

University of Minho
School of Engineering
Centre of Biological Engineering

RECONSTRUCTING GENOME-SCALE METABOLIC MODELS WITH MERLIN

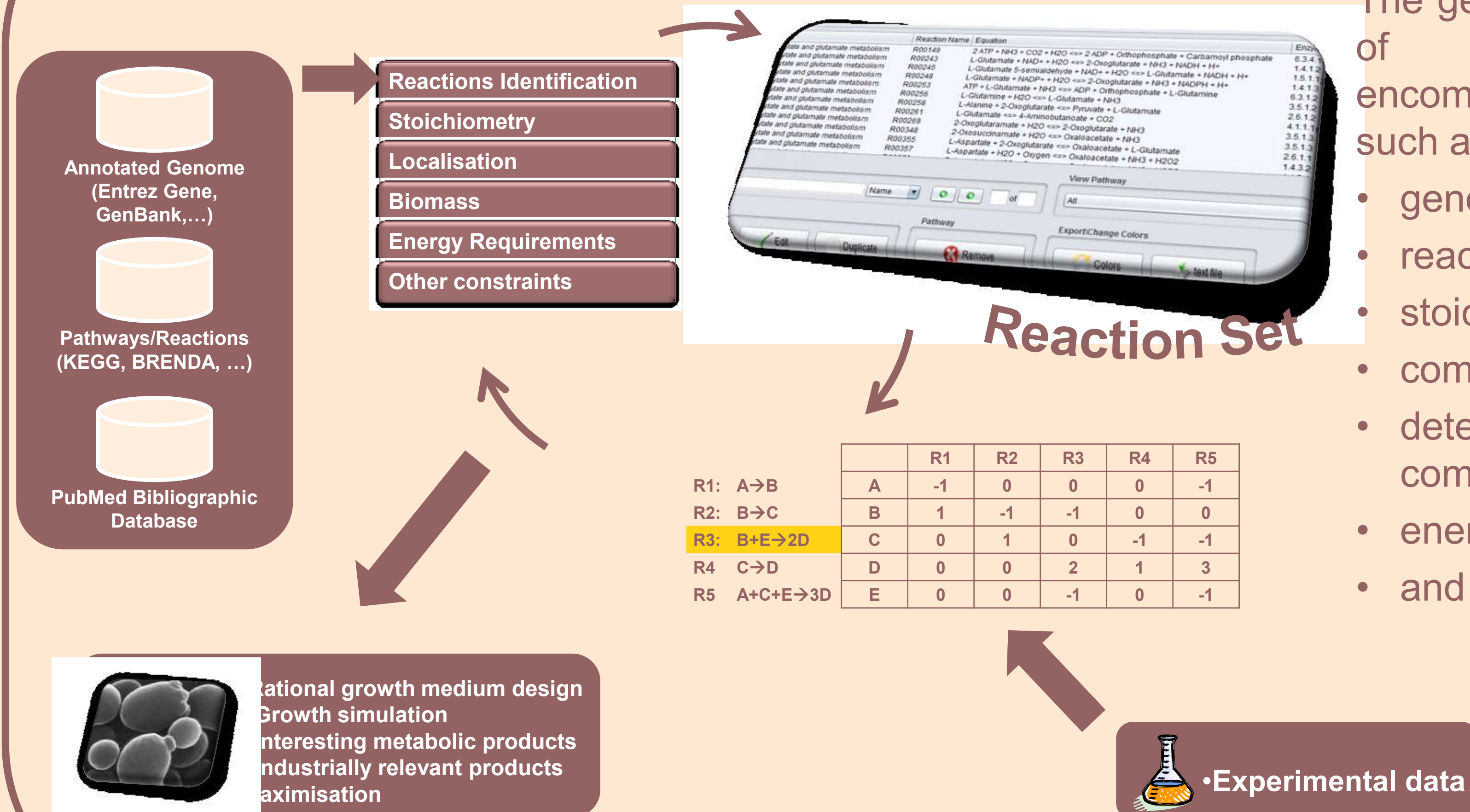
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GENOME-SCALE METABOLIC MODELS RECONSTRUCTION

