

merlin latest developments for pathways analysis

Oscar Dias, Miguel Rocha, Eugénio Campos Ferreira and Isabel Rocha

University of Minho, Braga, Portugal

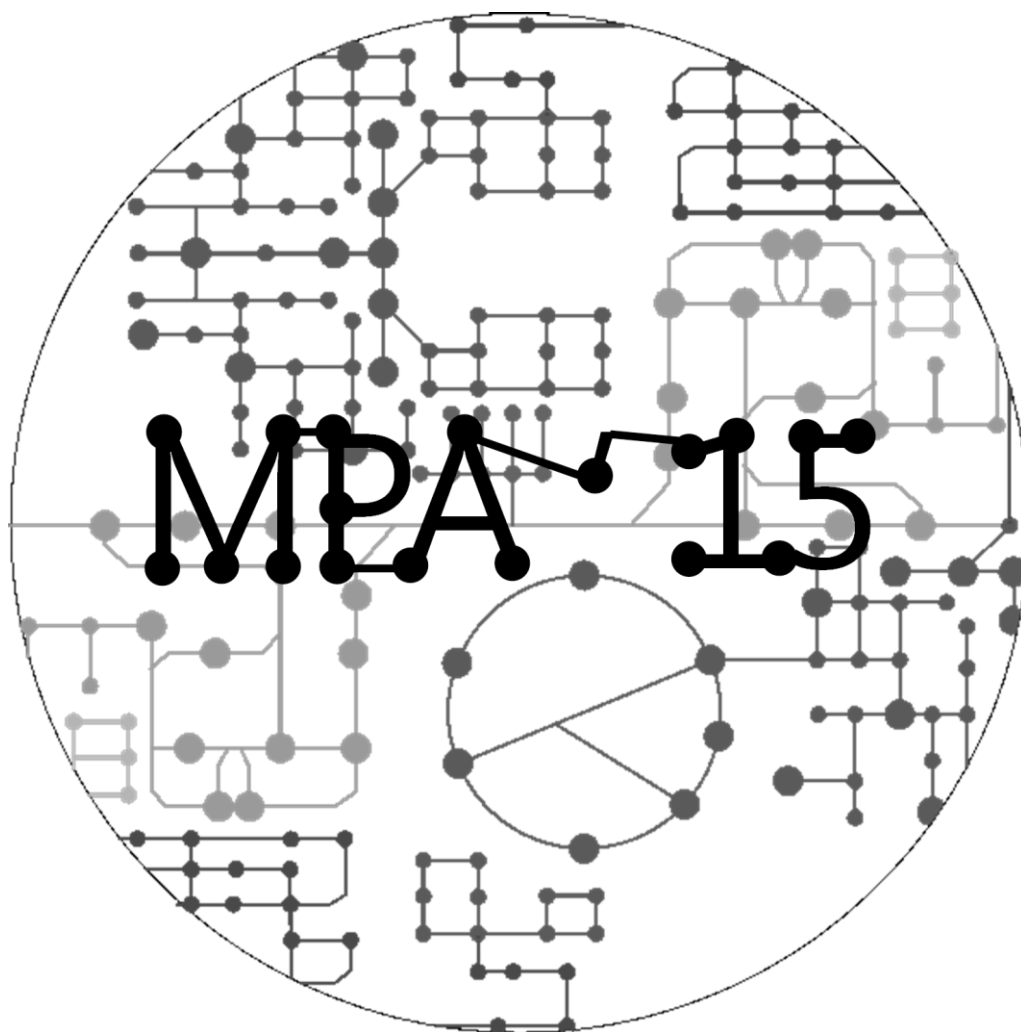
merlin is a user-friendly open-source software tool developed for the reconstruction of genome-scale metabolic models. These models are derived from sets of reactions, organised in pathways, which can be used to mimic the behaviour of microorganisms in different genetic and environmental conditions. One of the toughest challenges, when reconstructing models is the identification of gene-protein-reaction associations, a step usually performed by manually searching literature. Thus, a novel approach for automatically predicting, at the genome level, protein subunits using gene association rules retrieved from the KEGG BRITE database was developed and integrated in *merlin*. The presence or absence of the different pathways in the metabolic models may be related with several properties of the microorganism, namely the ability to survive in specific environments. Moreover, the analysis of metabolic pathways is important for finding gaps, which can impair model predictions by blocking the production of a by-product of interest, or a biomass component. Additionally, this analysis may propose more efficient pathways to increase the production of specific metabolites by, for instance, proposing knock-out or knock-in of genes. Therefore, an innovative reactions panel, which organises reactions by pathway allowing the visualisation and analysis of the constructed models' reactions in KEGG pathways was developed and integrated into *merlin*.

Programme & Abstracts

Metabolic Pathway Analysis 2015

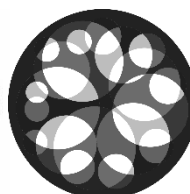
8-12 June

Braga – Portugal



www.biochemistry.org

Organized in partnership with the Portuguese
Biochemical Society (SPB) and the



**BIOCHEMICAL
SOCIETY**