

bayesnec: An R Package for C-R Modelling and Estimation of No-Effect-Concentration thresholds

Concentration-response (C-R) modelling is fundamental to assessing toxicity and deriving toxicity thresholds used in the risk assessments. Estimates of uncertainty in parameters and derived thresholds are critical to effective integration in risk assessment and formal decision frameworks. Bayesian methods that allow robust quantification of uncertainty with intuitive and direct probabilistic meaning provide a credible alternative to more traditional (Frequentist) approaches. However, Bayesian model fitting can be difficult to automate across a broad range of scenarios, particularly with respect to the identification of prior distributions and initial values. The bayesnec package in R has been developed to fit concentration(dose) - response curves (C-R) to toxicity data for the purpose of deriving No-Effect-Concentration (NEC), No-Significant-Effect-Concentration (NSEC), and Effect-Concentration (of specified percentage 'x,' ECx) thresholds from non-linear models using Bayesian MCMC fitting methods via brms and stan. In bayesnec it is possible to fit a single model, custom model-set, specific model-set or all of the available models. When multiple models are specified the bnec function returns a model weighted average estimate of predicted posterior values. A range of support functions and methods is also included to work with the returned single, or multi-model objects that allow extraction of raw, or model averaged predicted, ECx, NEC and NSEC values and to interrogate the fitted model or model-set. The statistical methods used ensure uncertainty in derived threshold values can be robustly quantified, including individual model fit and model selection uncertainty. This presentation will provide an overview of the package and a demonstration of its features using real examples.