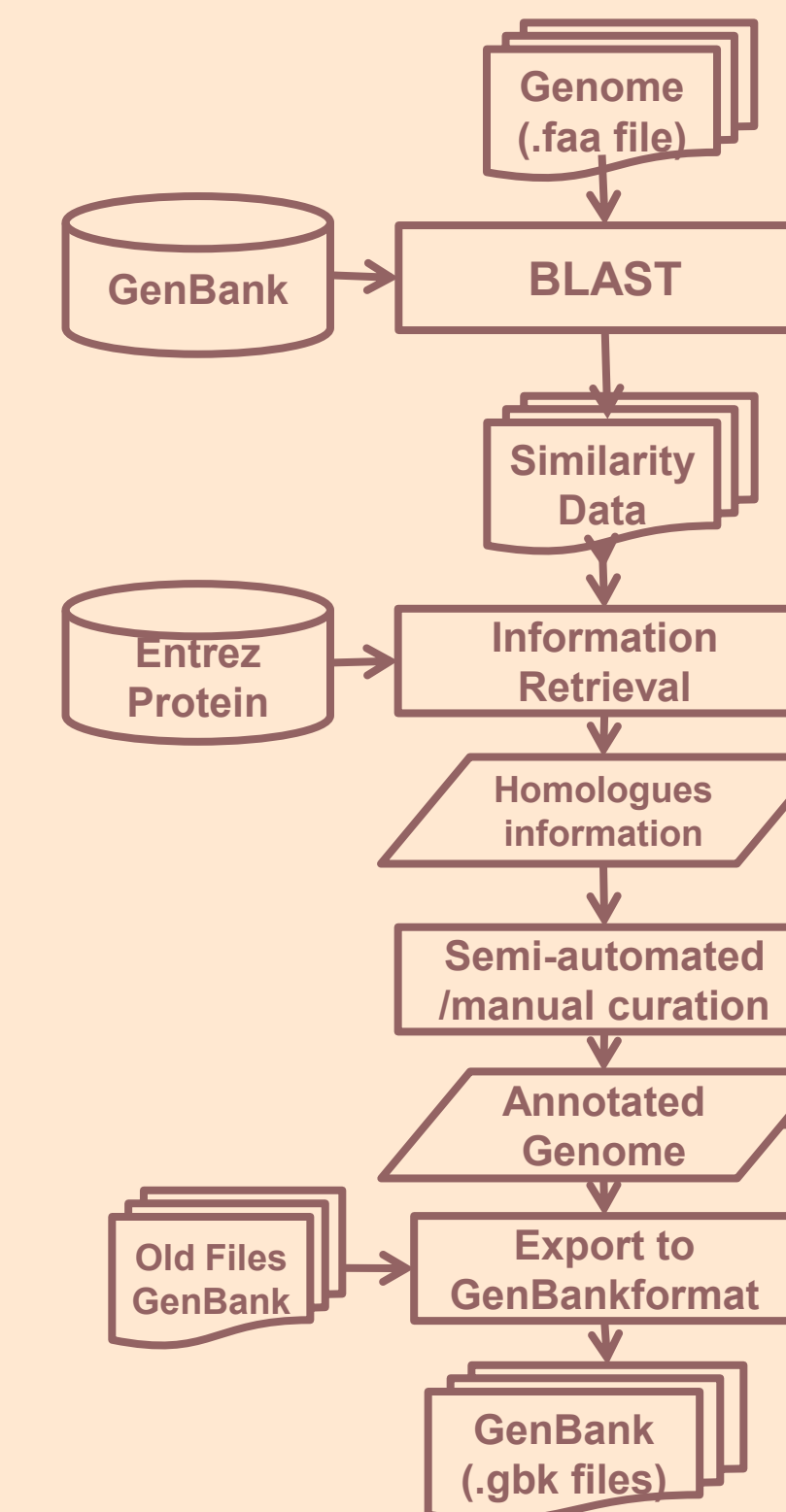


The genome-scale reconstruction of metabolic networks encompasses several steps, such as:

- genome annotation
- reactions identification
- stoichiometry determination
- compartmentation
- determination of the biomass composition
- energy requirements
- and additional constraints...

