

IDNMR: Establishing a low-barrier online tool for pre-publication NMR shift assignment evaluation



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While NMR has become one of the most powerful and versatile analytical techniques for molecular systems, the evaluation and documentation of NMR data is still mostly stuck in the pre-digital era. NMR data are usually published based on IUPAC recommendations from 1972,^[1] often without assignments, and valuable information like *J* couplings or 2D correlations are grossly discarded. The consequences are wrong assignments^[2] or incorrect structures in natural product and synthetic chemistry going unnoticed due to the lack of an appropriate evaluation.^[3]

While other areas like X-ray crystallography or biomolecular NMR have established means of electronic research data submission and automatic evaluation,^[4] there is only one such service for small molecules (CSEARCH robot referee) which is limited to ¹³C and does not offer a public research data repository.^[5] The aim of the IDNMR project is 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 NMRShiftDB.^[6]

The QuickCheck Interface

Using the existing NMR prediction tools of NMRShiftDB, a new QuickCheck interface was implemented for an easy, straightforward, and – if required – anonymous assessment of ¹H and ¹³C shift assignments (fig. 1).

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. Also, a blend of both methods is possible.

Upon submission of the assignment, users immediately receive a complete prediction and a quality report of the assignment (fig. 2). An automatic submission to the CSEARCH robot referee for a more detailed evaluation is also possible.

Direct Submission

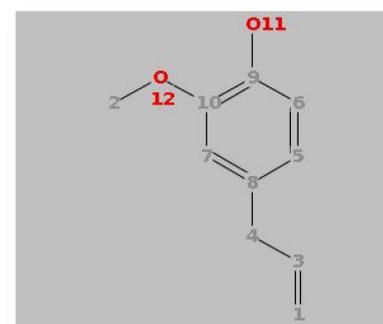
All assignments can be directly submitted to local or the public database (fig. 3). Therefore, checked assignments and thus

Figure 1. The QuickCheck Interface

valuable primary experimental data can be made accessible and searchable to the public after publication instead of being submerged in vast article supplements.

Integration of Workflows

In order to make the QuickCheck tool more accessible and attractive, we stress its integration into existing laboratory workflows. On one end, the underlying nmrshiftdb2 software provides a LIMS for NMR labs allowing to directly route recorded NMR data into the local and finally the public database. On the other end, we are currently exploring the possibility



Atom number	Shift	Deviation from prediction
1	115.53	0,16
2	55.84	0,13
3	137.81	0,14
4	39.9	0,00
5	121.14	0,11
6	114.21	0,24
7	111.05	0,25
8	131.91	0,04
9	143.85	0,15
10	146.39	0,26

Overall mark 9 (out of 1 to 10, 10 being best), recommendation: accept
Mean deviation from prediction: 1,48 ppm -> 0,15 Points
No. of red or missing shifts: 0.0 -> 0.0 Points
No. of yellow shifts: 0.0 -> 0.0 Points
Result: 9/accept

Figure 2. The quality report obtained after submitting

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' every-day work.

Figure 3. Assigned structures are ready for submission

References

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b) M. Elyashberg, A. J. Williams, K. Blinov, *Nat. Prod. Rep.* **2010**, 27, 1296–1328.
- [4] a) Cambridge Crystallographic Data Centre: <http://www.ccdc.cam.ac.uk/>
b) Biological Magnetic Resonance Data Bank: <http://www.bmrb.wisc.edu/>
- [5] CSEARCH Robot Referee: <http://nmrpredict.roc.univie.ac.at/c13robot/robot.php>
- [6] NMRShiftDB: <http://www.nmrshiftdb.org/>



NMRShiftDB
<http://www.nmrshiftdb.org/>



QuickCheck Tutorial
(German, English subtitles)
<http://youtu.be/ENJWRbF3vZU>