Supplemental File. One-Compartment Toxicokinetic Model: Diagram, Equations, and Error Propagaton by Quadrature.

The one-compartment toxicokinetic model is a well knowndescription of toxicokinetics as a function of a primary compartment in which the concentration is given by the amount (mg/kg body weight) of drug/chemical in the compartment divided by an apparent volume of distrbution (V_{dist}, L'kg body weight). For the serum, the model describes elimination from the body is described by a single, first-order (proportional to concentration) elimination rate (k_{elim}, 1/h). For the serum, oral exposure is modeled through an additional first-order rate (k_{abs}, 1/h) from the gut lumen. The fraction absorbed (F_{abs}) multiplies the overall dose and is valued between zero and 1. For the liver and kidney the absorption and elimination processes can be thought of as exchanges with the rest of the body. The one-compartment model is illustrated in Figure S1.

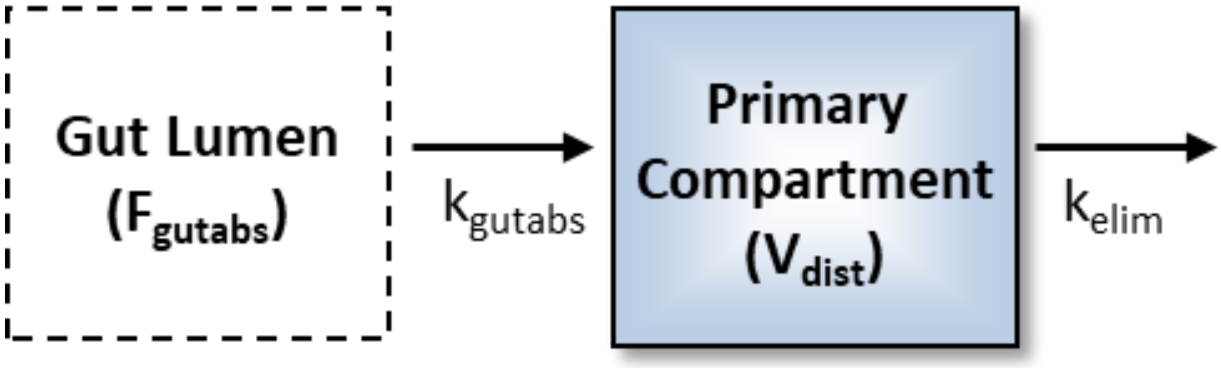

Figure S1: The One Compartment Model, relating a dose D (mg/kg body weight) introduced into the gut lumen. Chemical is subject to uptake into the body at rate k_{abs} and elimination from the body at rate kelim.

The mass-balanced differential equations for chemical concentration in the primary compartment (C, mg/L) and amount in gut (A_{gut}, mg/kg body weight) are:

$$\frac{dC}{dt} = k_{abs} * \frac{D}{V_d} - k_{elim} * C$$
$$\frac{dA_{gut}}{dt} = -k_{abs} * D$$

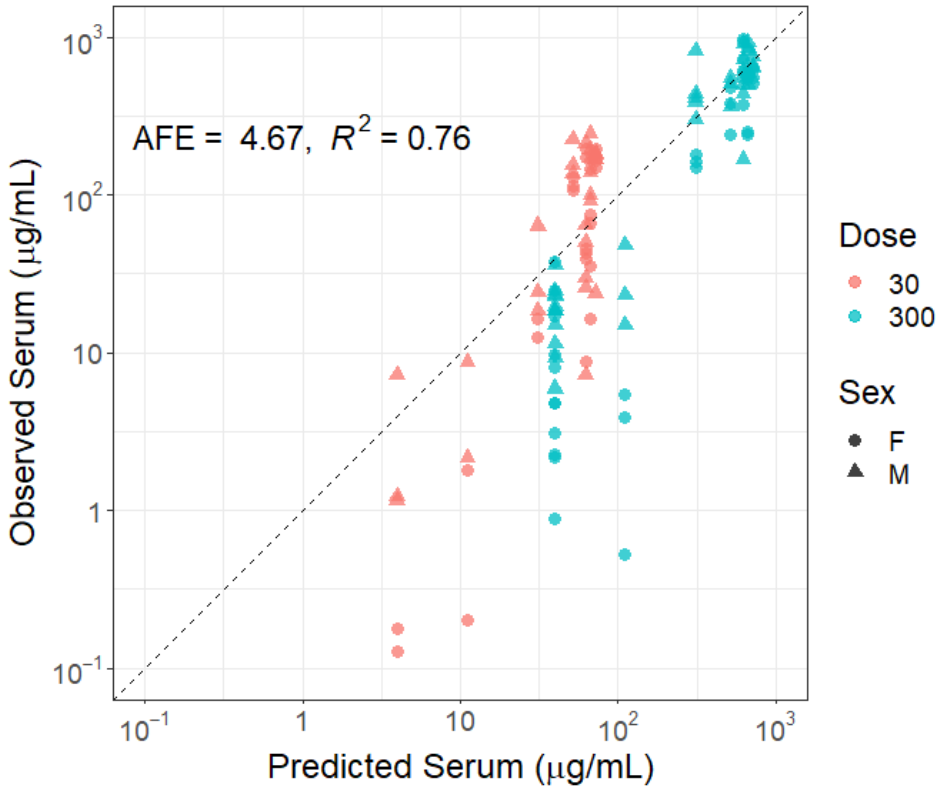

Figure S2: Evaluation of one compartment model fit to serum PFBS concentration data for both doses and genders.

