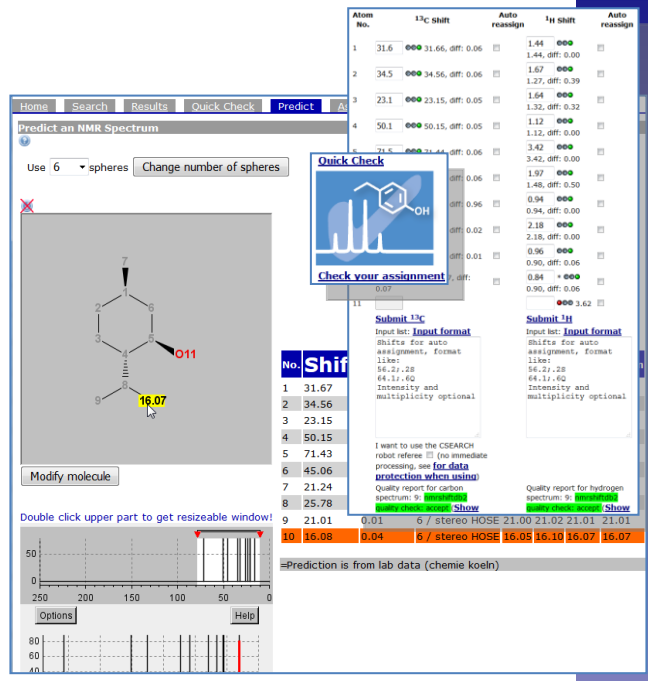
General Functionality

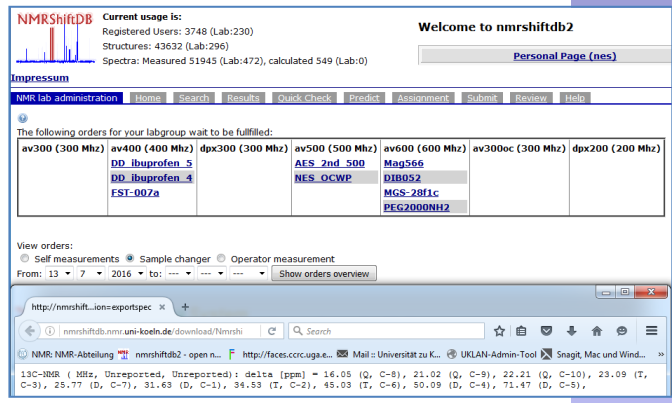
The public instance of nmrshiftdb2 offers the following features:

- **Search** by peak list or other properties (formula, weight, multiplicities, names…), combined queries can be executed
- **Prediction** of ^{13}C, ^{1}H and other nuclei (including stereochemistry for ^{13}C)
- **Automated assignment** integrated in the submission process
- **QuickCheck** function for assignment quality control
- **Database** repository includes original spectral data
- **HOSE code-based predictions**: transparent breakdown of prediction sources
- **Export function** for assignments in publication format

Individual datasets or the entire database content may be downloaded in various formats. These data can serve as base for research and algorithm development.



Database: *Prediction for a compound with diastereotopic CH_3 groups. Shifts for C9 and C10 are predicted differently. A QuickCheck tool allows assignment quality control (insert)*



Lab administration: *The administration interface as seen by a lab operator. The text editor shows the export of datasets in publication-ready format.*

LIMS

nmrshiftdb2 contains an integrated system for the administration of an NMR lab for electronic submission, administration and pickup of completed orders.

In contrast to traditional orders on paper, benefits for **lab users** include:

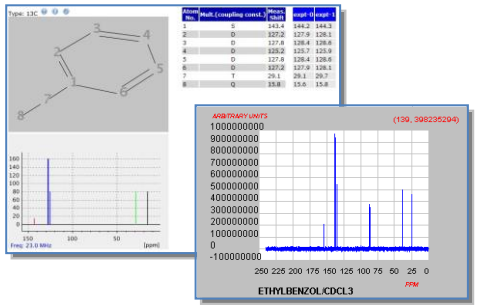
- **Overview and status** of orders always available
- Download of **spectra files** from any intranet connected computer
- All **nmrshiftdb2 functions** can be used with lab data
- **Export** of assigned spectra in **publication ready format**

For **facility administration** (NMR staff):

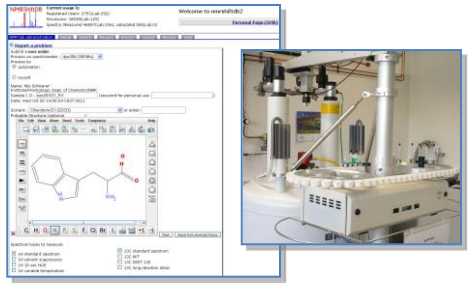
- **Overview** of orders on all spectrometers
- Reports of lab activity and statistics of usage for **accounting purposes**
- **Automated order handling** *via* sample changer through LIMS surface
- Creating an **in-house database** of assigned spectra is easy and improves prediction quality

Introduction

nmrshiftdb2 is an **open web database** for organic structures and their nuclear magnetic resonance (NMR) spectra. Data (including spectra) is available under an open content license at www.nmrshiftdb.org. It offers spectrum prediction (^{13}C, ^{1}H and other nuclei) as well as searching spectra, structures and other properties. Thus, nmrsnhiftd2 serves as a readily available tool for structure identification and elucidation.



An additional module in nmrshiftdb2 allows its use as a **lab information management system** (LIMS). Academic NMR labs can benefit from this, using the electronic lab administration and building their own inhouse database at the same time.



Contact

The public instance is available at:

www.nmrshiftdb.org

For any information contact

Stefan Kuhn
University of Cologne
info@nmrshiftdb.org

Since our primary goal is to improve reception and scientific treatment of NMR data in academia, comments and suggestions are welcome!

The developer page at

http://sourceforge.net/projects/nmrshiftdb2/

provides technical information and source code for those interested in the active development of this project.

nmrshiftdb2

NMRShiftDB

An open NMR Database and LIMS

www.nmrshiftdb.org