Technology Offer

Predicting concentrations, reactions rates and rate constants in biochemical networks

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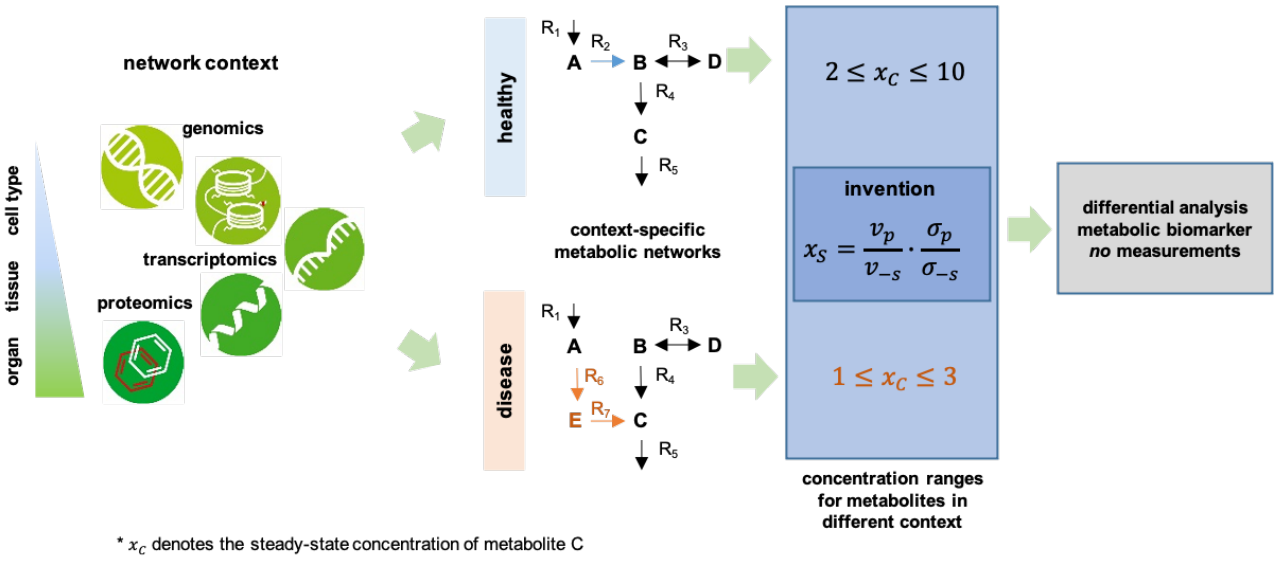
Background

Advances in systems biology are propelled by the availability of high-quality genome-scale metabolic reconstructions for many organisms. To cope with the associated high-dimensional data sets, diverse approaches have been applied, such as constraint-based modeling.
By neglecting the effect of concentrations on reaction rates, constraint-based approaches do not facilitate the usage of metabolic reconstructions to predict concentrations of metabolites, which are easily accessible by metabolomics techniques.
A method to predict component concentration ranges with limited knowledge about the underlying kinetic laws and parameter values would therefore allow direct integration and validation of genome-scale models with experimental data, enabling systems biology applications, from engineering intervention strategies to design of new drugs.

Technology

Scientists from the Max-Planck Institute for molecular plant physiology in Potsdam have invented a computer-implemented method that allows calculating concentration ranges of components within complex networks of biochemical reactions.
The invention provides simulation-free prediction of these ranges and is applicable to large networks, unlike other available methods. Moreover, it enables measurements of metabolite concentrations and information about selected parameters. Finally, does not require cumbersome experiments, such as isotope labeling to determine reaction rates.



* x_C denotes the steady-state concentration of metabolite C

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This invention facilitates comparison between different states (e.g. healthy vs diseased cells), in the absence of data, and will therefore allow for the modelling-driven discovery of biomarkers.
Moreover, since it is able to predict upper and lower concentration boundaries, the technology has the potential to be useful in diagnosing/monitoring diseases such as Type-2-Diabetes, where the change of ranges rather than absolute concentrations of the metabolite (i.e. glucose) is a better indicator of the disease.
The technology is not only applicable to the medical setting, but also to agriculture, for example to distinguish between two environments (drought vs ambient network states).

We are now looking for a licensing partner to further develop this technology.

Patent Information

A European priority establishing patent application was filed in 2018.

Publication

Küken et al (2019), doi: 10.1371/journal.pcbi.1006687

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