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## Metabolic models Reconstruction using genome scale Information (merlin) - assessment and validation

Merlin is a user-friendly Java application that performs the reconstruction of genome-scale metabolic models for every organism that has its genome sequenced. It performs several steps of the reconstruction process, including the functional genomic annotations of the whole genome.

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## MATHEMATICAL MODELING

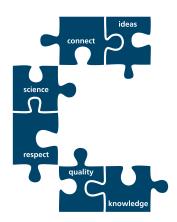
NOTES:

It includes tools for the identification and annotation of transport proteins encoding genes and for generating transport reactions for such carriers. Also, merlin includes tools for the compartmentalisation of the model that predict the localisation of the proteins encoded in the genome, and thus the localisation of the metabolites involved in the reactions induced by such proteins. Finally, merlin expedites the transition from genome-scale data to SBML metabolic models.

merlin has already been used to perform re-annotations and to reconstruct GSMMs for several organisms. For instance, merlin was used to perform the genome-scale metabolic re-annotations of K. lactis, A. gossypii and H. pylori. All of the above annotations were used as a basis for the reconstruction of GSMMs of the respective organisms.

For instance, the iOD907 K. lactis model was assessed to experimental data, performing very well. Moreover, the model proved accurate when predicting the biomass, oxygen and carbon dioxide yields and in silico knockouts accurately predicted in vivo phenotypes. Also, the iTR (H. pylori) model complies better than previous models with in vivo data. It shows the same specific growth rate verified in vivo whilst being the only in silico model able to use glutamate as carbon source and performs quite well on the essentiality tests.

Thus, merlin proved being useful for the reconstruction of these models.



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