

General Functionality

The public instance of nmrshiftdb2 offers the following functionality:

- search by peak list or other properties including formula, weight, multiplicities and names
- queries can be executed in various combinations
- prediction of ^{13}C , ^1H 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

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

Download of individual datasets or of the whole database content in various formats is possible. These data can serve as base for research and algorithm development.

The screenshot shows the nmrshiftdb2 web interface. At the top, there is a search mode selection: "Type of search Mode Value" with "HOSE code 1 C-4-c;C(=CC/C;CO)". Below this, it says "Results: 9" and "Browse: 1". The main area displays "Next structure" with four chemical structures and their corresponding chemical shifts: 18.3, 18.73, 18.8, and 18.7. Below the structures is a table with columns: "No", "Shift", "deviation", "spheres", "min", "max", "mean", "median", "values", and "HOSE code used".

No	Shift	deviation	spheres	min	max	mean	median	values	HOSE code used
1	137.88	2.96	3	132.80	141.20	137.88	139.10	9	C-3=C(C)C(C)CO
2	129.74	10.38	2	112.70	159.70	129.74	126.80	137	C-3=C(C)C(C)CO
3	64.00	0.42	3	63.70	64.30	64.00	64.00	2	C-3=C(C)C(C)CO
4	18.29	2.50	4	17.80	25.90	19.29	18.60	8	C-4=C(C)C(C)CO
5	24.98	0.48	4	18.90	35.93	24.66	25.90	2	C-4=C(C)C(C)CO
7	24.00	0.14	4	23.90	24.10	24.00	24.00	2	C-4=C(C)C(C)CO

Prediction for a compound with different CH_3 groups. Shifts for C4 and C5 are predicted differently. Clicking on one of the HOSE codes gives the structures used for prediction (inset).

The screenshot shows the NMRShiftdb administration interface. At the top, it says "Welcome to NMRShiftdb" and "Personal Page (testworker)". Below this, there are statistics: "Current usage of NMRShiftdb is: Registered Users: 1025, Structures: 19204, Spectra: Measured 22665, calculated 495". The main area is titled "Order fulfillment" and shows a list of orders waiting to be fulfilled. A text editor window is open, showing the export of datasets in publication-ready format.

Order ID	Frequency	Sample Name	Sample ID	Sample Name
ac250	250 (Mhz)	testhistory	muell2	muell2
ac300	300 (Mhz)	muell4	muell2	muell2
av300	300 (Mhz)			
av400	400 (Mhz)			
dpk300	300 (Mhz)	kris069d	kris069	kris069
drx500	500 (Mhz)			

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, lab users now benefit from

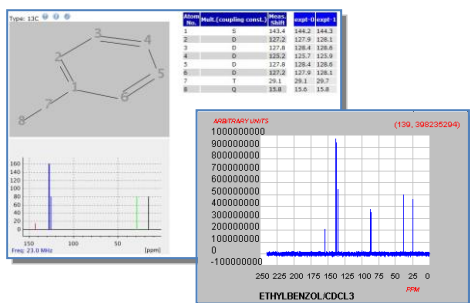
- easy overview of orders and their status
- download of the spectra files, from any intranet connected machine
- all nmrshiftdb2 functions can be used with lab data
- easy export of assigned spectral data for publication purposes

For facility administration by NMR staff it offers :

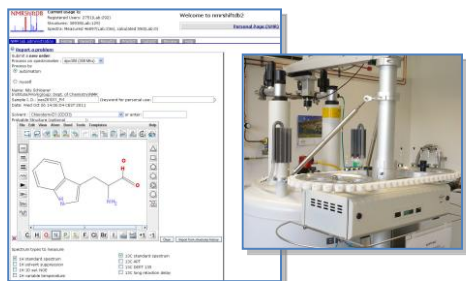
- easy overview of orders
- reports of lab activity and statistics of usage for accounting purposes
- automated handling of orders via sample changer without required interference by operators
- an in-house database of assigned spectra is automatically created over time

Introduction

nmrshiftdb2 is an **open web database** for organic structures and their nuclear magnetic resonance (NMR) spectra. Data is published under an open content license at <http://www.nmrshiftdb.org>. It allows for spectrum prediction (^{13}C , ^1H and other nuclei) as well as for searching spectra, structures and other properties. It therefore serves as a readily available tool for structure identification and elucidation. Last not least, it features peer-reviewed submission of datasets by its users.



An additional module in nmrshiftdb2 allows its use as a **lab information management system** (LIMS). Academic NMR labs can profit from this and build an inhouse database at the same time.



Contact

The public instance is available at:

<http://www.nmrshiftdb.org>

For any informations contact

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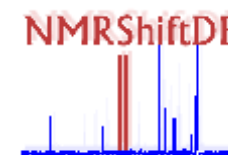
For the lab system, Nils Schlörer (nils.schloerer@uni-koeln.de), Universität zu Köln, and Raphael Stoll (raphael.stoll@rub.de), Ruhr-Universität Bochum, can also be contacted.

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

The developer page at

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

gives technical information and source code for those interested in the development of the project.



nmrshiftdb2

An open NMR database and LIMS

<http://www.nmrshiftdb.org>