicals to be included in our selection that only have enough data with the inclusion of in silico parameters. We will also customize several advanced parameters within this example.

General Parameters Tab

As with the previous example, we select *Parameter calculations* for the first drop down menu under the *Output* card. However, for this example, we select *Rat* for the first drop down under the *Species* card. Then, suppose we want to only use rat in vitro data instead of allowing human data to substitute for missing in vitro rat data, and so we select *No* for the second drop down under the *Species* card. The completed *General Parameters* tab should look like the image below.

INSTRUCTIONS

Fill out the prompts on each of the above tabs moving left to right. Then, click the 'Run Simulation' tab to run the simulation or reset all selections.

ToCS provides four toxicokinetic (TK) outputs: 1) Concentration-time profiles, which returns chemical concentrations in bodily compartments over time, 2) Steady state (SS) concentrations, which returns SS concentrations in bodily compartments from an oral infusion, 3) In vitro in vivo extrapolation (IVIVE), which returns oral equivalent doses to in vitro bioactive concentrations, 4) Parameter calculations, which returns elimination rates, volumes of distribution, tissue to unbound plasma partition coefficients, half-lives, and total plasma clearances.

This application uses the U.S. EPA's R package 'httk'. For more information on 'httk', refer to <https://doi.org/10.18637/jss.v079.i04> and/or <https://cran.r-project.org/web/packages/httk>

For additional guidance on ToCS, please refer to the vignettes (<https://github.com/KristenWindoloski/ToCS/tree/main/vignettes>). To report issues or suggestions for improvement, visit <https://github.com/KristenWindoloski/ToCS/issues>.

OUTPUT

Select the desired output.

Parameter calculations

SPECIES

Select the species to analyze.

Rat

Do you want to use human in vitro data if in vitro data for the selected species is missing?

No

The completed general parameters tab for example 2.

Model Specifications Tab

Our selections on this page are the same as example 1. The first drop down menu under the *Model* card is selected as 'Schmitt', and in the second drop down menu, we select *No* to not include chemical options with in silico generated parameters in place of in vitro data. The *Model Specifications* tab should look like the image below.

MODEL

Select a model to simulate.

Schmitt ▼

Select whether to use in silico generated parameters for compounds with missing in vitro data. These parameters will not overwrite existing in vitro data, and it will expand the number of compounds available.

No, do not load in silico parameters ▼

DOSING

No options for this category.

The completed model specifications tab for example 2.

Compound Selection Tab

We keep the first drop menu in the *Preloaded Compounds* card on *Choose from all available chemicals* and then we select five compounds from the drop down menu under the *Preloaded Compounds* card to simulate:

- Bisphenol-a (CAS: 80-05-7)
- Butylparaben (CAS: 94-26-8)
- Norethindrone (CAS: 68-22-4)
- Propylparaben (CAS: 94-13-3)
- Zoxamide (CAS: 156052-68-5)

Then, since there are no additional compounds we want to simulate, we advance to the next tab. The completed *Compound Selection* page should look like the image below.

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.

80-05-7, Bisphenol-a

94-26-8, Butylparaben

68-22-4, Norethindrone

94-13-3, Propylparaben

156052-68-5, Zoxamide

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

The completed compound selection tab for example 2.

Advanced Parameters Tab

In this example, we decide to change some of the default values of the advanced parameters under the *Model Conditions* card. Under the second drop down box, suppose that we want to not include protein binding when accounting for liver clearance. Therefore, we select *No, do not include protein binding*. Then, suppose we do not want to adjust the fraction unbound in the presence of plasma proteins for lipid binding. Therefore, we select *No, do not adjust the fraction of unbound plasma* for the third drop down. Finally, suppose that we want to lower the p-value threshold for the in vitro intrinsic hepatic clearance rate. Thus, we set the fifth box to *0.01* instead of *0.05*. The completed *Advanced Parameters* tab should look like the image below.

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

MODEL CONDITIONS

Enter the Ratio of Distribution coefficient D of totally charged species and that of the neutral form.

Select whether protein binding is taken into account in liver clearance.

