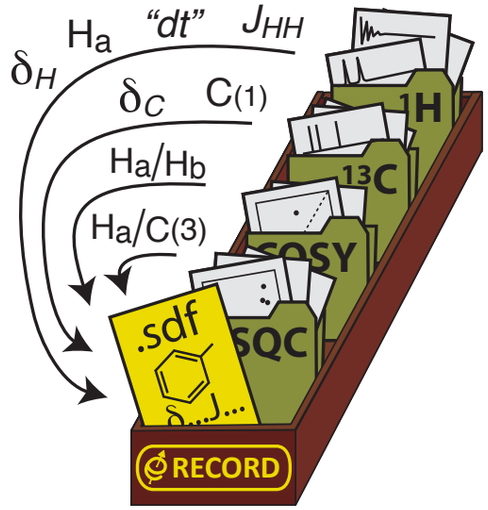
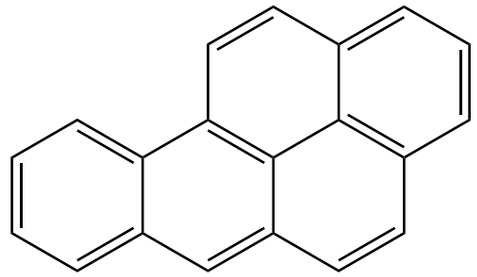
Validation of NMReDATA by spectral simulation

Validate, refine, complement, *etc*.

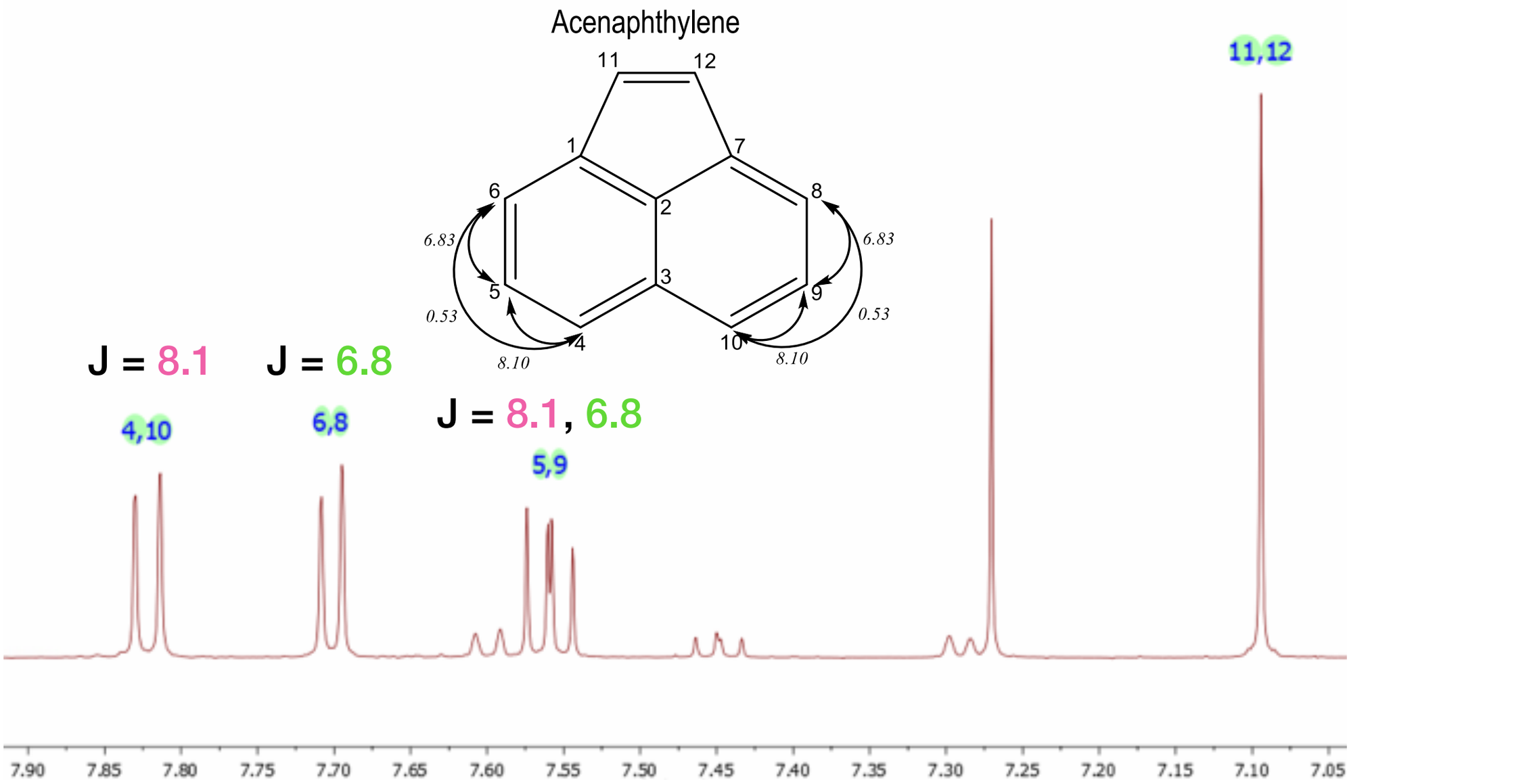
1) Computer-assited structure elucidation
2) Prediction of chemical shift and coupling constants



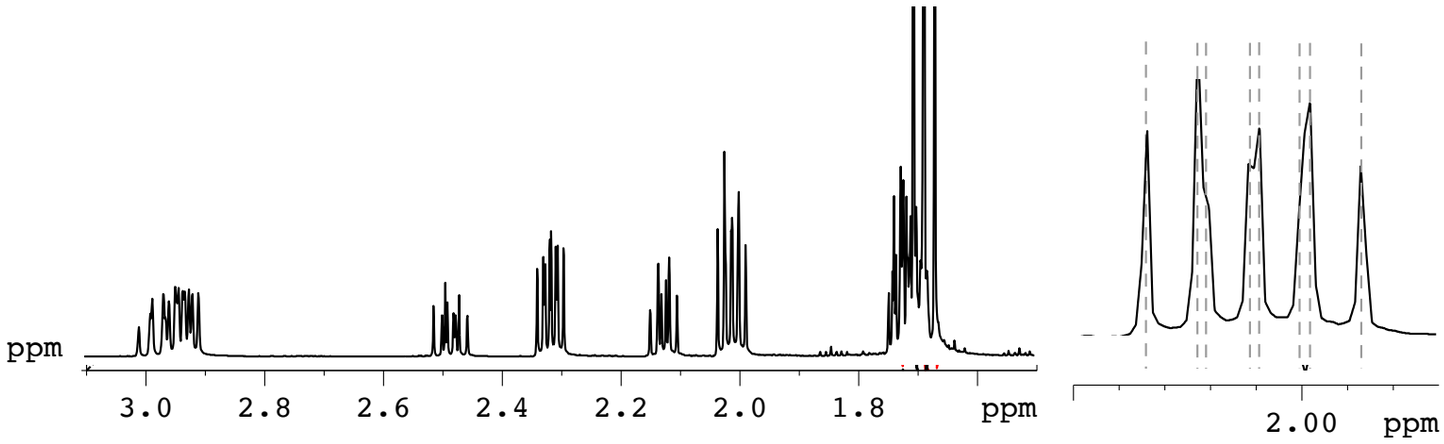


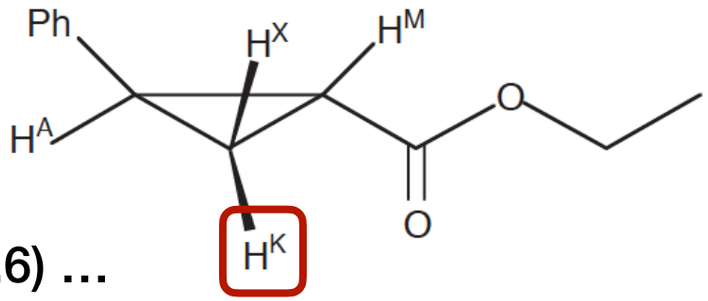
Validation of NMReDATA by spectral simulation

