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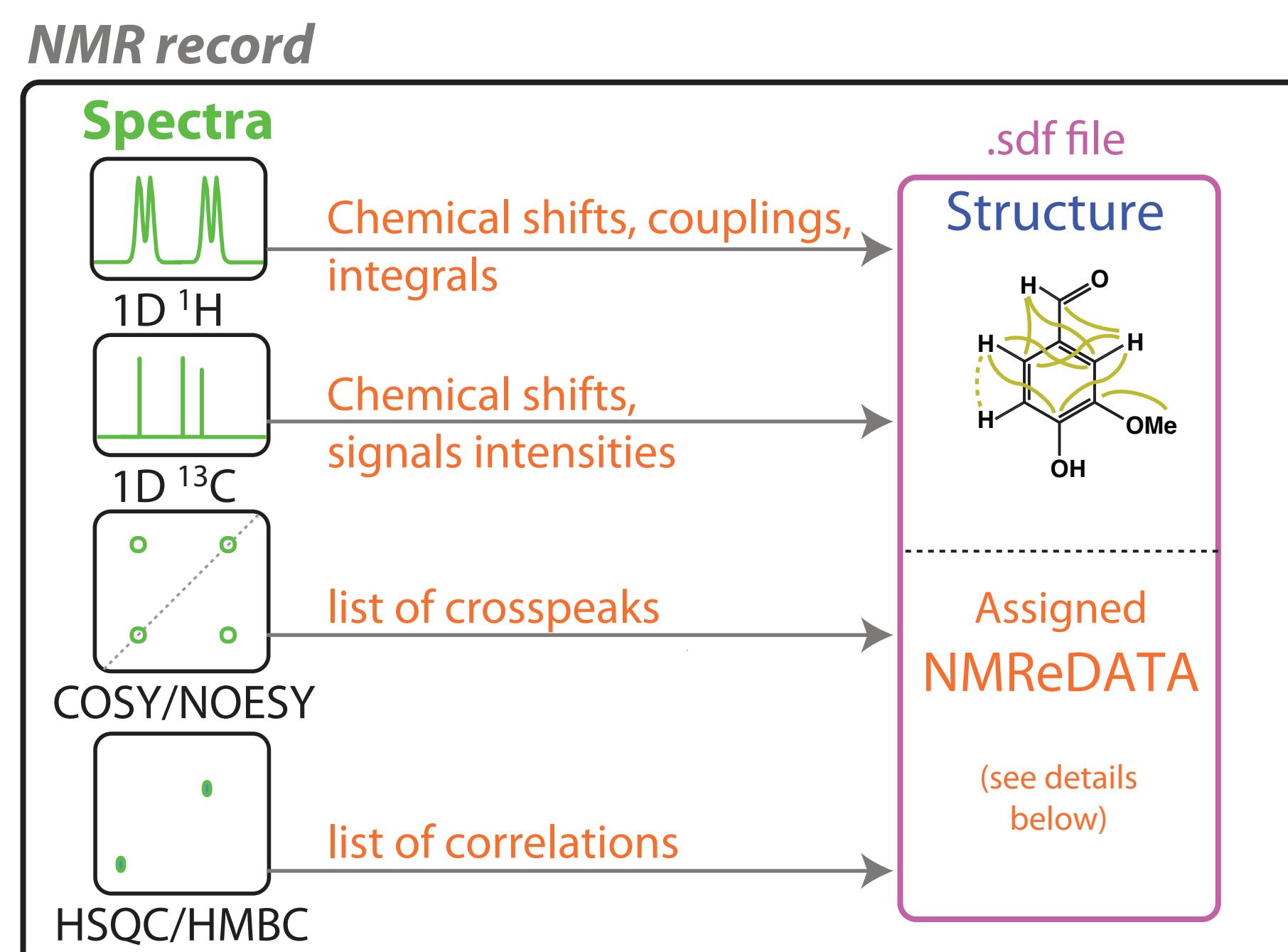
£ Executive journal editor