No, do not include protein binding

Select whether to adjust the chemical fraction unbound in presence of plasma proteins for lipid binding.

No, do not adjust the fraction of unbound plasma

Select whether to use regressions when calculating partition coefficients.

Use regressions (default)

Enter the p-value threshold for the in vitro intrinsic hepatic clearance rate where clearance assay results with p-values above this threshold are set to zero.

Enter the minimum acceptable chemical fraction unbound in presence of plasma proteins. All values below this will be set to this value.

MODEL SOLVER

No options for this category.

BIOAVAILABILITY

Enter a default value for the Caco-2 apical-to-basal membrane permeability (denoted Caco2.Pab, 10⁻⁶ cm/s).

Select whether to use the Caco2.Pab value set above to estimate F_{abs} (the in vivo measured fraction of an oral dose absorbed from the gut lumen into the gut) if bioavailability data is unavailable.

Use the Caco2.Pab value selected above (default)

Select whether to use the Caco2.Pab value set above to calculate F_{gut} (the in vivo measured fraction of an oral dose that passes gut metabolism and clearance) if bioavailability data is unavailable.

Use the Caco2.Pab value selected above (default)

Select whether to overwrite in vivo F_{abs} and F_{gut} data (if available).

Do not overwrite in vivo values (default)

Select whether to keep F_{abs} and F_{gut} at 100% availability (which overwrites all other bioavailability parameter settings above).

Do not keep Fabs and Fgut at 100% availability (default)

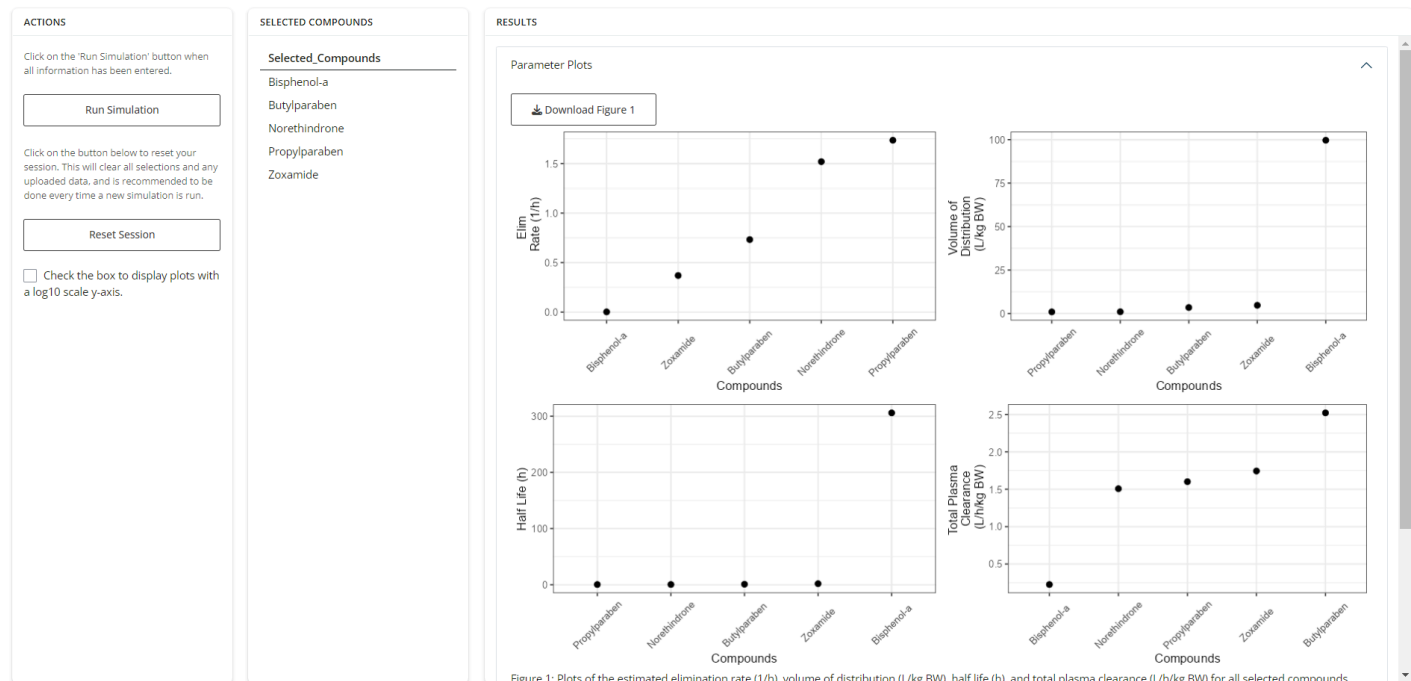
OUTPUT SPECIFICATION

No options for this category.