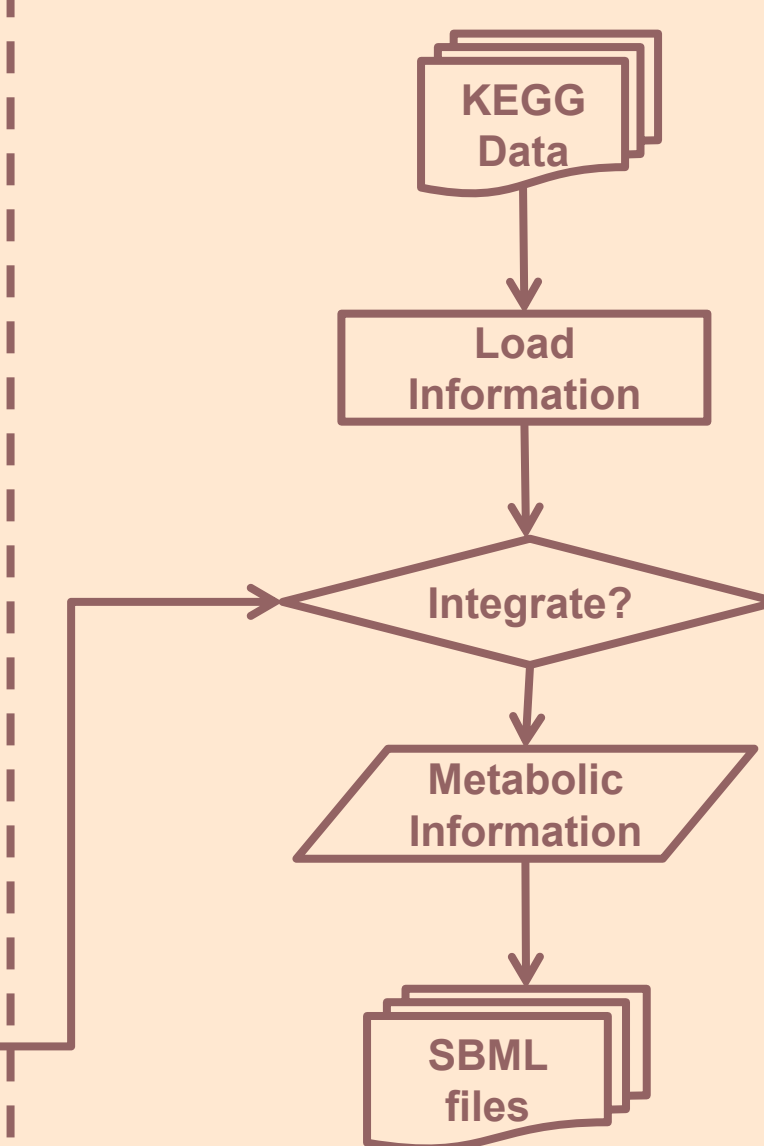
DYNAMIC ANNOTATION TOOL

- Performs BLAST similarity searches
- using user-defined parameters,
- Scoring the results with a quantifiable confidence level
- Allows to dynamically (re)-annotate each gene