The NMReDATA initiative

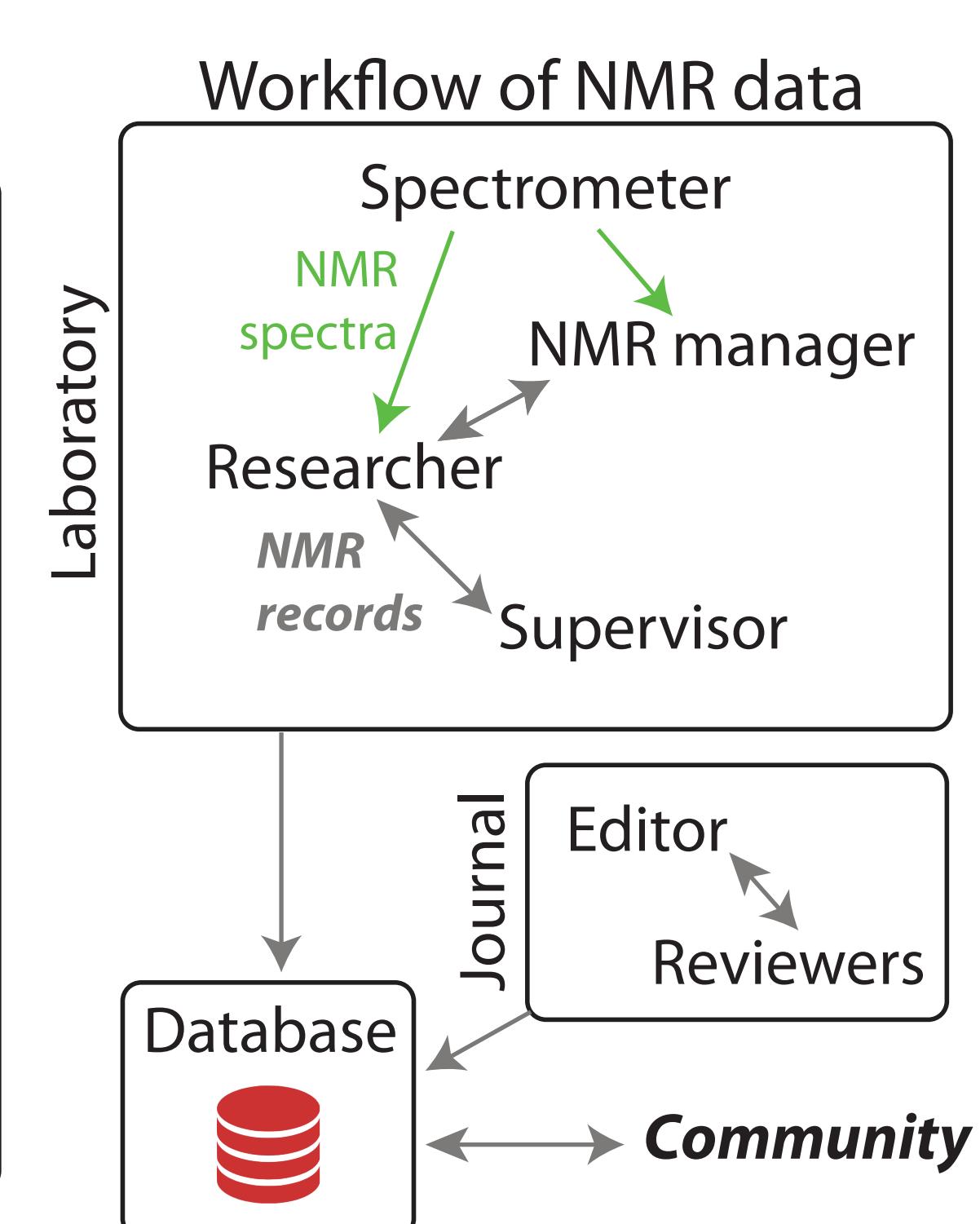
The goal of the NMReDATA initiative is to introduce a manner to associate the data extracted from a "full" NMR analysis (the NMReDATA) to a chemical structure.