The completed advanced parameters tab for example 2.

Run Simulation Tab

Now that all user selections have been made and all compounds appear under the *Selected Compounds* card, we can hit the *Run Simulation* button under the *Actions* card to initiate the simulation. Below is an image of what the *Run Simulation* tab should look like once the simulation is complete. The plots show each compound's elimination rate (1/h, top left), volume of distribution (L/kg BW, top right), half life (h, bottom left), and total plasma clearance (L/h/kg BW, bottom right). Users have the option to download the figure by clicking the *Download Figure 1* button.



The linear y-axis parameter plots under the parameter plots tab for example 2.

Since it is impossible to tell the volume of distribution and half life values for four of the five compounds in the plot above, we change the y-axis scale to be a log10 y-axis by clicking the checkbox under the *Actions* tab. Then, the plots should look like the image below, which allows the user to clearly see the magnitude of all parameter predictions.

RESULTS

Parameter Plots

Download Figure 1

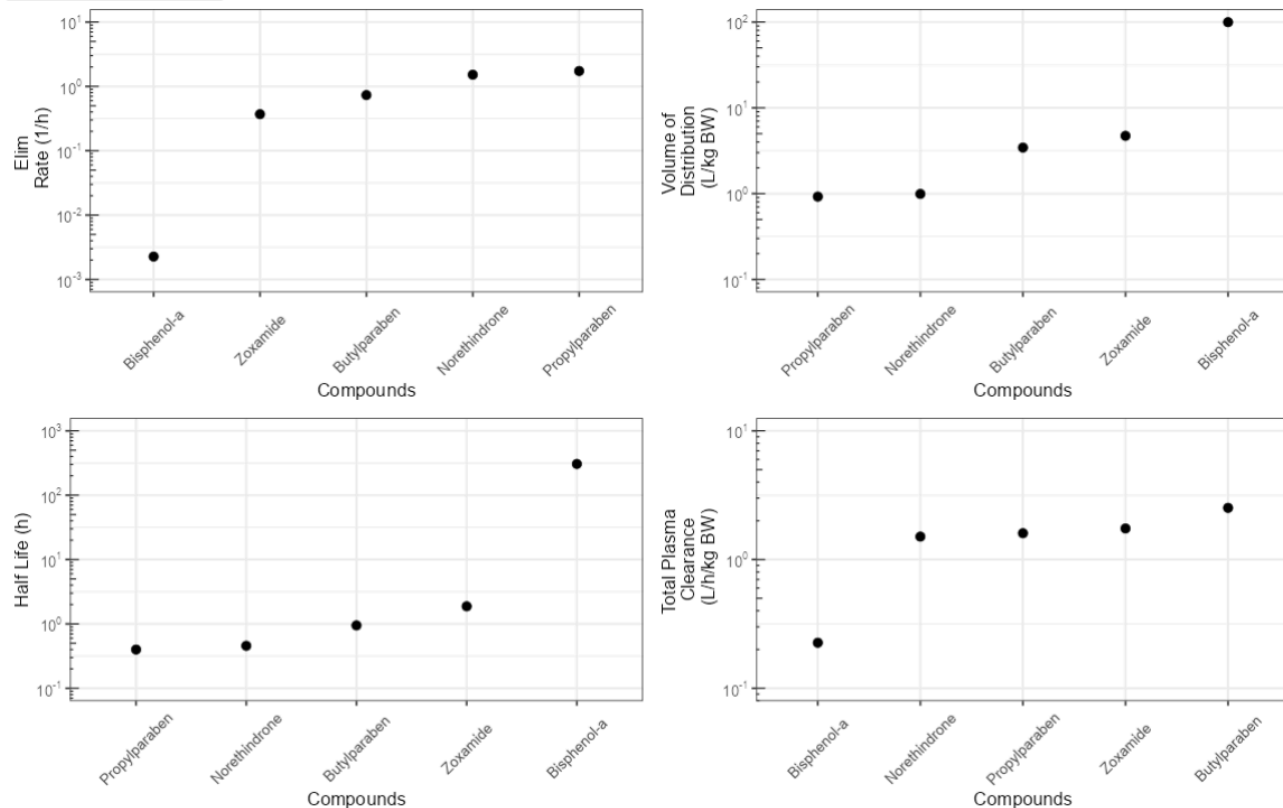


Figure 1: Plots of the estimated elimination rate (1/h), volume of distribution (L/kg BW), half life (h), and total plasma clearance (L/h/kg BW) for all selected compounds.

