General introduction to the repository.

A repository is a centralized place where to store useful data, in our case, useful calculation data. To achieve this goal, a sever has been installed and programmed at x-db.iciq.es.

To interface and interact with the repository there are two ways:

1. A Shell interface, that nowadays has the major functionalities.
2. A Web interface that allow us to search substructures into the repository drawing them.

To achieve this goal there are various user skills defined:

1. System Manager: Martin Gumbau
    1. System installation and maintenance.
2. Programmer & Designer: Joan Iglesias
    1. Designer of the application and programmer.
3. Data architects (in alphabetical order): Alexander Hamilton, Gerard Novell, Luca Bellarosa, Maria Besora , Mickael Gicquel (Also in the past Ataualpa Braga)
    1. Define what data to extract from a calculation and what concepts define what is a calculation.
4. Directors (alphabetical order) Carles Bo, Feliu Maseras, Nuria Lopez.
    1. Supervisors and directors of the repository functionalities.

The data-architect have defined using XSD files and XML files what concepts will be stored in the database and what parts of the calculation files to store.

The concepts were defined using an special XML file format, called XSD. You can check those concepts at:

http://datachem.iciq.es/xsd/calculation/chemicalDef.xsd

Data architects can clarify you any doubt you can have about this definition.

They also have defined the Areas, the texts pieces of your calculation files that will be stored on the database using the XML text format at:

http://datachem.iciq.es/xml/extraction/cutting-areas/

Those Areas in the future will be processed in more detail and each individual concept will be stored separately.

For more details about the repository functionalities see the other two tutorials that we have. X-db tutorial and the fuse tutorial.