

## Analyzing complex metabolomics data

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### **Abstract**

Systems biology is the study of biology as an integrated system of genetic-, protein-, metabolite-, cellular- and pathway events that are in flux and interdependent. Due to the availability of advanced instrumentation it is possible to generate very complex data sets and a systems biology approach becomes a possibility.

A part of systems biology is metabolomics. The amount of data generated in metabolomics studies is huge and the type of data can be very complicated. Such data can have a multiway-, multiset- or multilevel structure or combinations thereof. These data structures ask for special models to summarize and visualize the data in useful information. Moreover, there is an increasing awareness that time and spatially resolved metabolomics and fusing metabolomics data with other types of omics data is crucial for systems biology. One of the ultimate goals is to find the underlying network structure of a given biological process.

An overview will be given of the different kinds of complexities in metabolomics data. Some new methods will be presented that can deal with some of these complexities. All this will be illustrated with real-life metabolomics data sets from different origin, e.g., from the fields of mammalian and microbial metabolomics.