The log10 y-axis parameter plots under the parameter plots tab for example 2.

Under the second drop down menu and shown in the image below, the parameter values from the plots shown in the previous tab are stated in a table. Users can download this table by clicking the *Download Table 1* button at the top of the tab.

RESULTS

Parameter Plots



Parameter Table



Download Table 1

Show 10 entries

Search:

	CompoundName	EliminationRate	VolumeOfDistribution	HalfLife	TotalClearance
1	Bisphenol-a	0.002266	99.63	305.9	0.2258
2	Butylparaben	0.7324	3.442	0.9464	2.521
3	Norethindrone	1.519	0.9919	0.4563	1.507
4	Propylparaben	1.735	0.9228	0.3995	1.601
5	Zoxamide	0.3697	4.717	1.875	1.744

Showing 1 to 5 of 5 entries

Previous 1 Next

Table 1: Table of estimated elimination rates (1/h), volumes of distribution (L/kg BW), half lifes (h), and total plasma clearances (L/h/kg BW) for all selected compounds. Compounds are listed in ascending order of the elimination rate.

Partition Coefficient Plots



Partition Coefficient Table



The table of parameter plot values for example 2.

Under the third drop down menu in the *Results* card are 13 partition coefficient plots with one value per compound, as shown in the image below. Users can download these plots by clicking the *Download Figure 2* button at the top of the tab.