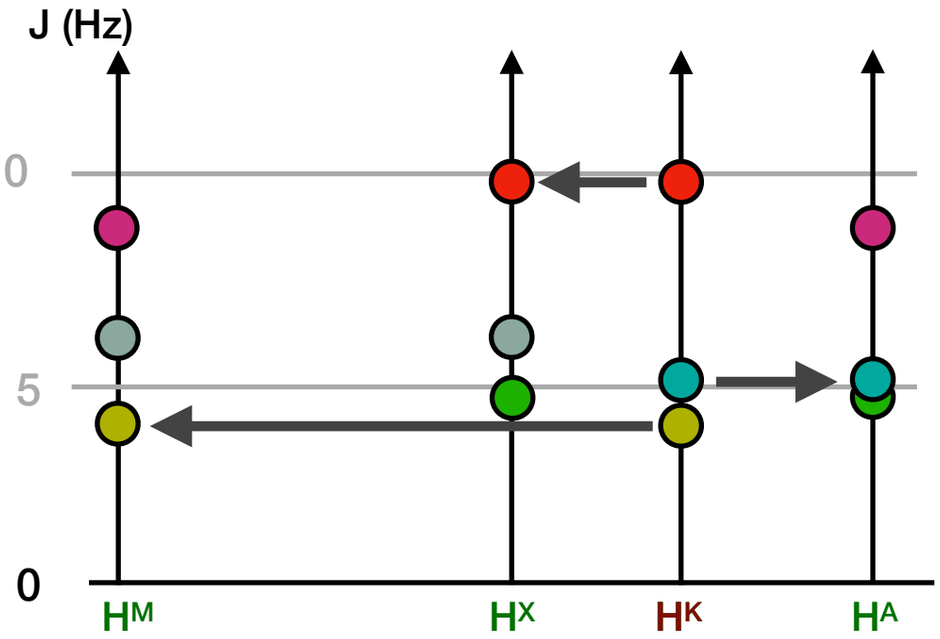
1) Computer-assited structure elucidation
2) Prediction of chemical shift and coupling constants



Validation of NMReDATA by spectral simulation

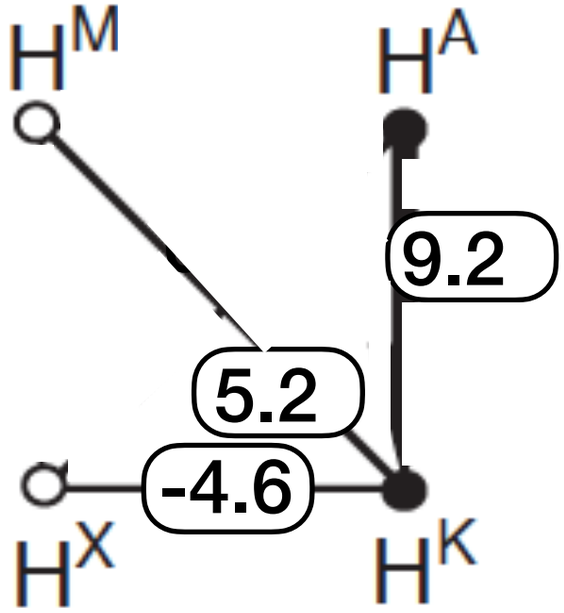






2.05 (H^K, ddd, J = 9.2, 5.2, 4.6) …

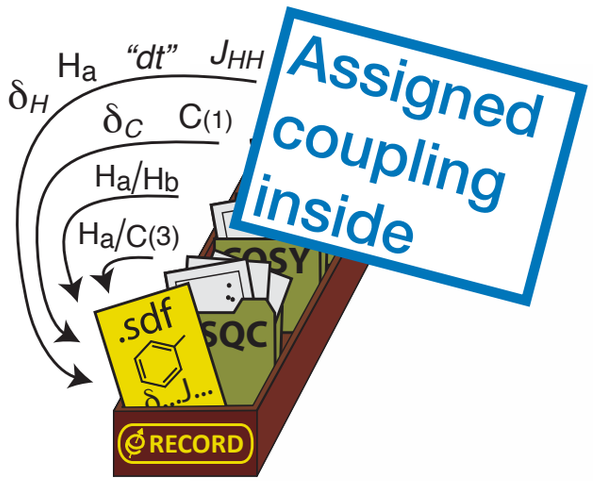
2.05 (H^K, ddd, J = 9.2(H^X), 5.2(H^A), 4.6(H^M)) …

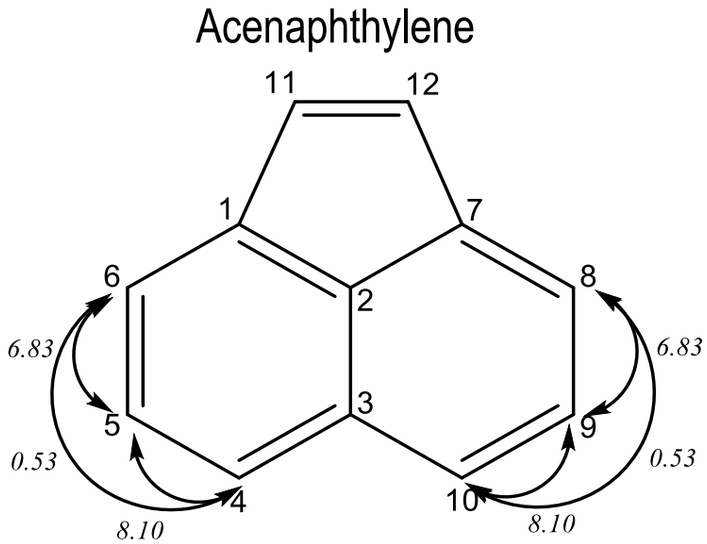


Jeannerat, D.; Bodenhausen, G., Determination of Coupling Constants by Deconvolution of Multiplets in NMR. *J. Magn. Reson.* **1999,** *141* (1), 133-140.

