

Function	Description
<code>add_chemtable</code>	Adds chemical data for HTTK analysis.
<code>available_rblood2plasma</code>	Retrieves $R_{blood2plasma}$ (measured preferred over predicted)).
<code>calc_analytic_css</code>	Calculates C_{ss} and blood concentrations for the four models used in the package from infusion dosing at a constant rate.
<code>calc_css</code>	Calculates the maximum and average steady state concentrations along with the day steady state is reached.
<code>calc_elimination_rate</code>	Calculates k_{elim} for a one compartment model due to the liver and kidneys, dividing the total clearance by V_{dist} .
<code>calc_hepatic_clearance</code>	Calculates the hepatic clearance for a well-stirred model or other type if specified (Ito and Houston 2004).
<code>calc_mc_css</code>	Calculates C_{ss} using Monte Carlo simulation, defaulting to HTTK-Pop simulator (Ring et al. 2017).
<code>calc_mc_oral_equiv</code>	Calculates an oral equivalent dose using C_{ss} from <code>calc_mc_css</code> .
<code>calc_rblood2plasma</code>	Calculates the blood:plasma chemical concentration ratio.
<code>calc_stats</code>	Calculates the area under the curve, mean, and peak values for the blood or plasma concentration of either a specified chemical or all chemicals for a given simulation.
<code>calc_total_clearance</code>	Calculates the total clearance rate for a one compartment model where clearance is equal to the sum of the well-stirred metabolism by the liver and glomerular filtration in the kidneys.
<code>calc_vdist</code>	Calculates the one compartment volume of distribution.
<code>export_pbtck_jarnac</code>	Exports the model pbtck to Jarnac (Sauro and Fell 2000).
<code>export_pbtck_sbml</code>	Exports the model pbtck to SBML (Hucka et al. 2003).
<code>get_cheminfo</code>	Provides a list of CAS numbers along with compound names, logP, pKa, molecular weight, Cl_{int} and its p value, and f_{ub} if specified for chemicals with sufficient data for a given model.
<code>get_httk_params</code>	Converts table generated by <code>httkpop_generate</code> to the corresponding table of htkk model parameters.
<code>get_rblood2plasma</code>	Retrieves <i>in vivo</i> $R_{blood2plasma}$.
<code>get_wetmore_cheminfo</code>	Provides the names and CAS numbers of chemicals with information from Wetmore et al. (2012), Wetmore et al. (2013), and Wetmore (2015).
<code>get_wetmore_css</code>	Retrieves C_{ss} as a result of oral infusion dosing from Wetmore et al. (2012), Wetmore et al. (2013), and Wetmore (2015).
<code>get_wetmore_oral_equiv</code>	Calculates an oral equivalent dose using C_{ss} from Wetmore et al. (2012), Wetmore et al. (2013), and Wetmore (2015).
<code>httkpop_generate</code>	Generates a virtual population.
<code>lump_tissues</code>	Lumps tissue flows, volumes, and input partition coefficients based on specified grouping.

Table 4: List of functions in the package – Part I. Models are described in Table 2. Parameters are defined in Table 1. Jarnac and SBML are external languages for systems biology models.