

Data table	Description
chem.invivo.PK.data	This data set includes time and dose specific measurements of chemical concentrations in tissues taken from animals administered control doses of the chemicals either orally or intravenously. These plasma concentration-time data are from rat experiments reported in public sources. Toxicokinetic data were retrieved from those studies by the Netherlands Organisation for Applied Scientific Research (TNO) using curve stripping (TechDig v2). These data are provided for statistical analysis as in Wambaugh et al. (2015) .
chem.invivo.PK.-summary.data	This data set summarizes the time course data in the chem.invivo.PK.data table. Maximum concentration (Cmax), time integrated plasma concentration for the duration of treatment (AUC.treatment) and extrapolated to zero concentration (AUC.infinity) as well as half-life are calculated. Summary values are given for each study and dosage.
chem.physical_and_-invitro.data	This data set contains the necessary information to make basic, high-throughput toxicokinetic predictions for compounds, including f_{ub} , Cl_{int} , molecular weight, logP, logMA (membrane affinity), and pKa.
tissue.data	This data set contains values from Ruark et al. (2014) describing the composition of specific tissues and from Snyder et al. (1975) and Birnbaum et al. (1994) describing volumes of and blood flows to those tissues, allowing parameterization of toxicokinetic models for human, mouse, rat, dog, or rabbit.
physiology.data	This data set contains additional physiological values necessary to parameterize a toxicokinetic model for human, mouse, rat, dog, or rabbit.
Wetmore.data	This data set gives the chemical-specific predictions for serum concentration at steady state resulting from infusion exposure at a constant rate, as published in a series of papers from Barbara Wetmore's group (Wetmore et al. 2012, 2013 ; Wetmore 2015) at the Hamner Institutes for Life Sciences. Predictions include the median and 90% interval in μM and mg/L. Calculations were made using the 1 and 10 μM <i>in vitro</i> measured clearances.

Table 3: List of data tables in the package. In [Ring et al. \(2017\)](#), a series of tables for generating populations based on variation in human physiology were added. They are described in that manuscript and vignettes.