

# An Integrated Method to the Study and Interpretation of Metabolic data for the Discovery of Plant Natural Products

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## Abstract

The creation of theories about the organisation and regulation of metabolic networks hinges on the discovery of molecular components and their functions. The path that leads to accurate computational modelling and prediction of metabolic outcomes is through iterative experimental testing of such assumptions. This information is particularly useful for comprehending the biology of natural compounds, whose metabolism is sometimes only vaguely characterised. A collection of reliable time-resolved and geographically characterised metabolite abundance data and accompanying information is essential to realising this objective. One of the most difficult aspects of metabolite profiling is the intricacy and analytical limitations of determining an organism's whole metabolome. Furthermore, metabolomics data must be curated in publically accessible metabolomics databases in order for it to be effectively used by the scientific community.

To incorporate genomic system-scale datasets, such databases require clear, consistent formats, easy access to data and metadata, data download, and accessible computational tools. Although transcriptomics and proteomics combine the genome's linear predictive capability, the metabolome represents the genome's nonlinear, final biochemical outputs, which are the outcome of the complex system(s) that control genome expression. For example, duplicated links between metabolites and gene-products muddle the relationship between metabolomics data and the metabolic network. The rules of chemistry, on the other hand, predict the linkages between metabolites. As a result, improving the metabolome's ability to integrate with anchor points in the transcriptome and proteome will improve the predictive value of genomics data.

## Keywords

Metabolic data, Metabolites, Genotypes, Genome

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## 1. Introduction

The steady-state levels of the intermediates and end products of the metabolic networks that make up a biological sample are defined by the metabolomes of that sample. As a result, metabolomics data reflect a genome's final expression (output) at the metabolic level. 1 & 2 As a result, by comparing the metabolomes of two samples with different metabolic outputs, one can learn about the structure of the metabolic network that supports these samples' metabolic outcomes [1]. Furthermore, because the structure of the metabolic network is the result of the genome's programmatic expression, which is modified by environmental inputs, metabolomics data, when combined with data from other ,omics levels, can provide insights into metabolic outcomes' systems level control and regulation. When combined with additional-omics level expression profiles, the quantitative determination of metabolomes of tissues/organs that express different levels of a specific metabolic endpoint can help identify genes/enzymes that are components of the biosynthetic pathway supporting that metabolic endpoint. Some specific plant

natural products are generated and stored in specialist structures at the extreme. If no intercellular trafficking is involved in the manufacture of the targeted metabolite, metabolic intermediates from its biosynthesis will occupy the metabolomes of cells that hyper accumulate the metabolite. In a simple metabolic model where transcriptional control determines biosynthetic capacity, one would expect the relative abundance of transcripts encoding enzymes involved in that biosynthetic pathway to be proportionate to the quantity of the process's output [2]. Correlating transcript levels to metabolic products and assigning function to the gene responsible for metabolism would be a statistically simple task in this situation. The regulatory intricacy of interrelationships among genes, gene products, and metabolites, on the other hand, frequently confounds multivariate dataset interpretation. The asymmetric nature of the analytical technologies that collect both datasets is a second hurdle in merging transcriptomics and metabolomics data. RNA-seq methods have the sensitivity to assess virtually the complete transcriptome of a sample, while current metabolomics technologies do not. It is critical to put metabolomics data in public databases that allow researchers

to deposit and analyse metabolomics data and metadata, as well as other data types, to best facilitate its use by researchers throughout the world. The intended applications of the deposited data must be considered while designing a database and its related user interface and software [3]. Programming a database that can effectively store and retrieve data from an increasing number of species, sample conditions, genotypes, analytical platforms, and metadata types, as well as provide a user-friendly, adaptable interface for biochemists, chemists, and biologists to analyse the data, necessitates careful planning and implementation. A more flexible and generalizable database is more difficult to develop and execute than a hard-coded database, but flexibility and generalizability are vital in metabolomics because they can better adapt to the rapid speed of technology advances in data analysis and computation. As a result of these factors, in the planning stage and thereafter, the combined knowledge of computer scientists, analytic chemists, and biologists/biochemists is necessary. Iterative cycles of alpha-testing by a wide range of intended users, followed by enhancements by designers/programmers, are also crucial. However, there are generally always significant gaps in comprehension between fields' concepts and vocabulary [4]. As a result, creating a usable database necessitates a significant time investment in meticulous planning and mutual knowledge of goals and capabilities among computer scientists, biologists, statisticians, and chemists, as well as continual contact among these groups during implementation. Metabolomics data analysis, which is primarily statistical, can be divided into three parts, with a fourth in some cases: Metabolomics data is processed and examined in its raw form. Replicate comparisons and quality assessments are made. The quantities and kinds of metabolites in different of the samples are compared. Metabolomics data can be combined with a wide range of other forms of information,

including transcriptomics, pathway and network annotations, and text mining data [5]. Data normalisation is necessary for data analysis since different sources of metabolomics data often utilise different scales. Normalization also aids in the reduction of noise caused by factors other than biological variability.

## 2. Conclusion

The acquisition of natural product and other metabolomics data takes a significant amount of time and money. Members of the research community can use this data on a worldwide scale for a number of reasons by storing it in a customizable database with a user-friendly interface. Researchers can analyse data quality, compare metabolite levels among samples, annotate, examine redundancies among different platforms in metabolite identification, and compare metabolomics to other data types using these databases. Even at the molecular level, biological systems are complicated and dynamic, and present models only capture a limited fraction of behaviour. Despite these drawbacks, modern approaches to systems-level research are allowing for extensive biological research. These advancements will be aided by incorporating metabolomics more deeply into the equation.

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