Spectral Database: from data model to web interface
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MetaboHUB is an infrastructure of metabolomics and fluxomics that provides tools, methods, and databases to analyze and interpret metabolic processes and fluxes. It is designed to support research in the fields of metabolomics and fluxomics, and to facilitate the sharing of data and knowledge among scientists.

Methods

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.

Light view of the data-model with main entities: both reference and putative compounds are linked to spectra. A specific entity, metadata, is dedicated to link spectra by their shared properties. The user entity is independent: it is used only for web-portal access control, not for spectra or compounds data ownership.

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

There are two ways to access the data: though a web-portal or a webservice. 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 plugin.

Interfaces and user access: some database queries are available for all users (get data), others require an authentication (add or modify elements, data curation).

“Spectral annotation tools” building is an aim of the MetaboHUB Spectral Database. We have to create the structure to be used to host and link all data provided by chemists.

We use a user-friendly framework (twitter bootstrap) to design web interfaces.

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).

Code architecture: the MVC pattern is better for code maintainability, team development and security.

Webservices are the way to open with bots data stored in the spectral database, submitting masses requests and hudge computing. We use popular technologies like REST and Jeon.

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.

To store data in the database, we use the Hibernate framework. We keep the model relations and constrains, with an abstraction of technologies used for SQL requests.

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.

Two milestones are coming: a first to provide a mechanism to import spectral data in the data-model and feed the database, a second to define metadata around spectral analysis.