Validation of NMReDATA by spectral simulation

1) Computer-assited structure elucidation
2) Prediction of chemical shift and coupling constants



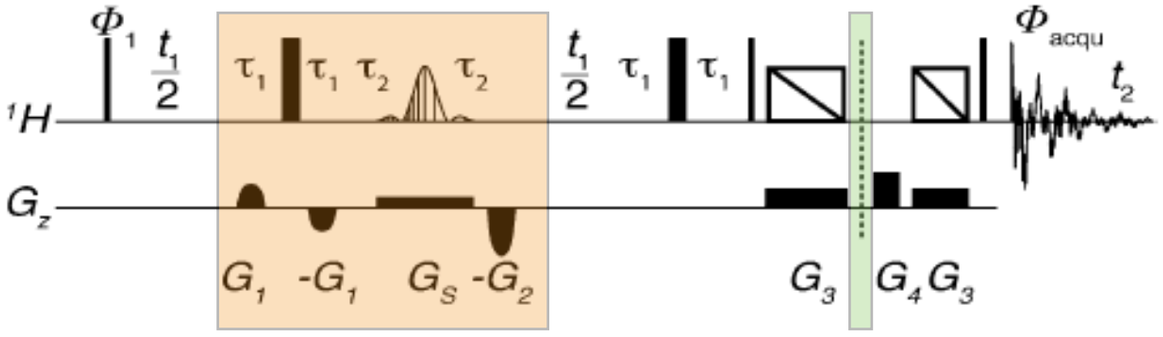


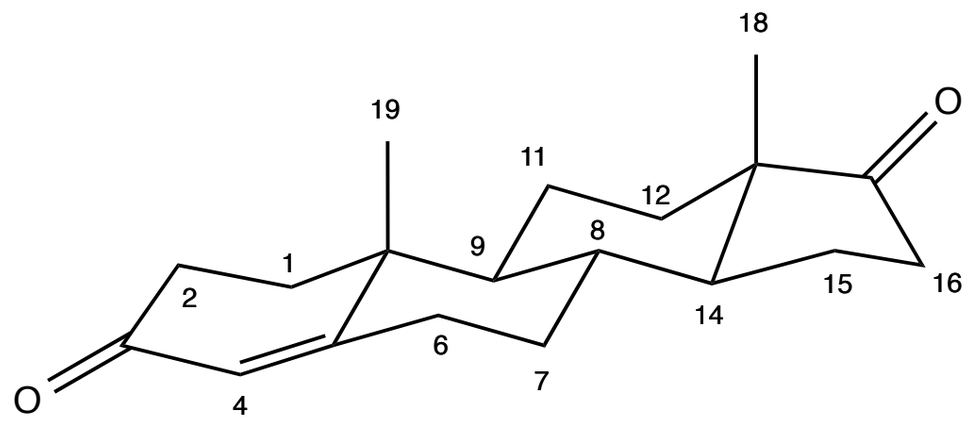
J = 8.1 J = 6.8

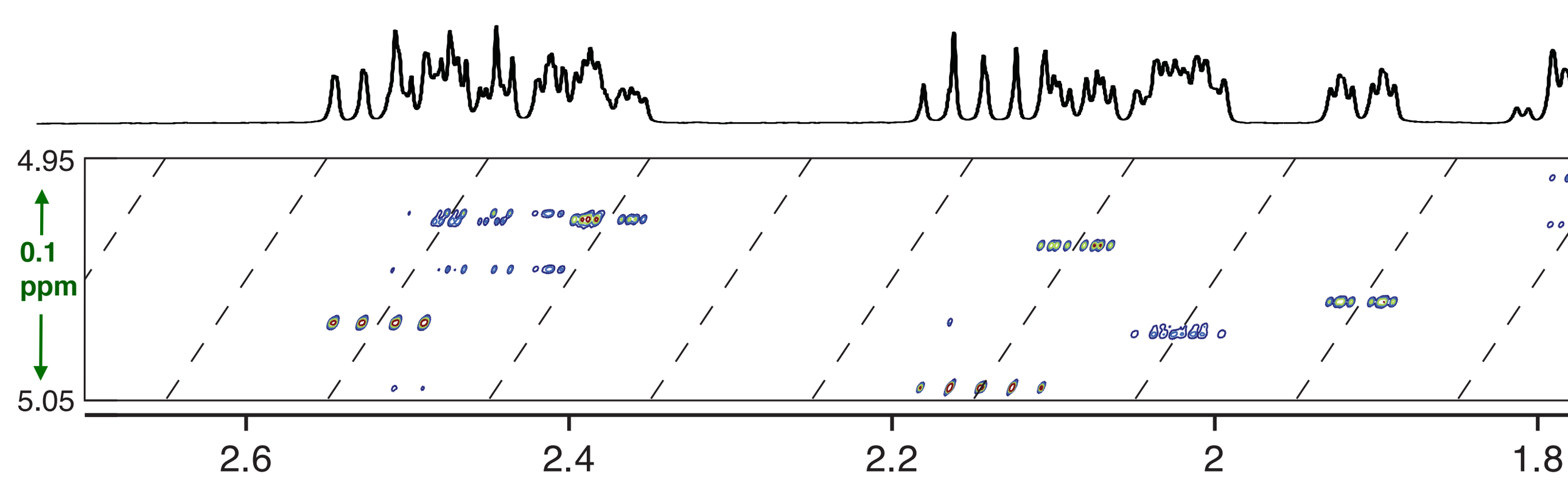
J = 8.1, 6.8

Validation of NMReDATA by spectral simulation

Methodology for top resolution NMR





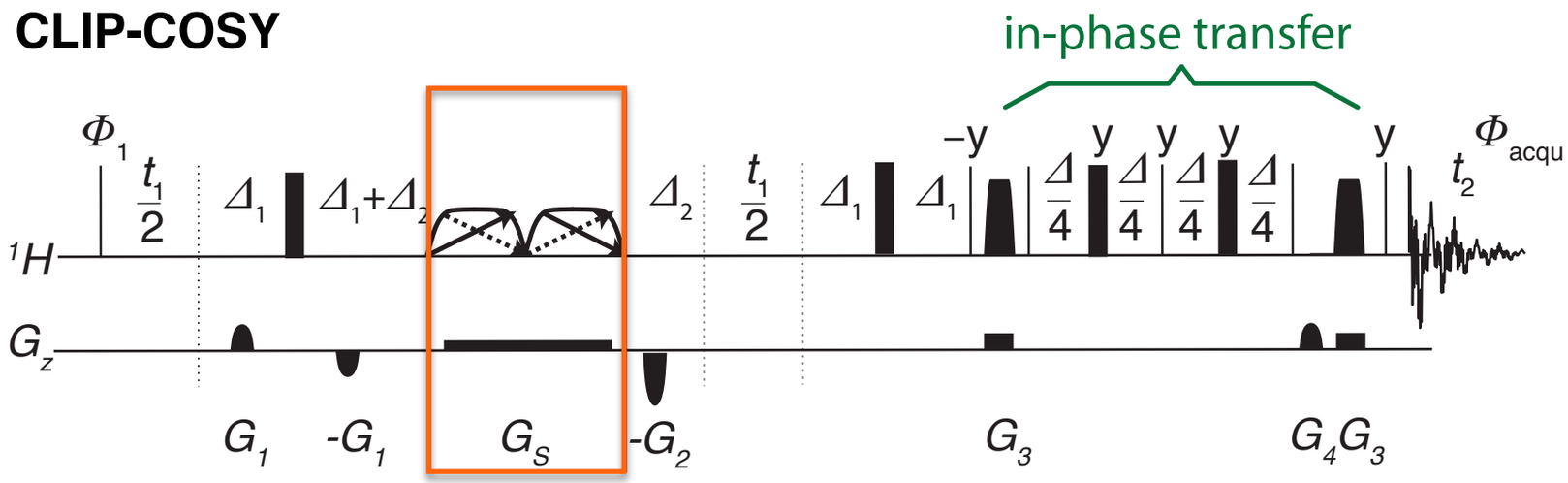


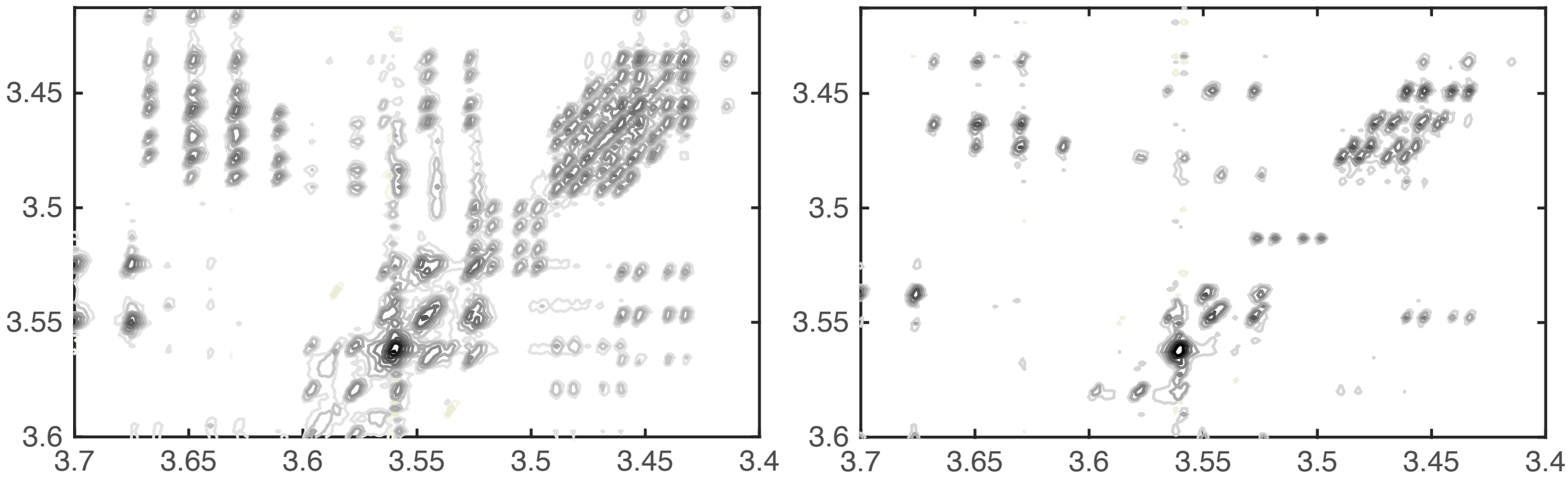
Cotte, A and Jeannerat, D, *Angew. Chem.* **2015**, *127, 6114–6116 10.1002/anie.201500831*