RESULTS

Partition Coefficient Plots

Download Figure 2

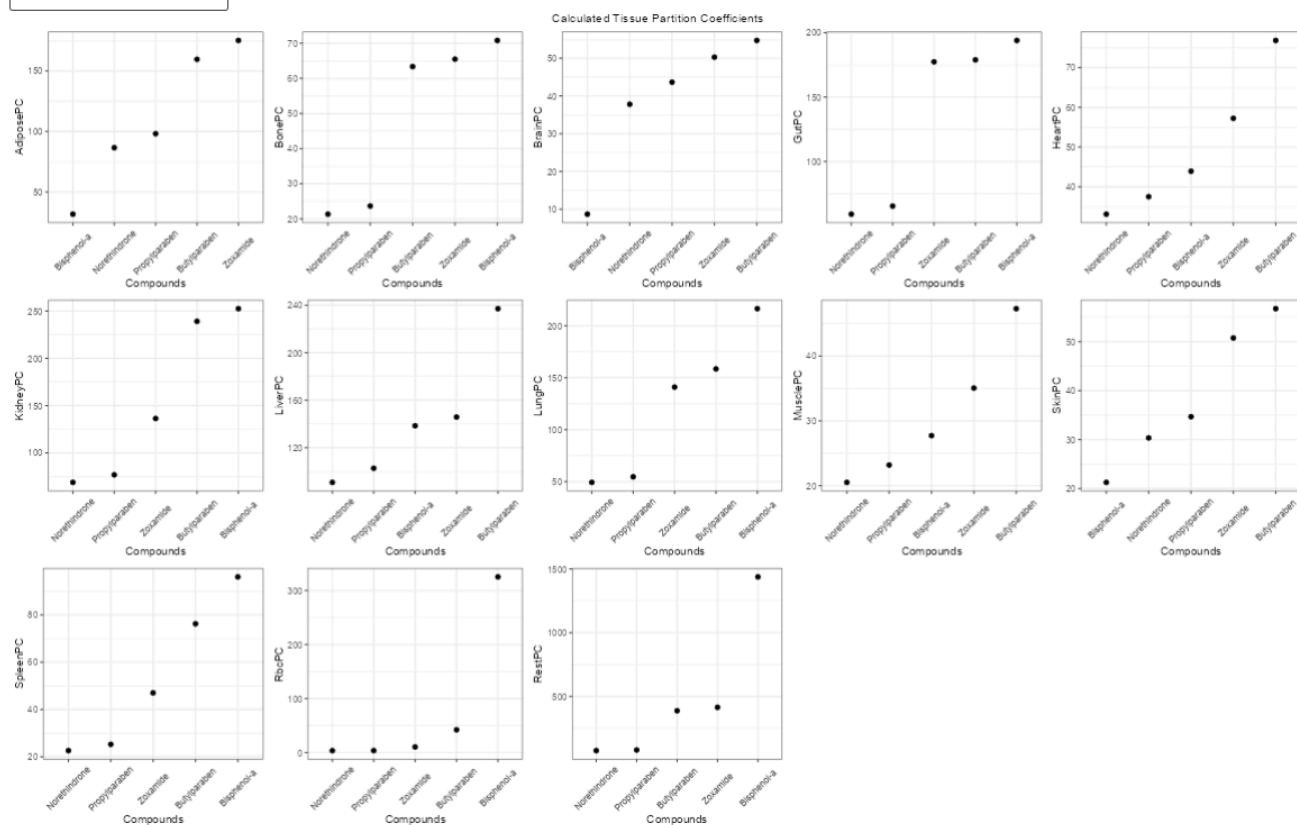


Figure 2: Plots of the estimated partition coefficients (no units) using Schmitt's method for all tissues available (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, spleen, red blood cells (rbc), testis, collectively from four species (mouse)). Compounds are arranged in ascending order based on the median partition coefficient for

The linear y-axis partition coefficient plots for example 2.

As with the plots under the first results tab, users can transform the scale of the y-axis to be a log10 scale by checking the box under the *Actions* card. This will produce the image shown below and give the user a better visual understanding of how the partition coefficients compare to one another.

