From chemical shift data through prediction to assignment and NMR LIMS – multiple functionalities of nmrshiftdb2

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Introduction

NMRShiftDB has been established for almost ten years as a free web database for organic structures and their nuclear magnetic resonance (NMR) spectra. Recently, there were some changes in the team and there was a slight rebranding to nmrshiftdb2 (available at **http://www.nmrshiftdb.org**). We continue to work in the open-data and open-source spirit and will improve the system mainly in the fields of features with immediate benefit for users and the recently added lab information management system (**LIMS**). The lab system features (i) easy administration of orders and the retrieved data, (ii) concise overview over lab workload and (iii) work accomplished. In addition to managing their orders, users can assign their spectra and therefore benefit from all nmrshiftdb2 functions. The NMR facility of the chemistry department at the **University of Cologne** is using the system for the (complete) lab management. Currently, this system is being installed at **RUBiospek** of the **Ruhr University of Bochum** and we are interested in additional users.

General Functionality

The public instance of **nmrshiftdb2** offers the following functionality:

- search by peak list
- search by other properties including formula, weight, multiplicities and names
- queries can be executed in various combinations
- prediction of ^{13}C, ^{1}H and other spectra
- semi-automated assignment of peaks to atoms during the submission process
- for HOSE code based predictions it is possible to examine where predictions come from

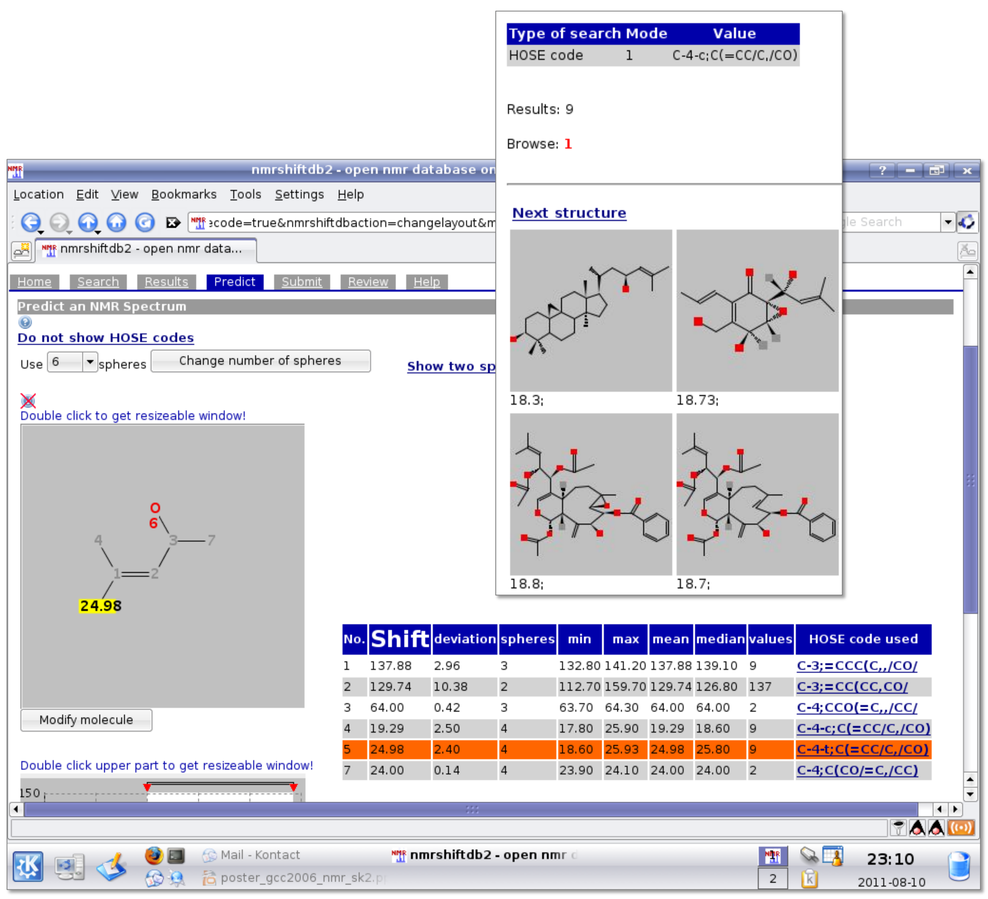

Fig. 1: Prediction for a compound with a 3D configuration. The shifts for 4 and 5 are predicted differently. Clicking on one of the HOSE codes gives the structures used for prediction (inset).

