

Prediction of acute toxicity of pesticides for *Americamysis bahia* using linear and nonlinear QSTR modelling approaches

The screenshot shows a web browser window displaying a ScienceDirect article. The browser's address bar shows the URL: <https://www.sciencedirect.com/science/article/abs/pii/S0013935122013111#preview-section-abstract>. The page header includes the journal name "Environmental Research", volume "214, Part 2", and date "November 2022, 113984". The article title is "Prediction of acute toxicity of pesticides for *Americamysis bahia* using linear and nonlinear QSTR modelling approaches". The authors listed are Karol D'Águez-Santana, F.A.W. Manoel, Marcos Nadimibe-Nayandi, Amílcar Paris, and Rolán Torres Gutiérrez. The abstract text is partially visible, starting with "Globally, pesticides are toxic substances with wide applications. However, the widespread use of pesticides has received increasing attention from regulatory agencies due to their various acute and chronic effects on multiple organisms. In this study, Quantitative Structure-Toxicity Relationship (QSTR) models were established using Multiple Linear Regression (MLR) and five Machine Learning (ML) algorithms to predict pesticide toxicity in *Americamysis bahia*. The most influential descriptors included in the MLR model are RBF, JGI2, nCH, nRCOOR, nRSR, nPO4 and 'Cl-090', with positive contributions to the dependent variable (negative decimal logarithm of median lethal concentration at 96-h). The Random Forest (RF) regression model was superior amongst the five ML models. We observed higher values of R^2 (0.812) and lower values of RMSE (0.595) and MAE (0.462) in the cross-validation training set and external validation set. Similarly, this study had a high level of fitness and was internally robust and externally predictive."