RESULTS

Partition Coefficient Plots

Download Figure 2

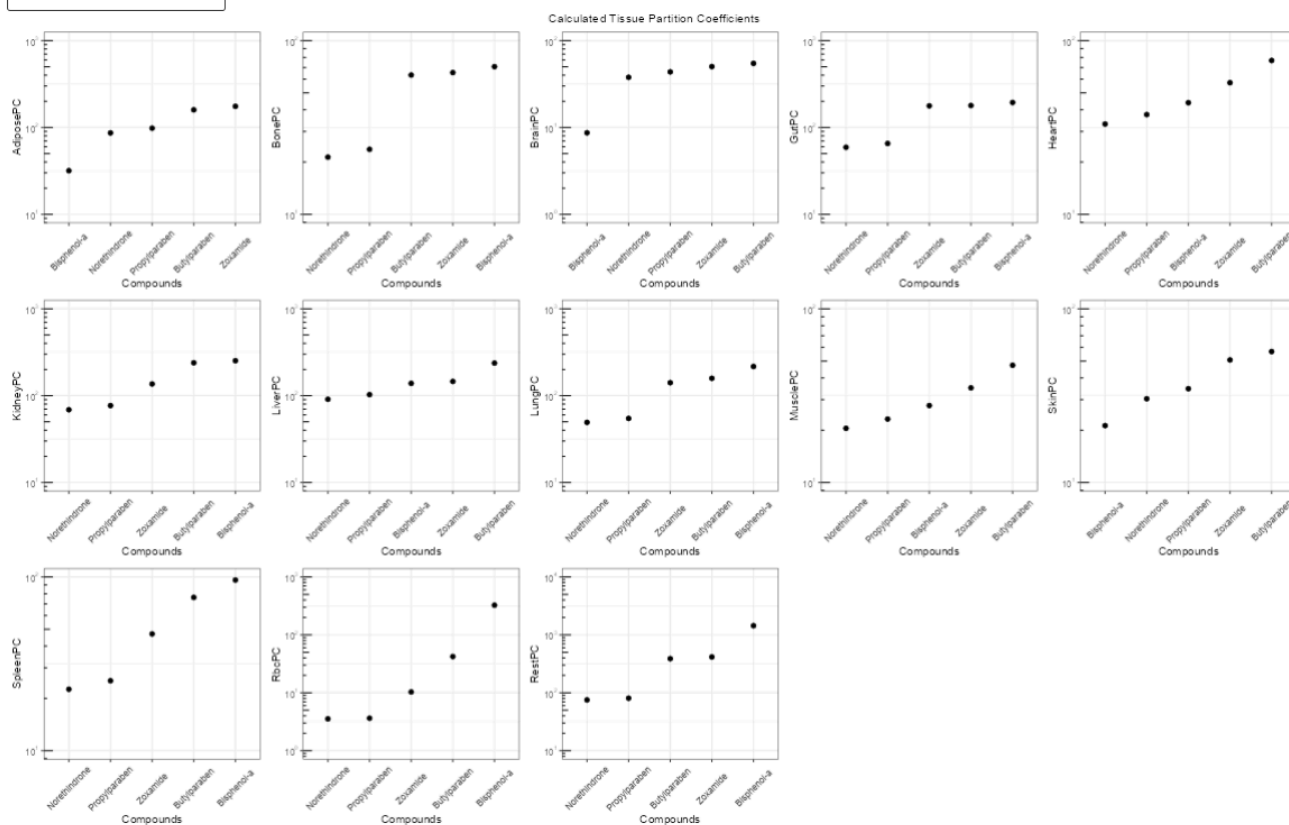


Figure 2: Plots of the estimated partition coefficients (no units) using Schmitt's method for all tissues available (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, skin, spleen, and testis). The compounds are arranged in ascending order based on the median partition coefficient for each tissue.

The log10 y-axis partition coefficient plots for example 2.

Under the fourth drop down menu (shown in the image below), the parameter values from the plots shown in the previous tab are stated in a table. Users can download this table by clicking the *Download Table 1* button at the top of the tab.

RESULTS

Parameter Plots

Parameter Table

Partition Coefficient Plots

Partition Coefficient Table

Download Table 2

Show 10 entries

Search:

	CompoundName	AdiposePC	BonePC	BrainPC	GutPC	HeartPC	KidneyPC	LiverPC	LungPC	MusclePC	S
1	Bisphenol-a	31.77	70.8	8.686	194	43.92	252.5	138.5	216.5	27.73	
2	Butylparaben	159.5	63.36	54.7	178.9	76.83	239.1	237.1	158.5	47.31	
3	Norethindrone	86.6	21.33	37.79	59.12	33.11	68.84	90.79	49.26	20.51	
4	Propylparaben	98.15	23.66	43.64	65.4	37.51	76.84	102.7	54.62	23.19	
5	Zoxamide	175.1	65.46	50.27	177.4	57.23	136.4	145.8	141	35.06	

Showing 1 to 5 of 5 entries

Previous 1 Next

Table 2: Table of partition coefficients for all selected compounds in each of the available tissues (adipose, bone, brain, gut, heart, kidney, liver, lung, muscle, skin, spleen, red blood cells (rbc), rest - collective term for remaining tissues). The compounds are listed in ascending order based on the median partition coefficient of each compound across all tissues. The median partition coefficient for each compound is shown in the last column of the table.

Simulation Parameters

The partition coefficients table for example 2.

The final drop down tab under the *Results* card gives the user the option to download all model parameters and chemical information for all 5 chemicals.

RESULTS

Parameter Plots

Parameter Table

Partition Coefficient Plots

Partition Coefficient Table

Simulation Parameters

Download Simulation Parameters

The simulation parameters tab for example 2.

As with the previous example, we suggest that the user clicks the *Reset Session* button if they want to run another simulation.