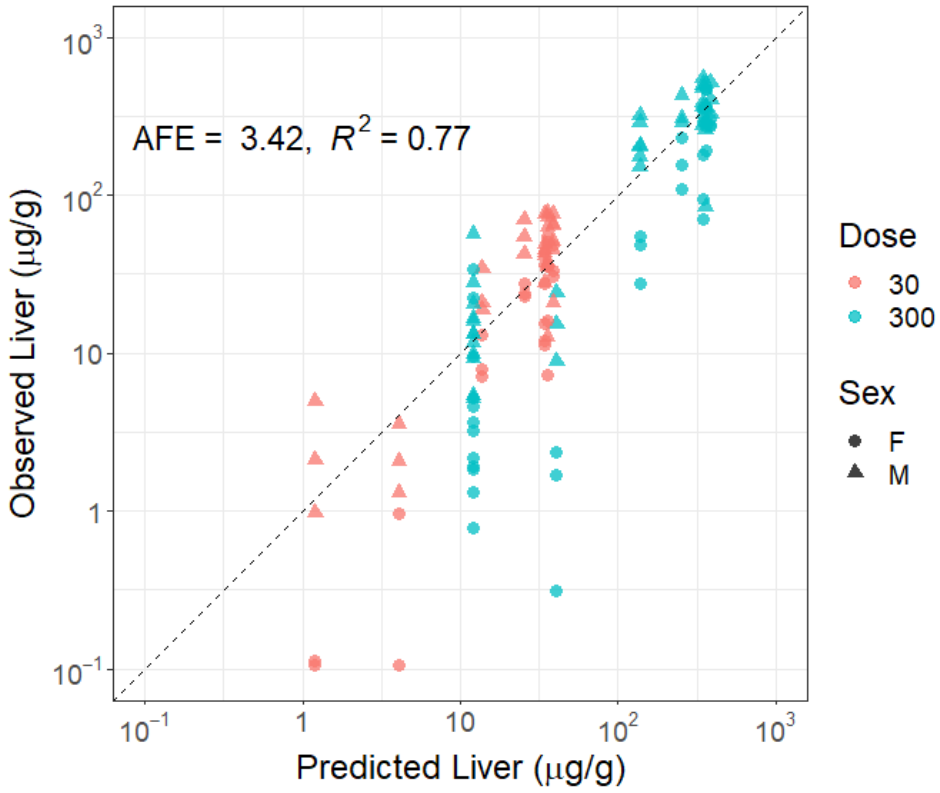

Figure S3: Evaluation of one compartment model fit to liver PFBS concentration data for both doses and genders.

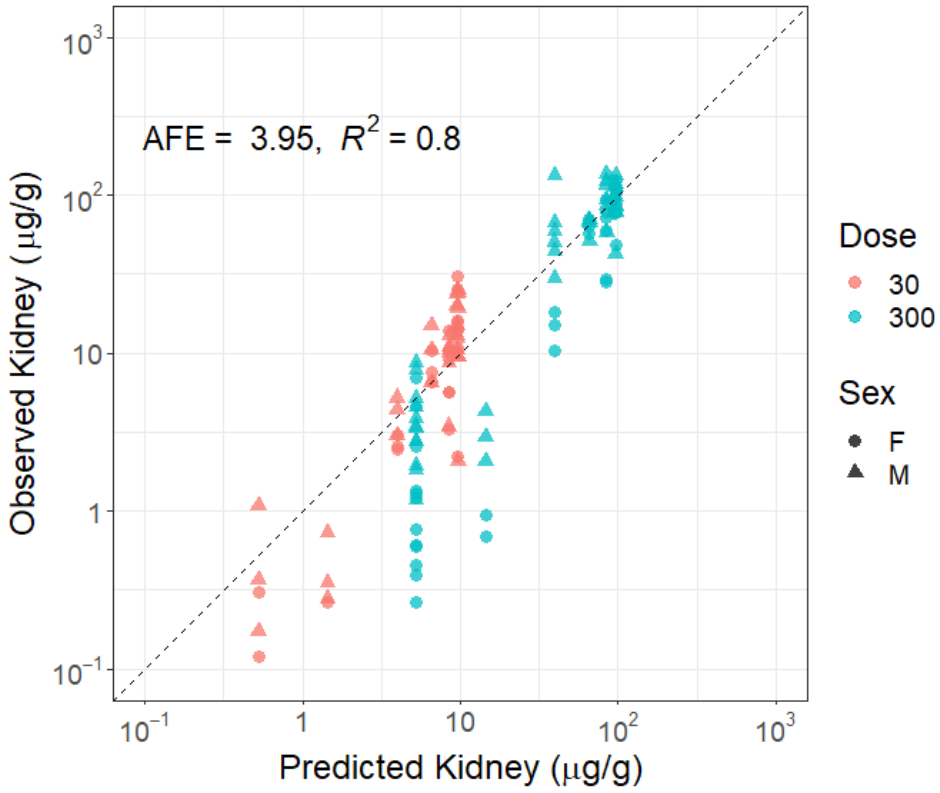

Figure S4: Evaluation of one compartment model fit to kidney PFBS concentration data for both doses and genders.