DRomics

Keywords

dose response modelling / benchmark dose (BMD) / environmental risk assessment / transcriptomics / proteomics / metabolomics / toxicogenomics / multi-omics

Overview

DRomics is a freely available on-line tool for dose-response (or concentration-response) characterization from omics data. It is especially dedicated to omics data obtained using a typical dose-response design, favoring a great number of tested doses (or concentrations) rather than a great number of replicates (no need of three replicates).

After a first optional step which consists to import, check and if needed normalize/transform the data (step 1), the aim of the proposed workflow is to select monotonic and/or biphasic significantly responsive items (e.g. probes, metabolites) (step 2), to choose the best-fit model among a predefined family of monotonic and biphasic models to describe the response of each selected item (step 3), and to derive a benchmark dose or concentration from each fitted curve (step 4).

In the available version, DRomics supports single-channel microarray data (in log2 scale), RNAseq data (in raw counts) or metabolomics data (in log scale). In order to link responses across biological levels based on a common method, DRomics also handles apical data as long as they are continuous and follow a Gaussian distribution for each dose or concentration, with a common standard error.

All sources of DRomics are available at
https://github.com/aursiber/DRomics
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The package

The **limma** and **DESeq2** packages from Bioconductor must be installed for the use of DRomics:

- *if (!requireNamespace("BiocManager", quietly = TRUE)) {install.packages("BiocManager")}*
- *BiocManager::install(c("limma", "DESeq2"))*

The **stable version of DRomics** can be installed from CRAN using:

- *install.packages("DRomics")*

The **development version of DRomics** can be installed from GitHub (remotes needed):

- *if (!requireNamespace("remotes", quietly = TRUE)) {install.packages("remotes")}*
- *remotes::install_github("aursiber/DRomics")*

Finally **load** the package in your current R session with the following R command:

- *library(DRomics)*

Vignette and cheat sheet

A vignette and a cheat sheet are attached to the DRomics package. See below the pdf.

This vignette can be reached in your R session by:

- *vignette("DRomics_vignette")*

Note that, by default, the vignette is not installed when the package is installed through GitHub. The following command (rather long to execute because of the large size of the vignette) will allow you to access the vignette of the development version of the package you installed from GitHub:

- *remotes::install_github("aursiber/DRomics", build_vignettes = TRUE)*

The shiny app

The shiny app DRomics is available :

- on the LBBE shiny server at http://lbbe-shiny.univ-lyon1.fr/DRomics/inst/DRomics-shiny/
- in the Biosphere cloud, if you or your lab is a partner of the IFB (Institut Français de Bioinformatique), at https://biosphere.france-bioinformatique.fr/catalogue/appliance/176/
- locally in your R session doing:
    - *install.packages(c("shiny", "shinyBS", "shinyjs", "shinycssloaders"))*
    - *shiny::runApp(system.file("DRomics-shiny", package = "DRomics"))*

This shiny app is runing with the development version of DRomics.

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If you have any need that is not yet covered, any feedback on the package / Shiny app, or any training needs, feel free to email us at dromics@univ-lyon1.fr.

Citation

If you use Dromics, you should cite:

- Larras F, Billoir E, Baillard V, Siberchicot A, Scholz S, Wubet T, Tarkka M, Schmitt-Jansen M and Delignette-Muller ML (2018). *DRomics: a turnkey tool to support the use of the dose-response framework for omics data in ecological risk assessment.* Environmental Science & Technology. https://pubs.acs.org/doi/10.1021/acs.est.8b04752

You can find this article at :
https://hal.archives-ouvertes.fr/hal-02309919
You can also look at the following citation for a complete example of use:

- Larras F, Billoir E, Scholz S, Tarkka M, Wubet T, Delignette-Muller ML, Schmitt-Jansen M (2020). *A multi-omics concentration-response framework uncovers novel understanding of triclosan effects in the chlorophyte Scenedesmus vacuolatus.* Journal of Hazardous Materials. https://doi.org/10.1016/j.jhazmat.2020.122727

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