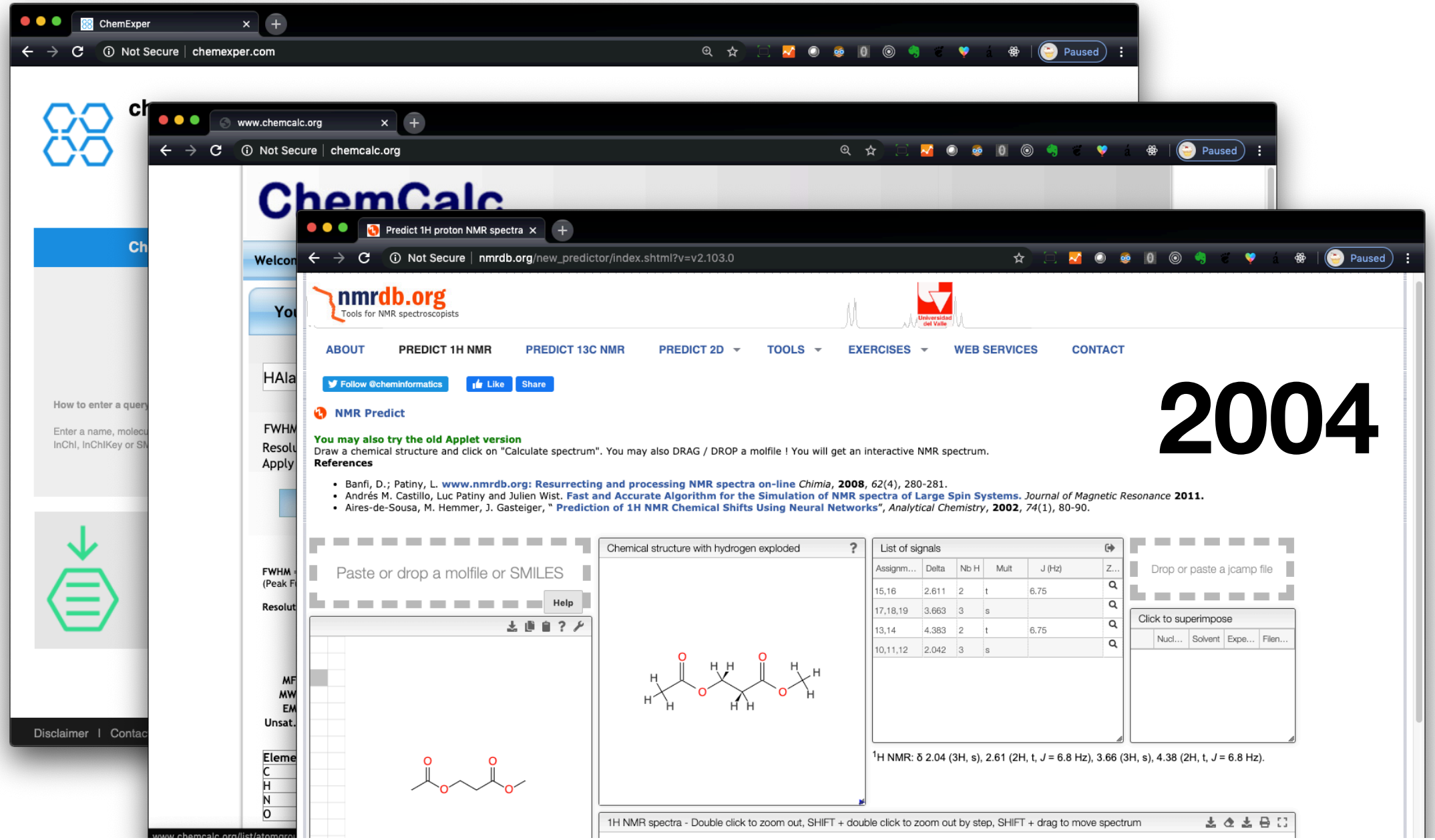
Processing NMR spectra in the web-browser