Validation of NMReDATA by spectral simulation

Marta Bruka

Simplified structure by ***Homodecoupling***





M. R. M. Koos, G. Kummerlowe, L. Kalschnee, C. M. Thiele, B. Luy, Angew. Chem. Int. Ed. 2016, 55.

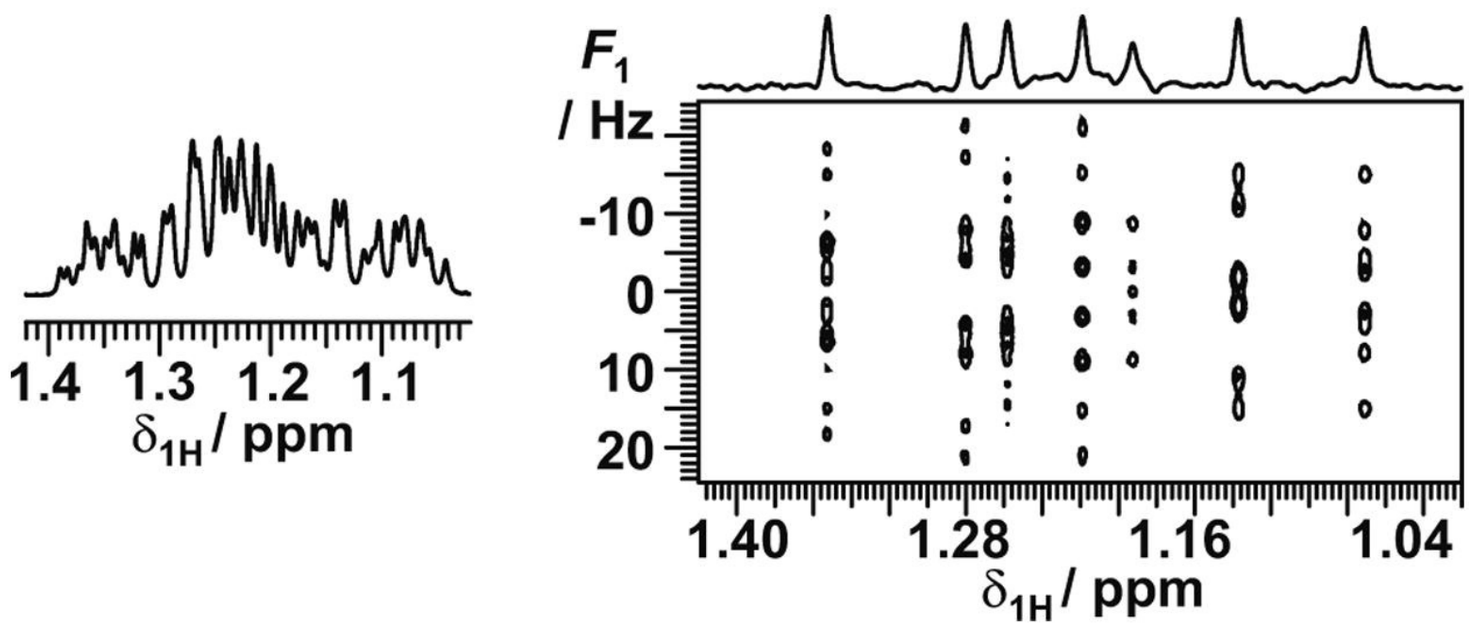
Validation of NMReDATA by spectral simulation

Chemical Physics Letters
Volume 683, 1 September 2017, Pages 398-403

Research paper

Anatomising proton NMR spectra with pure shift 2D *J*-spectroscopy: A cautionary tale

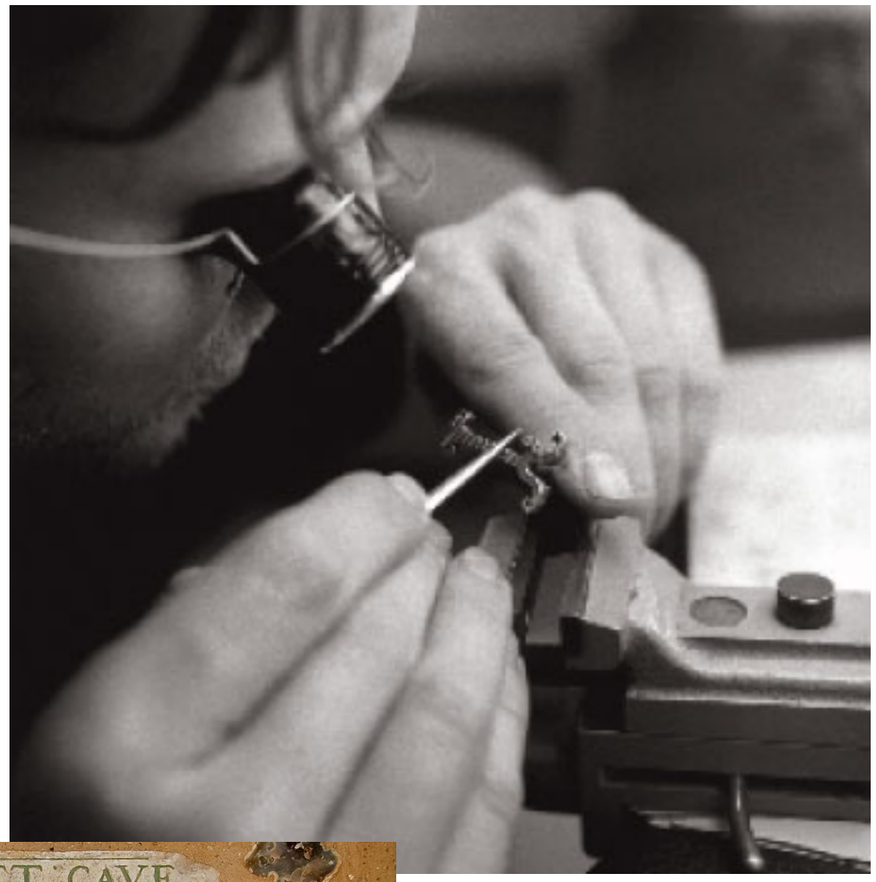
Peter Kiraly, Mohammadali Foroozandeh, Mathias Nilsson, Gareth A. Morris