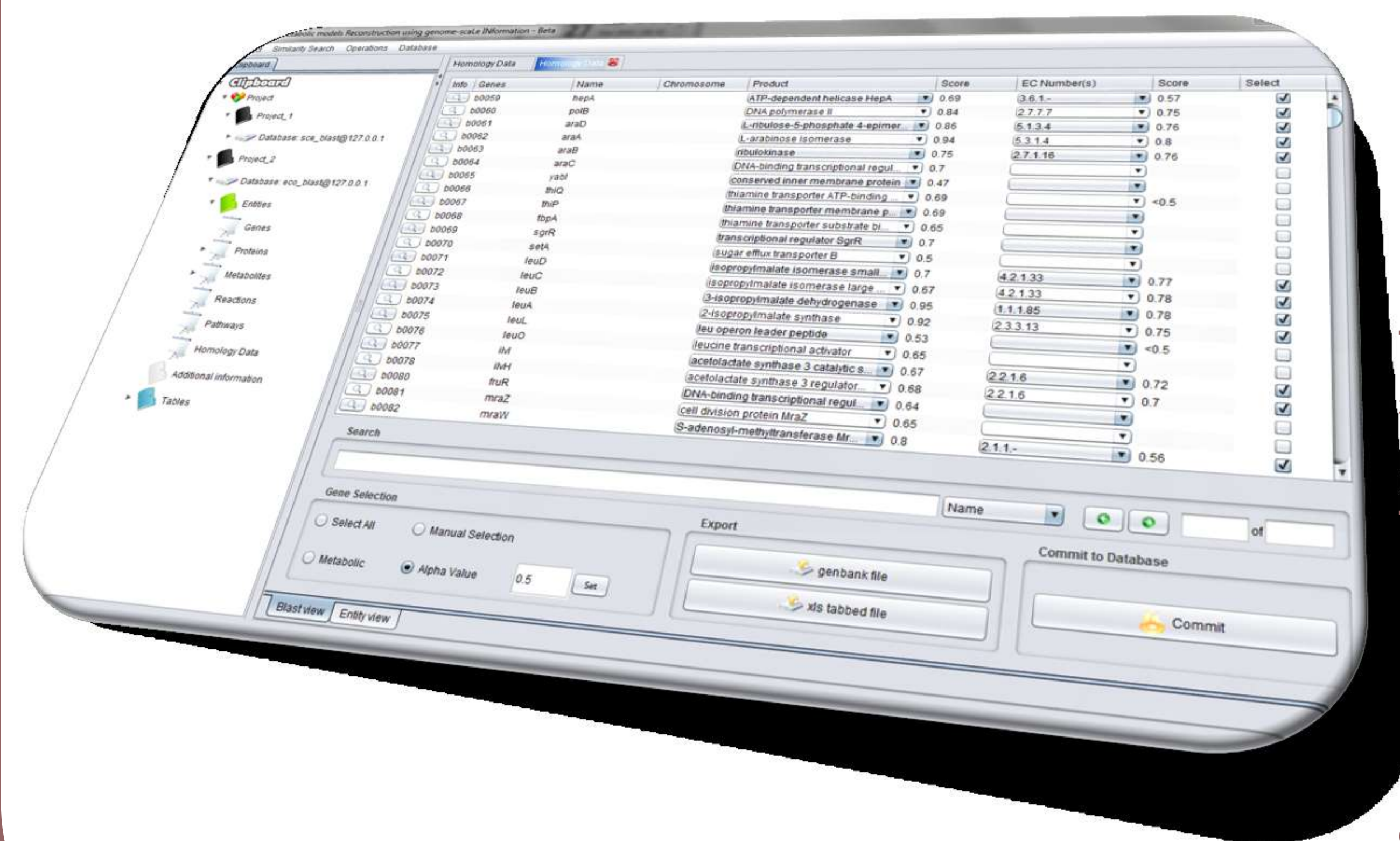


MODELS RECONSTRUCTION TOOL

- Loads information from the Kyoto Encyclopedia of Genes and Genomes (KEGG);
- Integrates the loaded data with information from the previous module
- Build the metabolic model and store it in the well accepted SBML implementation.



