ToxicR

An open-source R package for computational toxicology and dose-response analyses, utilizing the core functionality of EPA's BMDS and NTP's BMDexpress.

https://github.com/NIEHS/ToxicR

Overview

ToxicR is an open-source R programming package developed by the Biostatistics and Computational Biology Branch of the National Institute of Environmental Health Sciences (NIEHS), in cooperation with the National Toxicology Program (NTP) and the US Environmental Protection Agency (EPA).

Product Overview and Key Benefits

ToxicR was created to provide a stable, open-source codebase attached to a programming language (R) that allows researchers to implement new algorithms and create custom analysis pipelines, addressing the limitations of existing software that often relies on pre-specified workflows. By utilizing the same core model source libraries as the EPA's Benchmark Dose Software (BMDS) and the NTP's BMDExpress, ToxicR ensures regulatory alignment while offering increased flexibility and customizability.

Main Features and Capabilities

The ToxicR platform implements many of the standard analyses used by the NTP and EPA, including:

Dose-Response Analysis: Supports both continuous and dichotomous data.

Modeling Methods: Employs Bayesian, Maximum Likelihood, and Model Averaging (MA) methods for dose-response analysis.

Standard Toxicology Tests: Includes standard NTP tests such as the Poly-K and Jonckheere trend tests.

Custom Workflows: Provides a programming interface that allows users to develop personalized analysis pipelines within the R environment.

Performance: Takes advantage of multicore computers using the OpenMP library to increase computational speed for model averaging fits.

Visualization: Provides a unified platform for plotting graphics, generating customizable `ggplot2` objects for model fits and density plots (`cleveland_plot`, `MAdensity_plot`).

Target Users and Use Cases

ToxicR is primarily targeted at computational toxicologists, researchers, and risk assessors in regulatory and academic settings. Primary use cases include:

Computational Toxicology: Implementing and testing novel dose-response methodologies.
Toxicogenomic Data Analysis: Developing custom workflows for analyzing high-throughput toxicogenomic and other omic data platforms.
Benchmark Dose (BMD) Estimation: Performing BMD analysis using methods aligned with EPA and NTP standards.
Risk Assessment: Providing transparent, code-based analysis for regulatory submissions (when combined with R Markdown).

Key Features

- Dose-Response Analysis (Continuous/Dichotomous)
- Bayesian Modeling
- Model Averaging (MA) Methods
- Maximum Likelihood Estimation
- Standard NTP Trend Tests (Poly-K, Jonckheere)
- Custom Analysis Pipeline Creation
- Multicore Processing (OpenMP)
- ggplot2-based Plotting

Pricing

Model: free

Open-source R package released under the MIT (source code) and LGPL (>= 3) licenses. Free to download, use, and modify.

Target Company Size: startup, small, medium, enterprise

Integrations

R programming environment, Rcpp, ggplot2, shiny, tidyverse, plotly, R Markdown