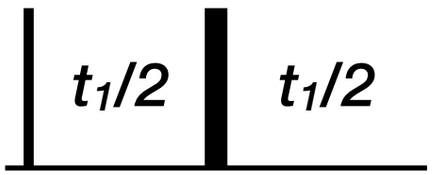


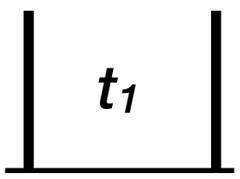
Validation of NMReDATA by spectral simulation

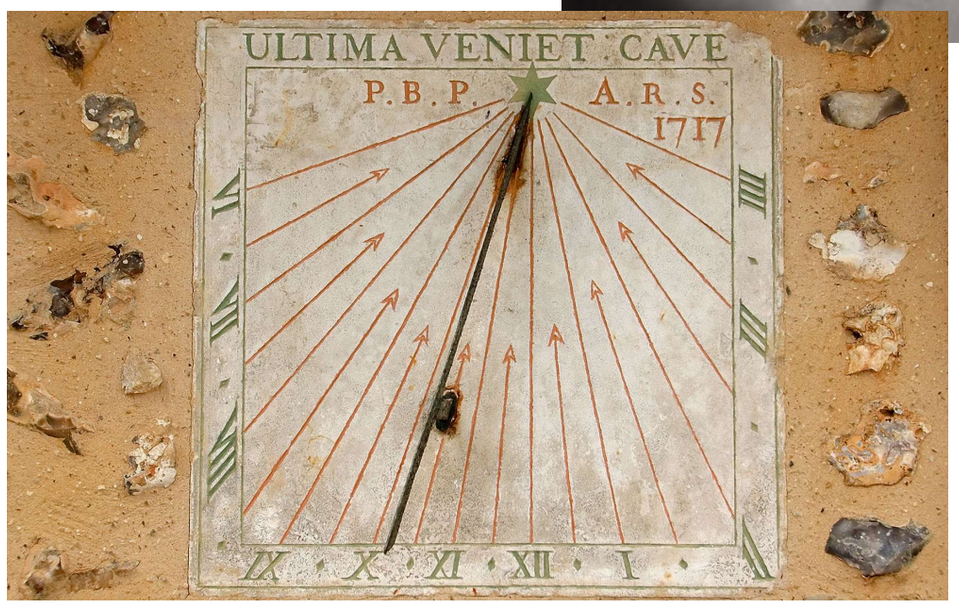
"Clean"
- high resolution
- high interpretability
- many pulses
- low sensitivity

"Crude"
- robust
- high sensitivity
- information-rich artifacts
- high value for validation



