Computational Approaches for Developing Informative Prior Distributions for Bayesian Calibration of PBPK Models

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Using Bayesian statistical methods to quantify uncertainty and variability in human PBPK model predictions for use in risk assessments requires prior distributions (priors), which characterize what is known or believed about parameters' values before observing *in vivo* data. Experimental *in vivo* data can then be used in Bayesian calibration of PBPK models to refine priors when it exists. However, when little or no *in vivo* data is available for calibration efforts, parameter estimates and uncertainties can be obtained from priors. We present approaches for specifying *informative* priors for chemical-specific PBPK model parameters based on information obtained from chemical structures and *in vitro* assays. Means and standard deviations (or coefficients of variation) for priors are derived from comparisons of predicted values from computational (e.g., QSAR) methods or *in vitro* assays and experimentally-determined chemical-specific values for a data set of chemicals. *This abstract does not necessarily reflect U.S. EPA policy.*