Recent extensions include limited 3D usage in ^{13}C predictions, storage of original JCAMP-DX files for spectra and significant improvements “under the hood”.

Our primary goal is to make the system more useful and better suitable for daily tasks. All comments and suggestions are welcome!

The Lab System

We have built a system for the administration of an NMR lab integrated with nmrshiftdb2. It offers electronic submission, administration and pickup of completed orders.

In contrast to traditional orders on paper, **lab users** now benefit from

- easy overview of orders and their status
- download of the spectra files, from any intranet connected machine
- all nmrshiftdb2 functions can be used with lab data
- easy export of assigned spectral data for publication purposes

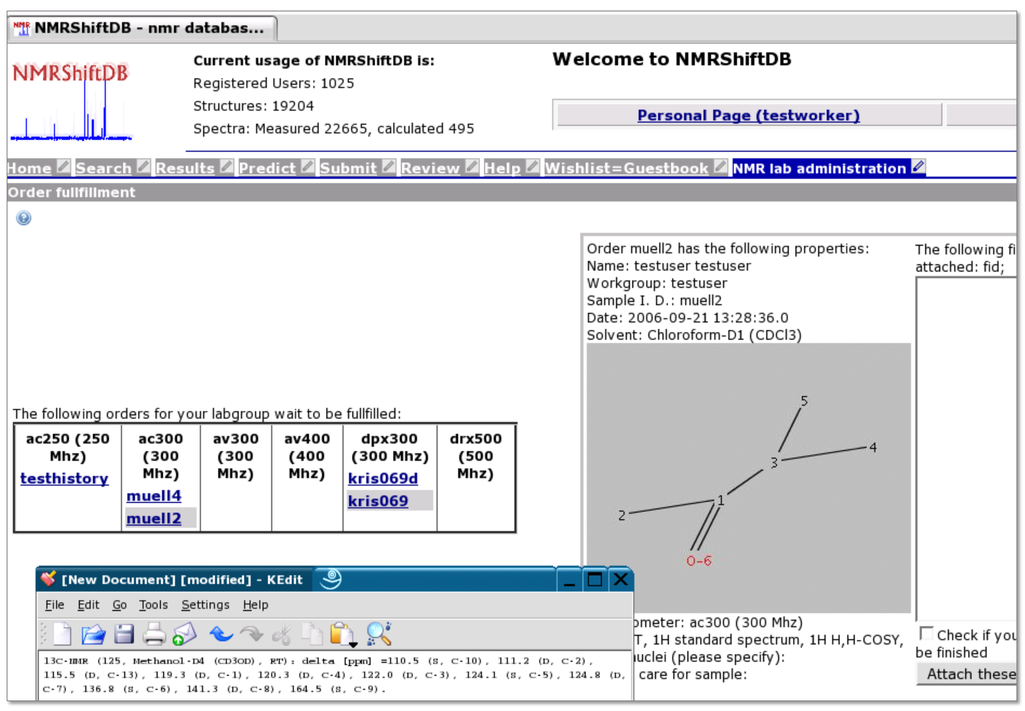

Fig. 2: The administration interface as seen by a lab operator. The text editor shows the export of datasets in publication-ready format.

For facility administration by **NMR staff** it offers :

- easy overview of orders
- reports of lab activity and statistics of usage for accounting purposes
- automated handling of orders via sample changer without required interference by operators
- an in-house database of assigned spectra is automatically created over time

Summary

nmrshiftdb2 continues as an open tool for all NMR users. The lab system offers advantages for both, user and lab, in comparison to paper-based orders still present in many institutions. The integration of **LIMS** with database enhances functionality for every-day use and en route introduces lab users to functionalities of the database.

Literature

[1] Steinbeck, C.; Kuhn, S. NMRShiftDB – compound identification and structure elucidation support through a free community-build web database. Phytochemistry 2004, 65, 2711-2717.

[2] Steinbeck, C.; Kuhn, S.; Krause, S. NMRShiftDB - Constructing a Chemical Information System with Open Source Components. Journal of Chemical Information & Computer Sciences 2003, 43, 1733 - 1739.

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