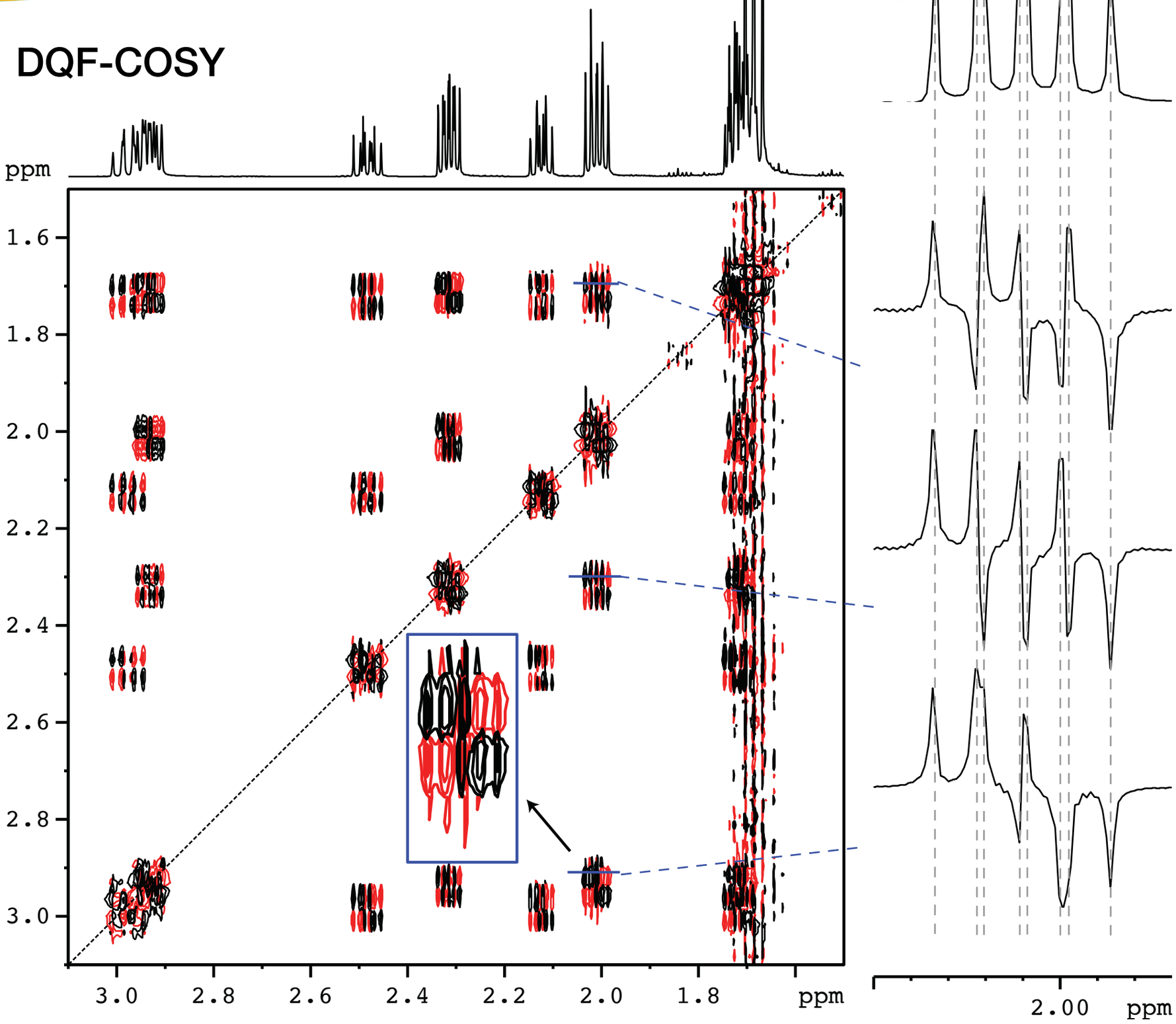




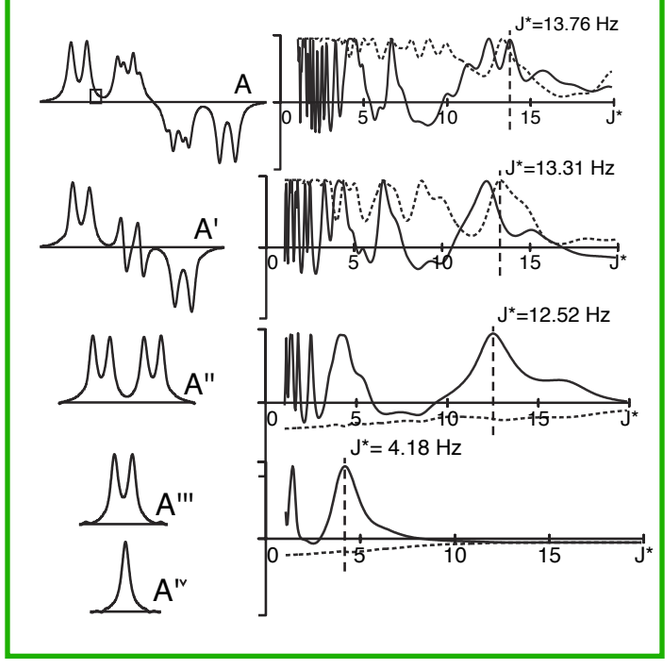


Validation of NMReDATA by spectral simulation

DQF-COSY

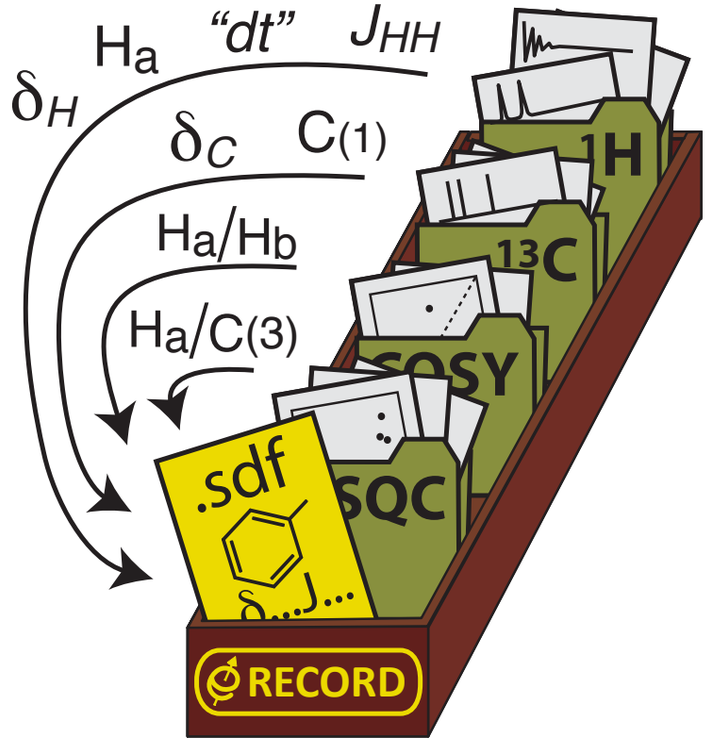


Multiplet deconvolution



Validation of NMReDATA by spectral simulation

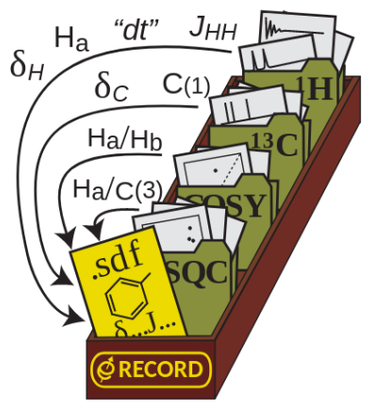
- Assignment of the coupling
- Tools to analyse modern “top-resolution” spectra
- (re)consider simple J-resolved and DQF-COSY spectra



Julien Wist and Luc Patiny's developments

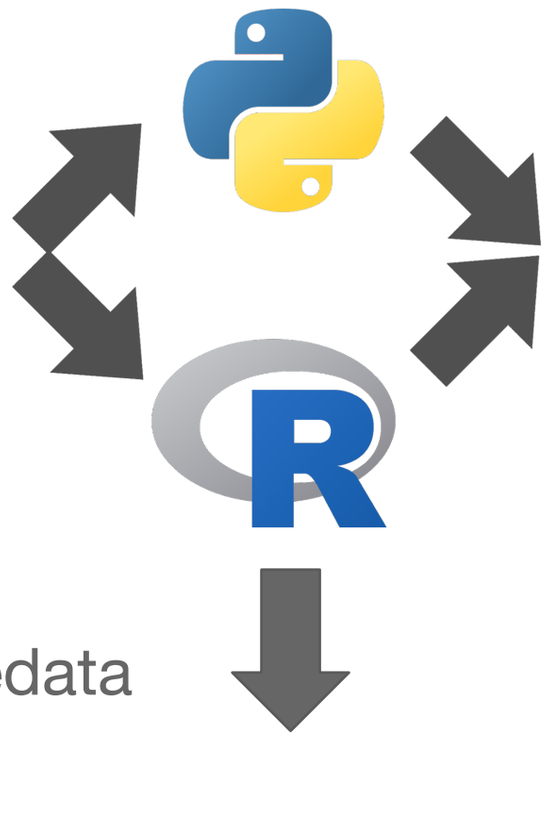
NPM package for node.js

nmredata library



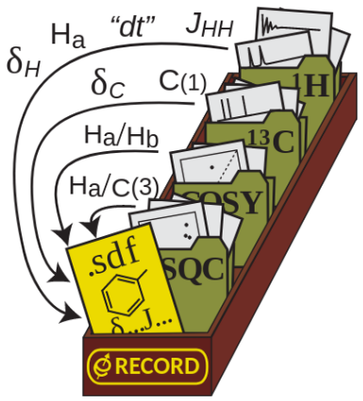
readNMR()

JSON Object



writeNMR()

JSON Object



github.com/cheminfo/nmredata

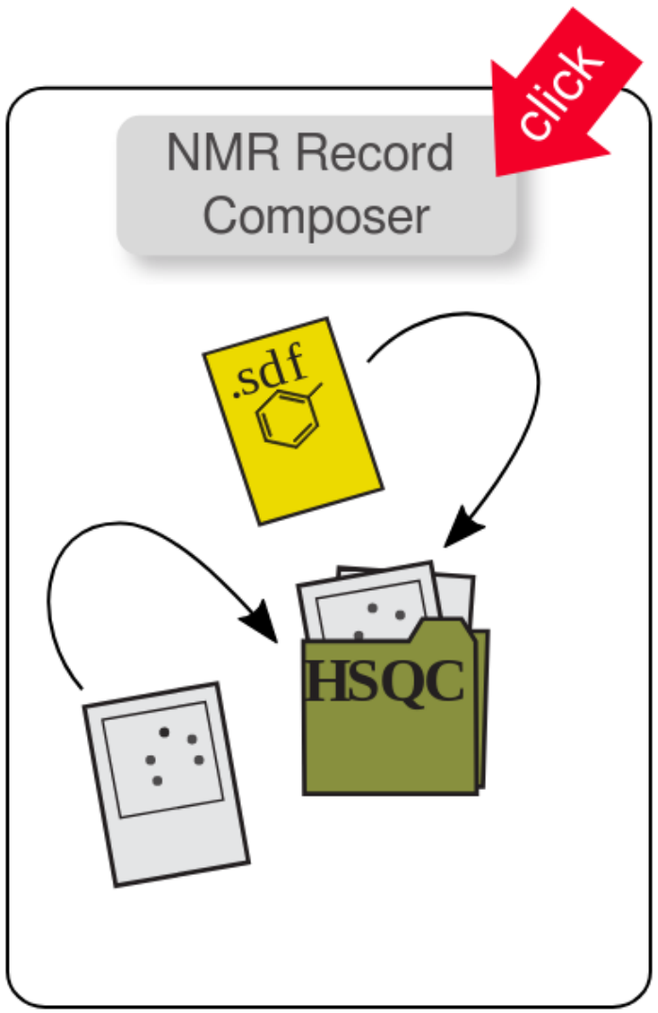
- Open source and free
- Github issues and ticket to report anomalies
- Github pull request for those willing to contribute
- Part of the **nmredata.org** initiative

