Details

NMR database for small molecules with LIMS implementation for academic research laboratories (nmrshiftdb2)

Nmrshiftdb2 is a free database with additional functionalities for NMR structure analyses and quality control of spectra assignments. The software can be locally installed and used to set up a local spectra database. At the same time, full access to all nmrshiftdb2 data on our www server is granted. Such, local data collections can be stored separately and protected from public access. As an option, nmrshiftdb2 offers an integrated Laboratory Information and Management System (LIMS) for academic NMR laboratories. The web-based system provides a complete electronic order processing and is independend of operating systems. It allows connection to a scheduling system and possesses a range of reporting functions.

Address: Greinstrasse 4
50939 Köln
Nordrhein-Westfalen
Deutschland
To website

Host Institution

Universität zu Köln, Department für Chemie
Greinstrasse 4
50939 Köln
Nordrhein-Westfalen
Deutschland
http://nmr.chemie.uni-koeln.de/
Regionales Rechenzentrum der Universität zu Köln (RRZK), Institut für Informatik
Robert-Koch-Strasse 10, Gebäude 52
50931 Köln
Nordrhein-Westfalen
Deutschland
http://vis.uni-koeln.de/

Scientific Domain

Primary Subjects:
- Chemistry

Secondary Subjects:
- Biology

Category

Research data repositories

Scientific Services

In addition to a tool for the prediction of chemical shifts in NMR spectra, nmrshiftdb2 offers a broad range of search options: Possible criteria are (amongst others) chemical shifts, (sub)structures, structure similarities, molecular formula or meta data. Also, a tool for semi-automated assignment is provided. If a user submits an assignment to the database, the quality of the assignment will be checked by comparision with stored data and a CSEARCH prediction. The result is visualized and can be corrected before the input is actually submitted to the referee system for assessment. Integration of a LIMS allows a complete electronical order processing by NMR facilities through a web-based interface. Such, mmrshiftdb2 is independent of operating systems. It enables integration of a scheduling system and comes with reporting functionalities for archiving, user statistics and accounting. The LIMS module is directly connected to the database and therefore provides the opportunity to set up a local, internal database, as well as accessing the tools of the www database for scientific and educational purposes.

Scientific Equipment

Keywords

- NMR spectroscopy
- automated NMR
- LIMS
- dereplication
- spectra search
- prediction of NMR chemical shifts
- assignment tools
- spectra database
- archiving of spectral data
- quality control of NMR assignments
- paper-free NMR laboratory

Networks

Users per annum

Internal Users: 400
External Users in total: 12.000
External Users:
External Users in the EU:
External Users outside of EU: