Chemistry Identifier Mapping to Pathway Databases using Ontologies: Expanding metabolomics analysis in WikiPathways with ChEBI

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1. Introduction

Health research uses large scale (omics) methods to study the state of an individual, organs, and increasingly tissues and single cells. These methods can measure gene expression, epigenetic modification, and protein abundances. Metabolomics complement the aforementioned methods by studying the abundances of small molecular compounds in e.g. bodily fluids, tissue samples and breath.

Changes in metabolism are relevant for many diseases, such as metabolic diseases, hereditary diseases, various forms of cancers, and the symbiotic interaction of the gut microbiome and the (human) body. Pathway and network approaches are extensively used to integrate various data types and other information sources, in order to understand measurements and results in their biological context. Unfortunately, not all measured metabolites can be linked to metabolite identities present in biological pathway models, which make it more complicated to use metabolomics data in pathway and network analysis.

2. Approach

In order to overcome this intrinsic mismatch between metabolomics experiments and knowledge bases, we use the ontological information from ChEBI [1]. With this, we create additional mappings to metabolites in the pathway database WikiPathways [2]. With this approach, we can connect compounds classes (e.g. fatty acid, lipids), tautomers and/or charge states (e.g. ionisation into acid or base) to individual molecules in a data set. By applying this method on various publicly available datasets in the MetaboLights [3] repository, we want to estimate the increased mapping that chemical ontologies can provide.

References

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