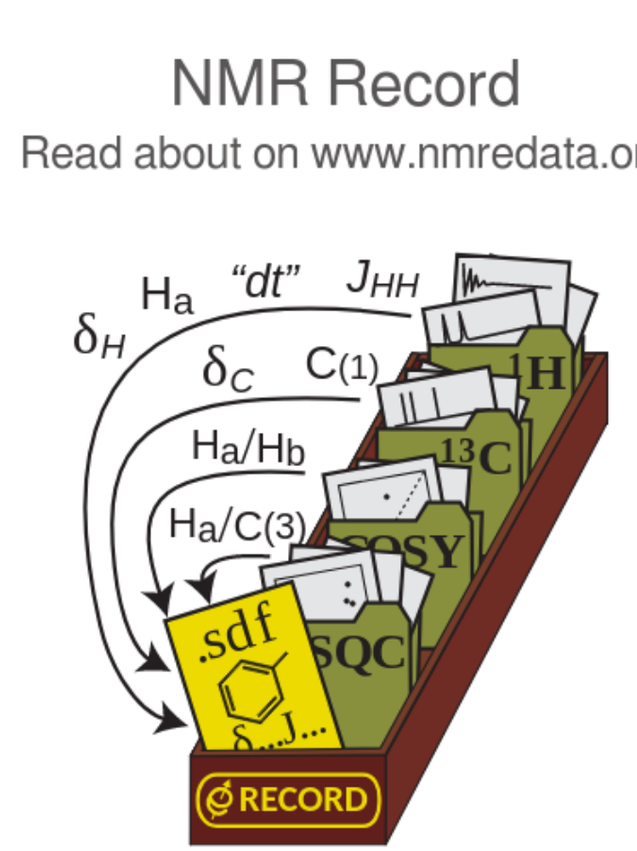
Alejandro Bolaños Universidad del Valle, Cali, Colombia

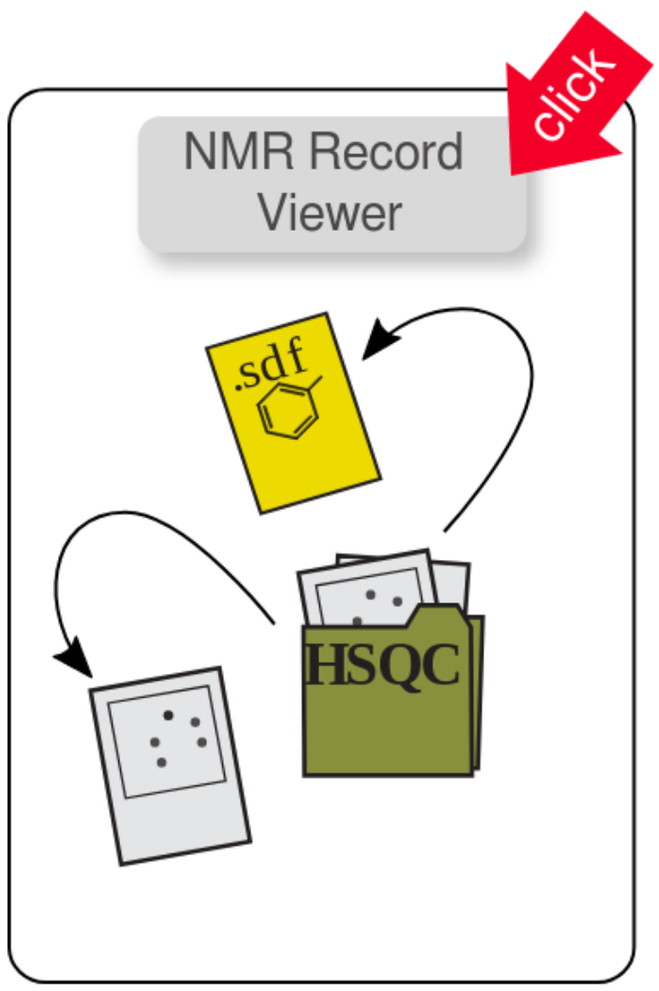
Julien Wist and Luc Patiny's developments

