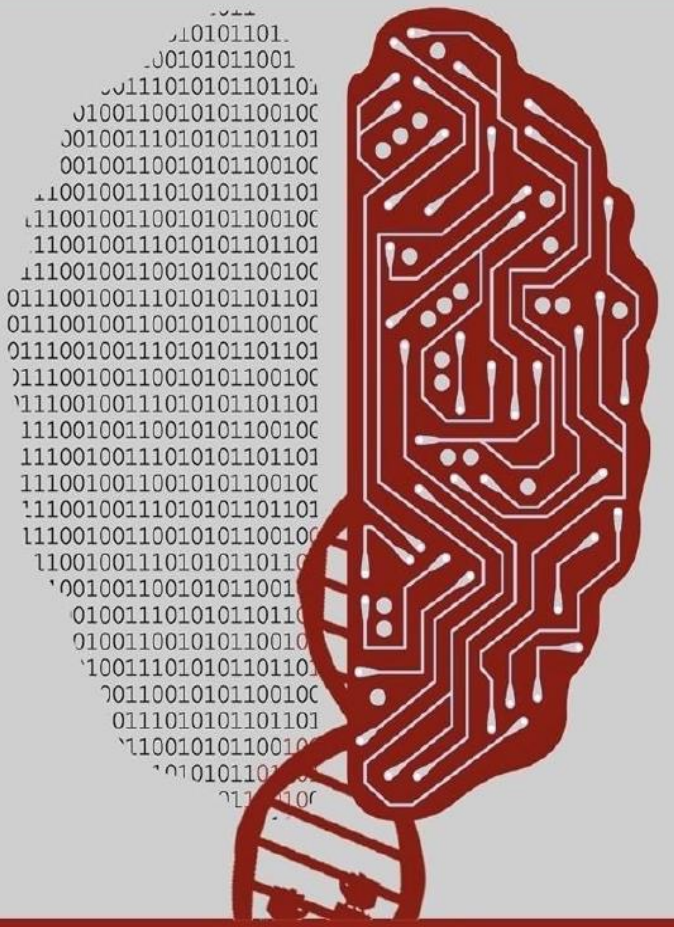
# Bioinformatics Open Days

www.bioinformaticsopendays.org



# BOOK OF ABSTRACTS

Ciências ULisboa

NEBIUM

# BIOINFORMATICS OPEN DAYS

Campus de Gualtar, Universidade do Minho

18th and 19th of February 2016

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## An R package for the integrated analysis of metabolomics and spectral data

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Recently, there has been a growing interest in the field of metabolomics, materialized by a remarkable growth in experimental techniques, available data and related biological applications. Indeed, techniques as Nuclear Magnetic Resonance, Gas or Liquid Chromatography, Mass Spectrometry, Infrared and UV-visible spectroscopies have provided extensive datasets that can help in tasks as biological and biomedical discovery, biotechnology and drug development. However, as it happens with other omics data, the analysis of metabolomics datasets provides multiple challenges, both in terms of methodologies and in the development of appropriate computational tools. Indeed, from the available software tools, none addresses the multiplicity of existing techniques and data analysis tasks.

In this work, we make available a novel R package, named specmine, which provides a set of methods for metabolomics data analysis, including data loading in different formats, pre-processing, metabolite identification, univariate and multivariate data analysis, machine learning, and feature selection. Importantly, the implemented methods provide adequate support for the analysis of data from diverse experimental techniques, integrating a large set of functions from several R packages in a powerful, yet simple to use environment.

The package, already available in CRAN, is accompanied by a web site where users can deposit datasets, scripts and analysis reports to be shared with the community, promoting the efficient sharing of metabolomics data analysis pipelines.