We introduced a file format based on the commonly used "Structure Data Format" (.sdf) to combine the chemical shifts, couplings, lists of 2D correlations and assignment (NMReDATA) with a chemical structure in the .mol format.

NMR records (NMR spectra + NMReDATA) including the .sdf file will be generated by computer-assisted structure elucidation software or web-based tools under development.



D. Jeannerat, Magn. Res. in Chem., 2017, 55, 7-14.
J. Bisson, C. Simmler, S.-N. Chen, J. B. Friesen, D. C. Lankin, J. B. McAlpine, G. F. Pauli, Nat. Prod. Rep., 2016, 33, 1028



Important benefits of the new format

- Improved quality of the NMR data for researchers and the community
- Straightforward inclusion of NMR data in reports and journal articles
- Simplified referee work
- Compatibility with electronic storage in database
- Easier comparison of dataset
- Improved searchability of NMR data

Detailed structure of NMR records

benzo[a]pyrene.nmredata.zip

This section provides a detailed look at the contents of the benzo[a]pyrene.nmredata.zip file, specifically focusing on the "structure" part of the file and the "NMReDATA" part of the file.

"Structure" part of the file: This part contains the chemical structure of benzo[a]pyrene in mol format, along with a list of atoms with coordinates and a list of bonds. It also includes explicit structures for all hydrogen atoms.

"NMReDATA" part of the file: This part contains the NMR spectra and extracted data in sdf format. It includes sections for 1D spectra, 2D spectra (e.g., COSY, HSQC), and 3D spectra (e.g., HMBC). The data includes chemical shifts, coupling constants, and signal intensities. A detailed description of the file structure and its components is provided, including the use of tags like <NMREDATA_ASSIGNMENT> and <NMREDATA_LITERATURE>.

Timeline of the initiative

Mid-2016: Proposition by the members of the Associate editorial board of Magnetic resonance in Chemistry to request authors to submit NMR spectra and the extracted data in a manner allowing serious reviewing and to become a source or reliable peer-reviewed NMR data.

September 2016: Decision of the Editorial board of Magnetic Resonance in Chemistry to request NMR data for structure papers.

Until March 2017: Elaboration of a beta version of the format to include NMR data in .sdf files.

July 2017: Official announcement of the Initiative at the Euromar 2017, Warsaw, Poland.

By August 2017: Elaboration and tests of the cheminfo.org web-based platform to host the embargoed NMR records during the peer-review process and open them to the public upon acceptance for publication.

By September 2017: Implementation of import/export features by the providers of computer-assisted structure elucidation software.

September 19th 2017: Round-table discussion at the SMASH conference (Baveno, Italy) and decision on the version 1.0 of the file format.

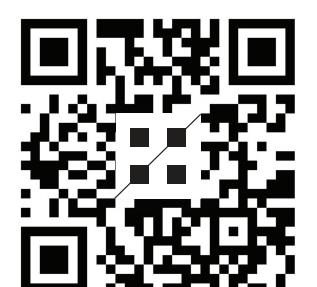
September 28th 2017: Presentation of the Initiative at the IG "Small Molecules", 39th FGMR Annual Meeting, Bayreuth.

From January 2018: NMReDATA and spectra will be requested for all structure papers submitted to Magnetic Resonance in Chemistry.

Mid-2018: Evaluation of the initiative. If satisfactory, invitation to other journals to join the initiative.

During 2018: Contact with IUPAC to consider changes in the recommendation to report small-molecule NMR data.

Follow the progress of the initiative on
www.nmredata.org



Acknowledgments

Damien Jeannerat thanks the State of Geneva and the Swiss NSF funds 200021-147069, 200020-126650, 206021-1288746 for financial support. This work does not necessarily reflect U.S. EPA policy.