Metabolic Networks : Visual Analysis of Elementary Flux Modes.

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Metabolic networks are characterized by their size and the high level of interactions between nodes. Several formalisms can be used to analyze these networks, most of them use tools based on graph theory. Searching Elementary Flux Modes (EFMs) is a way to identify feasible routes through the metabolic networks respecting steady state constraints (Schuster et al. Nat. Biotechnol., 18 (3), 2000). EFMs are useful to find essential metabolites/reactions or to discover alternative process when a gene is knocked-out. Nevertheless, it is well-known that computing EFMs could produce huge results, impracticable to analyze by hands. The lack of user-friendly tools to help biologists to analyze EFMs limits drastically their spread into the community.

We proposed a graphical tool to classify EFMs following shared common set of reactions. This tool, available through a web interface, uses a plot technique based on parallel coordinates (A. Inselberg. The Visual Computer, 1985) to build a diagram of EFMs. It allows the user to visualize associated reactions within different EFMs. A pre-processing step based on K-mean clustering provides a customized view of EFMs as a set of data aggregated by value, depending on if the reaction is present (taking into account the forward or backward direction) or if it is missing. In a second step, editing operations available in the interface allows the user to interact with the representation, making possible to customize the axes order, thus emphazing links between reactions, or to highlight subsets of interest for example, guiding the user for the dataset exploration. To conclude, this editor offers a way to dynamically experiment arrangements between axes, in order to extract new information from EFMs sets.