



浙江中醫藥大學
ZHEJIANG CHINESE MEDICAL UNIVERSITY

Seminar

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Representation

Documentation

MCnebula2

November 16, 2022

Title MCnebula algorithm integrated in S4 system of R.

Version 0.0.0.9000

Description MCnebula2 was used for metabonomics data analysis. It is written in the S4 system of object-oriented programming. Its workflow, i.e., MCnebula workflow, is a complete metabolomics data analysis process, including initial data preprocessing (data format conversion, feature detection), compound identification based on MS/MS, statistical analysis, compound structure and chemical class focusing, multi-level data visualization, output report, etc.

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Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.0

Website

Hugo + Netlify + Github + Blogdown

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MCnebula2: R package for LC-MS/MS metabolic dataset analysis

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Next Schedule

Overall

- Data filtering and arranging system. ✓
- Visualization system. ✓
- LC-MS runing in XCMS.
- Statistic system. ✓
- Report. ✓
- Documentation. ✓
- Website. ✓
- Test in Linux, Windows, Mac
- Figures for article.
- Rewrite article.