Spectral Database: from data model to web interface
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Introduction

MetaboHUB is an infrastructure of metabolomics and fluxomics that provides tools to researchers and partners. A full package focuses on bioinformatics tools design and development, including one called MetaboHUB’s Spectral Database. The tool is designed to gather and share knowledge and data from both Mass and NMR Spectra.

Methods

For the MetaboHUB’s Spectral Database code architecture, we use modelling concepts and objects-objects relations to represent mass / nuclear magnetic resonance (NMR) spectrometry complexity. Manipulated entities and their links are based on data / metadata used by chemists in laboratory routine. Our work is split in three levels with data-model building, users services designing and code engineering.

Removing the complexity of the full data-model allows us a better understanding of it; the first schema proposes a light view of relation entities, others are focused on parts of it.

Parts of the data-model are specific for spectra techniques (like MS-MS), others are created for future developments (like biological matrix spectra annotation).

There are two ways to access the data: a web portal or a web service. Each service on the web-portal gets its own specific interface, with user control access. Additional interfaces, like spectral annotation tools, will be implemented later as plug-in.

Code architecture and frameworks are an originality of this project. Developers use java frameworks and common generic toolbox to keep to the time scheduled and interoperability. There are three levels of architectures: the spectral database core (figure 2), implemented in both webservices and the web portal model-view-controller (MVC) (schema 5).

The core of the database is split in stand-alone blocks, which allow the community to re-use them in others projects. Each block is specific to one function.

Conclusion

Still in early development phase, some functional blocks are already being tested. The first challenge was to validate this data-model and the use cases with chemists. We are currently testing the chemical library module with data provided by MetaboHUB partners.

It was designed with spectrometry experts knowledge; their experience will also be required to build an interactive identification interface for spectral analysis.

This database will be available through a web portal and open for each partner of the MetaboHUB consortium in a first time, to the whole community later.