Further Activities

Ongoing and planned activities geared towards improving shift assignment quality and better use of NMR data in publications are:

- Workshop on the improvement of data quality in NMR, bringing together NMR specialists, to discuss the inadequate use of NMR data in shift assignments and publications.
- Meet and dialogue with synthetic chemists via roadshows on the need for better shift assignments and NMR data use as well as introduction to the use of the QuickCheck tool.
- Continuous development to further improve on the quality of the nmrshiftdb2 prediction tool. More testers will be recruited during the road show from participating institutions.
- Introduce and encourage new users to adopt the new approach in NMR data evaluation and presentation.

Contact

Scientific Board

Dr. Nils Schlörer (University of Köln)

Dr. Johannes Liermann (University of Mainz)

Technical Advisor

Stefan Kuhn (University of Köln)

Project Manager

Dr. Cletus Itambi (University of Köln)

Website

http://www.nmr.chemie.uni-koeln.de/idnmr.html

nmrshiftdb2

http://www.nmrshiftdb.org

Funding

GDCh Gesellschaft Deutscher Chemiker

DFG

The IDNMR Project

Development of an
Integrated and Open

- NMR Assignment QuickCheck
- Open NMR Assignment Repository

IDNMR

Initiative Data Quality in NMR Spectroscopy

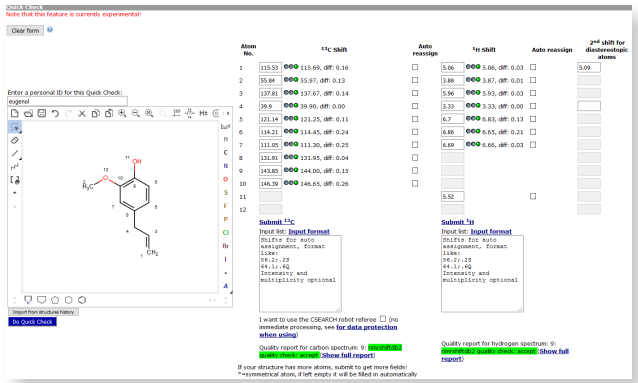
Background

The evaluation and documentation of NMR data is mostly stuck in the pre-digital era, despite NMR being a powerful and versatile analytical technique for molecular systems.

- NMR data is still usually published based on IUPAC recommendations from 1972, often without assignments.
- Valuable information such as *J* couplings or 2D correlations is grossly discarded.
- Wrong assignments or incorrect structures of natural and synthetic compounds go unnoticed due to the lack of appropriate evaluation.
- No established electronic research data submission and evaluation for small molecules NMR data (in contrast to areas like X-ray crystallography or biomolecular NMR).
- The only available tool for evaluation of small molecules NMR assignments, CSEARCH robot referee, is limited to ^{13}C and does not offer a public research data repository.

The IDNMR project aims to address these issues in an integrated strategy by fostering the development of new features and workflows for this purpose based on the existing open NMR database nmrshiftdb2.

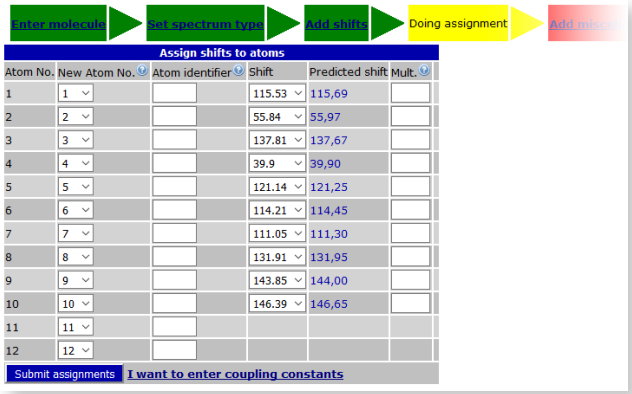
The QuickCheck Interface



Using the existing NMR prediction tools of nmrshiftdb2, a new QuickCheck inferface was developed.

- It allows an easy, straightforward, and – if required – anonymous assessment of ^{1}H and ^{13}C shift assignments.
- The structure can either be drawn directly in the structure editor or copied from any molecular drawing tool.
- Users can choose between explicitly assigning their shifts or providing a shift list which will be tentatively assigned by the system according to the prediction.
- A complete prediction and quality report of the assignment is immediately available to the user upon submission of the assignment.
- A submission to the CSEARCH robot referee for a more detailed evaluation is also possible.

Direct Submission



All assignments can be directly submitted to a local or the public database. Therefore, checked assignments and thus valuable primary experimental data can be made accessible and searchable to the public after publication instead of being submerged in vast article supplements.

Integrated Workflows

In order to make the QuickCheck tool more accessible, we intend to promote its integration into existing laboratory workflows.

- The underlying nmrshiftdb2 software provides a laboratory information management system (LIMS) for NMR labs allowing to directly route recorded NMR data into the local and finally, the public database.
- We will explore possibilities to provide interfaces to commonly used NMR analysis software.
- The final objective is to make this functionality just one additional click away from NMR users' everyday work.