Luc Patiny
luc@patiny.com

Prof. Julien Wist


ChemExper
Not Secure | chemexper.com
Paused
www.chemcalc.org
Not Secure | chemcalc.org
ChemCalc
Predict 1H proton NMR spectra
Not Secure | nmrdb.org/new_predictor/index.shtml?v=v2.103.0
nmrdb.org
Tools for NMR spectroscopists
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You may also try the old Applet version
Draw a chemical structure and click on "Calculate spectrum". You may also DRAG / DROP a molfile ! You will get an interactive NMR spectrum.
References
Banfi, D.; Patiny, L. www.nmrdb.org: Resurrecting and processing NMR spectra on-line Chimia, 2008, 62(4), 280-281.
Andrés M. Castillo, Luc Patiny and Julien Wist. Fast and Accurate Algorithm for the Simulation of NMR spectra of Large Spin Systems. Journal of Magnetic Resonance 2011.
Aires-de-Sousa, M. Hemmer, J. Gasteiger, " Prediction of 1H NMR Chemical Shifts Using Neural Networks", Analytical Chemistry, 2002, 74(1), 80-90.
2004
Paste or drop a molfile or SMILES
Help
Chemical structure with hydrogen exploded
List of signals
Assignm...
Delta
Nb H
Mult
J (Hz)
15,16
2.611
2
t
6.75
17,18,19
3.663
3
s
13,14
4.383
2
t
6.75
10,11,12
2.042
3
s
Drop or paste a jcamp file
Click to superimpose
Nucl...
Solvent
Expe...
Filen...
1H NMR: δ 2.04 (3H, s), 2.61 (2H, t, J = 6.8 Hz), 3.66 (3H, s), 4.38 (2H, t, J = 6.8 Hz).
1H NMR spectra - Double click to zoom out, SHIFT + double click to zoom out by step, SHIFT + drag to move spectrum

Why the browser ?

- No installation
- Always up-to-date
- Cross-platform
- Optimised graphical rendering
- JavaScript: direct processing in the browser

NMRium: visualise and process 1D NMR spectra

Dr Nils Schloerer

University of Cologne

Dr Johannes Liermann

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

JG|U

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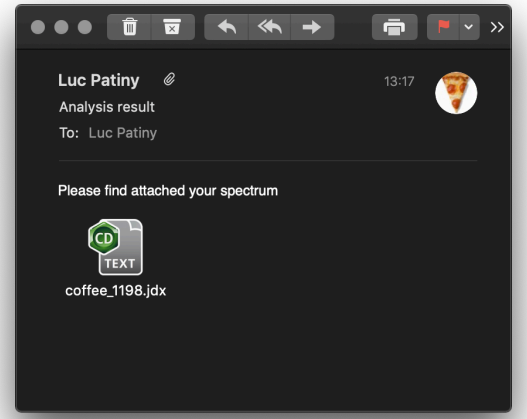
NMRium: Current status

- Free, open-source MIT licence
- 7 months old, 1.5 full-time developper + 6 contributors
- Processing in the browser, no data is transmitted
- LB, zero filling, FT, phase correction, peak picking, integration
- Save, Load, Copy as image, Save as SVG
- Commercial support and database integration on request

Straightforward workflow

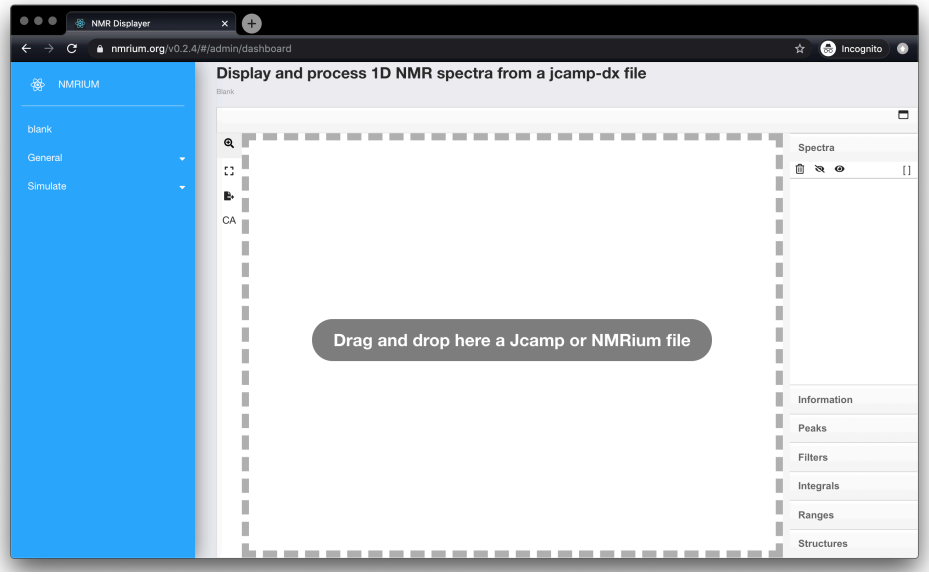
Bruker TopSpin™

NMR facility



Students
Researchers

www.nmrium.org



Metabolomics data preprocessing

https://www.cheminfo.org/flavor/metabolomics

Prof. Jeremy Nicholson
Prof. Elaine Holmes