Magellan: a database application to store and help the analysis of mass spectrometry and gas chromatography data.

Yann LIENHART, IGBMC
CERBM, University of Strasbourg

Chemistry databases are centered on chemicals and their reaction data is extracted from scientific literature. They are usually given in non-standardized conditions and in general nothing is available about reactions that did not occur or exhibit a low yield. Thus, it can be difficult to compare reactions and chemical transformations because of the specific experimental conditions and the missing data.

The Magellan information system, a chemical reaction-centric database, is built on Java open-source technologies. It allows to collect high-throughput data from mass spectrometry or gas chromatography experimentations realized in standardized conditions.

The Magellan application enables the chemist to read and store experimental results, provides tools to help data analysis and query the collected data.