An example of application

nmredata.com





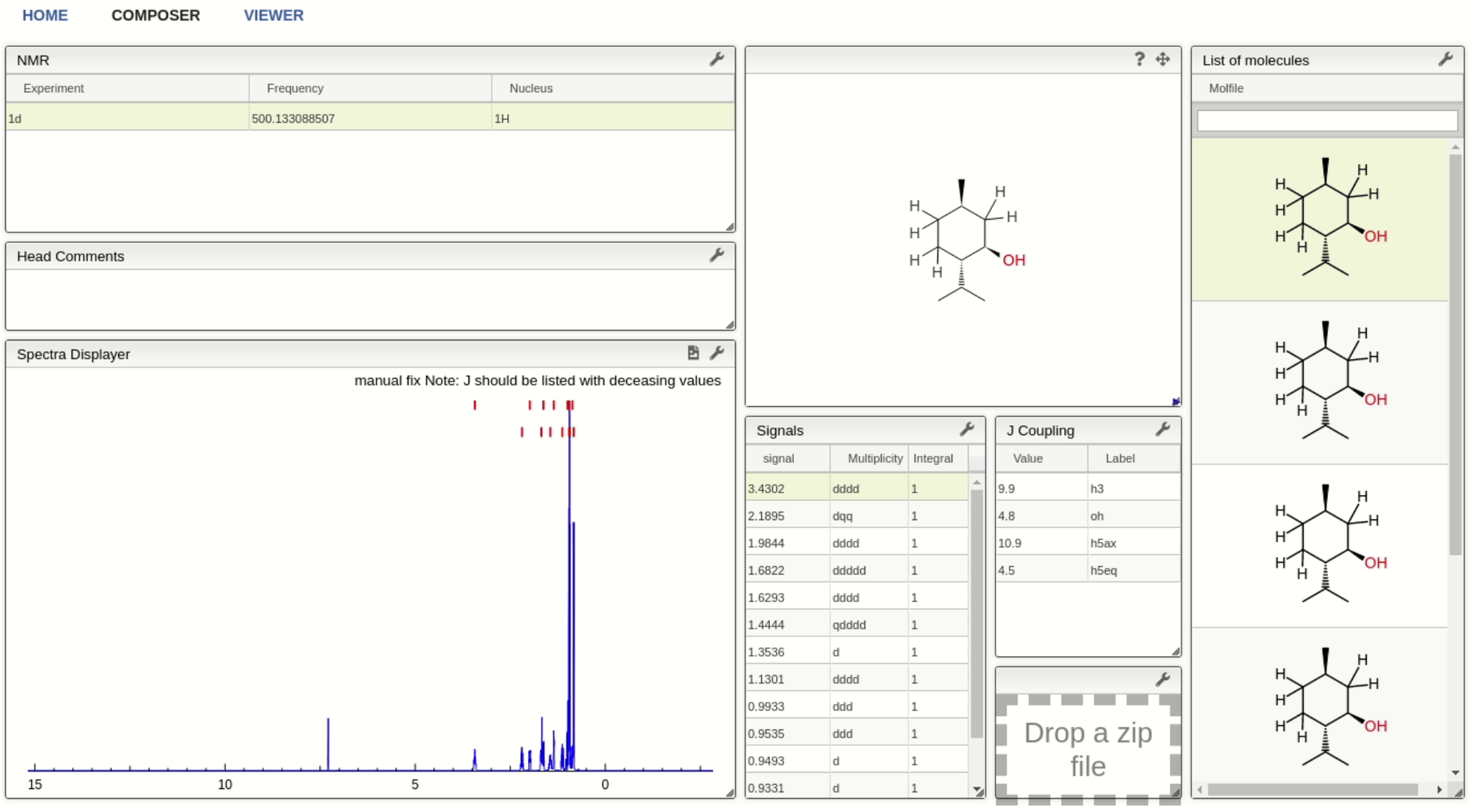


or cite us: doi: 10.1002/mrc.4737

powered by github.com/cheminfo/nmredata

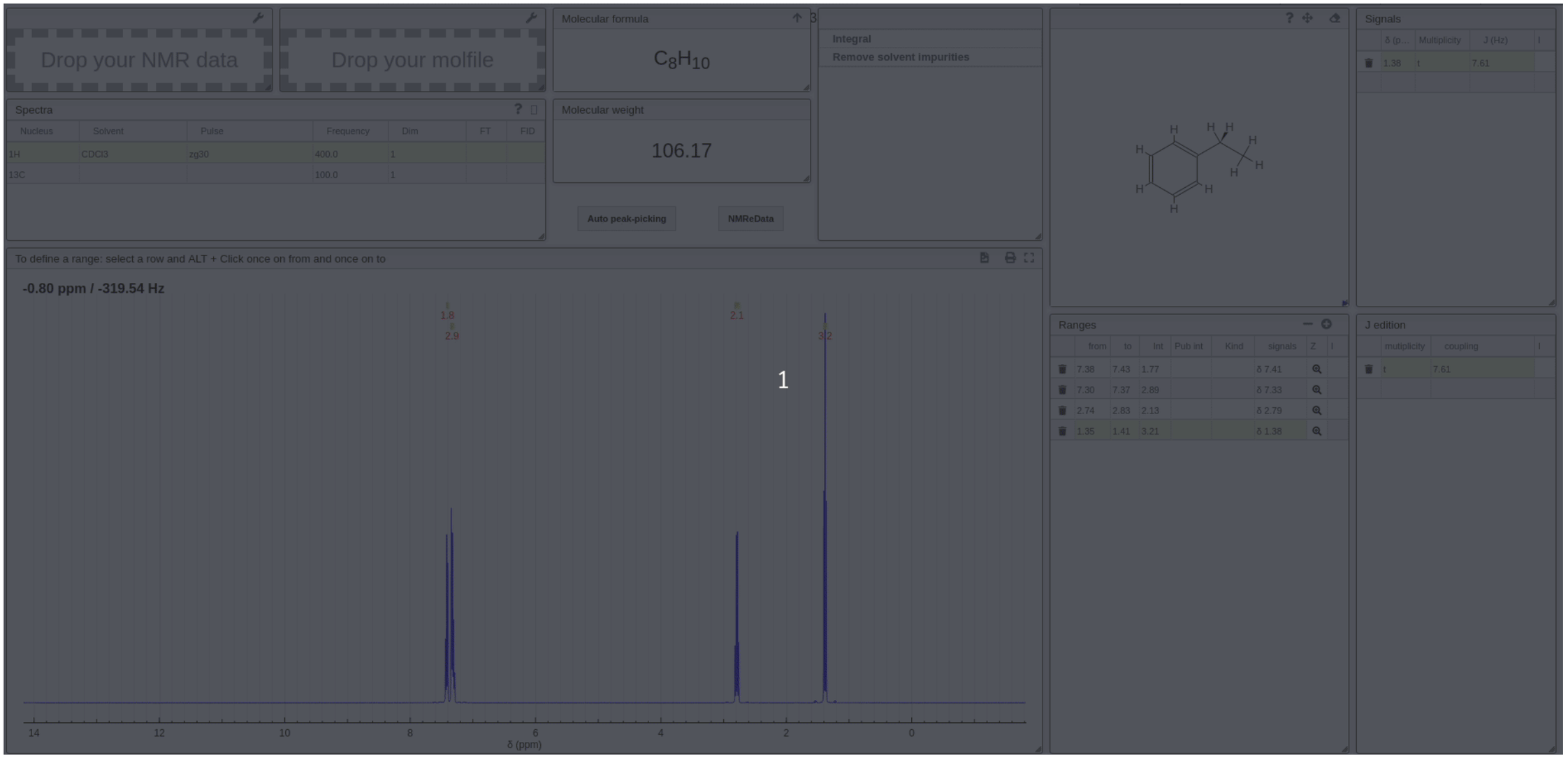
Displaying the information from the JSON object

NMR record viewer



Writing to NMR record

NMR record composer



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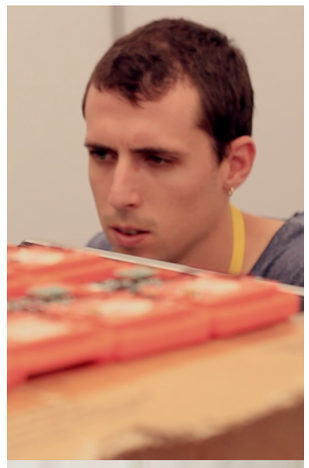
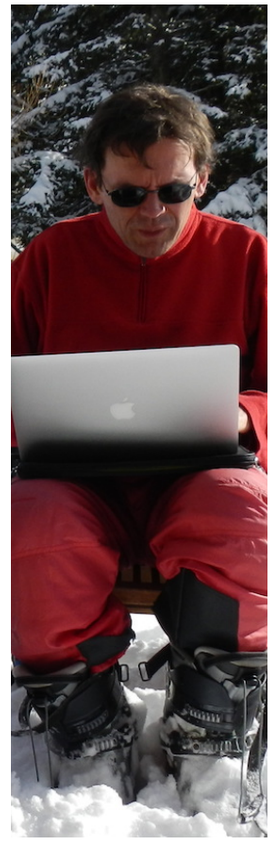
Luc Panity





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ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

ZAKODIUM

cheminfo.org

Validation of NMReDATA by spectral simulation

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Dr. Eduard Sistaré Guardiola
Kirill Shebertov

IUPAC

Leah McEwen
Greg Banik
Dave Davidson
Bob Hanson
…

Programmers

Angel Herraez

Julien Wist
Luc Patiny
…

NMReDATA

Nils Schlörer
Stefan Kuhn
Jean-Marc Nuzillard
Paul Trevorrow (Wiley)

Workshop

FAIR Chemical Data
Publishing Guidelines Workshop
Chemical Structures and Spectra

NSF OAC – Award No. 1838958 and 1838960

Visualizer

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES

DLCM 2.0