Merlin is composed by two modules



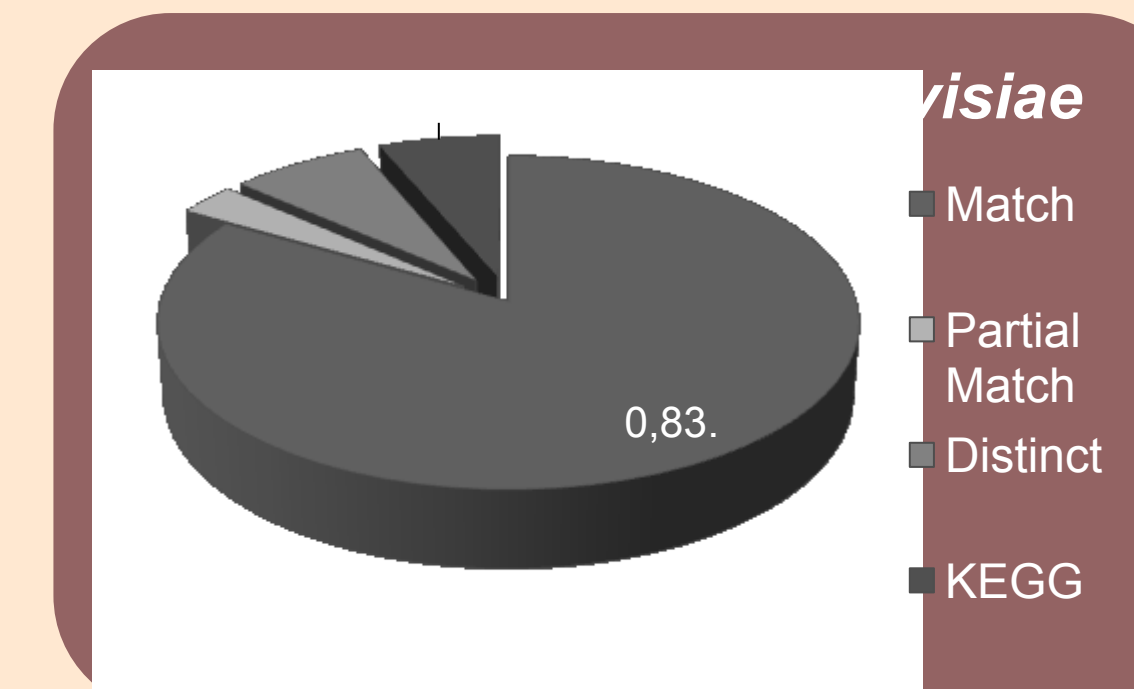
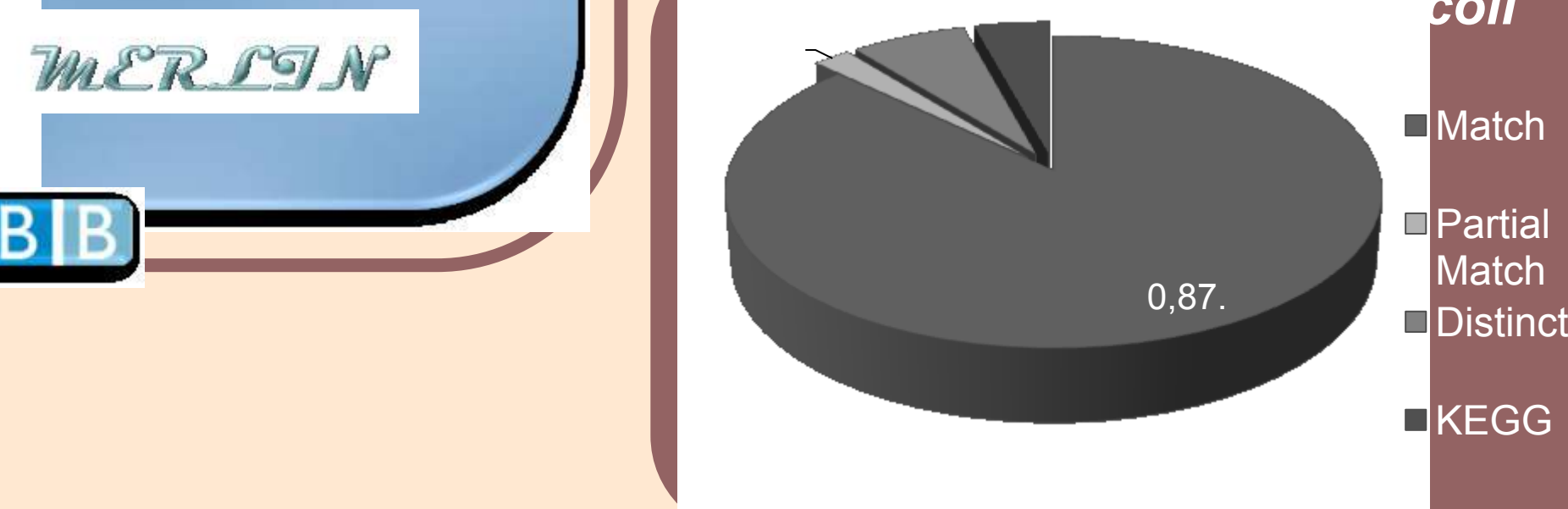
METHODOLOGY

Two of the most well known organisms were selected :

- *Escherichia coli* str. K-12 subset. W3110
- *Saccharomyces cerevisiae*

The enzymes selected by the BLAST scorer were matched with the data retrieved from KEGG

The assessment of the agreement between the information retrieved by homology with the data loaded from the KEGG database, can be used to evaluate the relevance of the results selected by Merlin



The results for the EC numbers integration are similar for *E. coli* and *S.cerevisiae*

With the ever increasing amount of genomic data becoming available, every tool developed to interpret and make sense of such bulk loads of data can be very tedious and time consuming

Hence, *merlin* is proposed as:

- a user-friendly tool
- which provides comprehensible information
- allows a semi-automated dynamic annotation with up to date information
- exports model in the SBML format for *in silico* processing

RESULTS AND CONCLUSIONS