

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.

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Website

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



nmrshiftdb2

<http://www.nmrshiftdb.org>



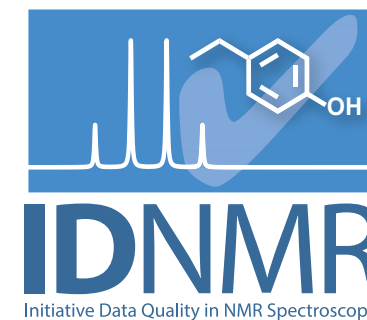
Funding



The IDNMR Project

Development of an
Integrated and Open

- NMR Assignment QuickCheck
- Open NMR Assignment Repository



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

The screenshot shows the QuickCheck interface. On the left, there is a chemical structure editor with a benzene ring substituted with a methyl group, a hydroxyl group, and an ethyl group. The atoms are numbered 1 through 12. On the right, there is a table of NMR assignments. The table has columns for Atom No., New Atom No., Atom identifier, Shift, and Predicted shift. Below the table, there are two 'Submit' buttons: 'Submit 13C' and 'Submit 1H'. The 'Submit 13C' button has a tooltip that says 'I want to use the CSEARCH robot referee...'. The 'Submit 1H' button has a tooltip that says 'Quality report for carbon spectrum...'. At the bottom, there are two checkboxes: 'I want to enter coupling constants' and 'I want to enter carbon spectrum...'. There are also some links like 'Show full report' and 'Show full report'.

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

- It allows an easy, straightforward, and – if required – anonymous assessment of ^1H 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

The screenshot shows the Direct Submission interface. At the top, there is a workflow diagram with four steps: 'Enter molecule', 'Get spectrum from', 'Add shifts', and 'Doing assignment'. Below the diagram, there is a table titled 'Assign shifts to atoms'. The table has columns for Atom No., New Atom No., Atom identifier, Shift, and Predicted shift. The table contains 12 rows of data. At the bottom, there are two buttons: 'Submit assignments' and 'I want to enter coupling constants'.

Atom No.	New Atom No.	Atom identifier	Shift	Predicted shift	Mult.
1	1		115.53	115,69	
2	2		55.84	55,97	
3	3		137.81	137,67	
4	4		39.9	39,90	
5	5		121.14	121,25	
6	6		114.21	114,45	
7	7		111.05	111,30	
8	8		131.91	131,95	
9	9		143.85	144,00	
10	10		146.39	146,65	
11	11				
12	12				

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.