Department of Chemistry

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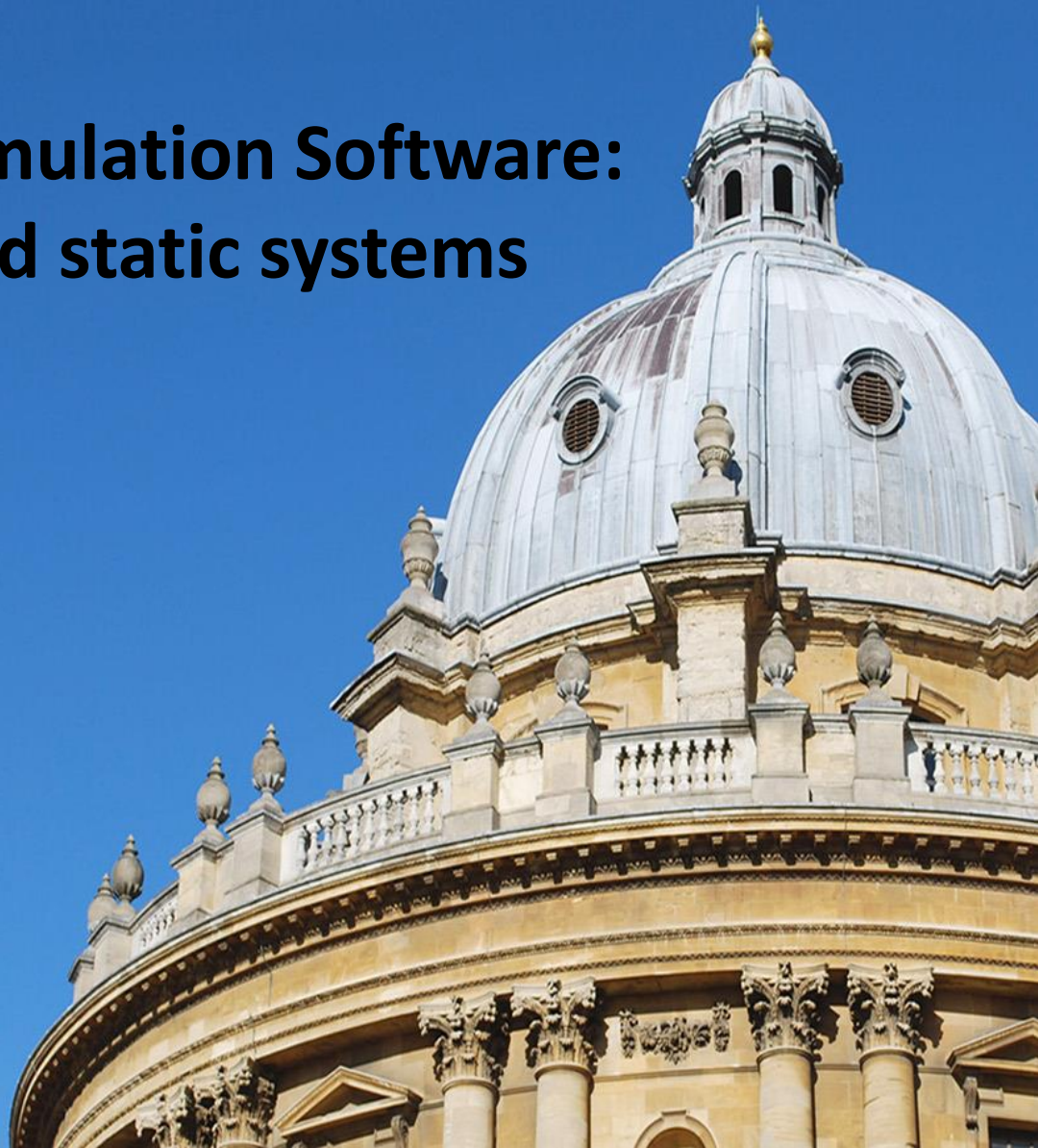
NMR Spectrum Simulation Software: for dynamic and static systems

Nick Rees



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Which computer programs:

- Simulate 1st and 2nd order NMR spectra based on input values of δ, J and number of nuclei.
- Simulate the effects of exchange on the appearance of NMR spectra.
- Allow the iteration of input parameters of simulated against experimental spectra.

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What is your experience:

- Which packages do you use or are familiar with?
- Do old programs still work on new operating systems?
- Can you still get some programs as web pages disappear and links to websites break?

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The packages I have used:

1. gNMR
   home.cc.umanitoba.ca/~budzelaa/gNMR/gNMR.html
2. WinDNMR-Pro
   www.chem.wisc.edu/areas/reich/plt/windnmr.htm
3. Spinworks (Mexico & DNMR3)
   home.cc.umanitoba.ca/~wolowiec/spinworks/
4. Topspin (DNMR) www.bruker.com

Other packages I know of:

1. iNMR www.inmr.net
2. SpinEvolution spinevolution.com
3. XNMR www.seimet.de/en/simulation.html

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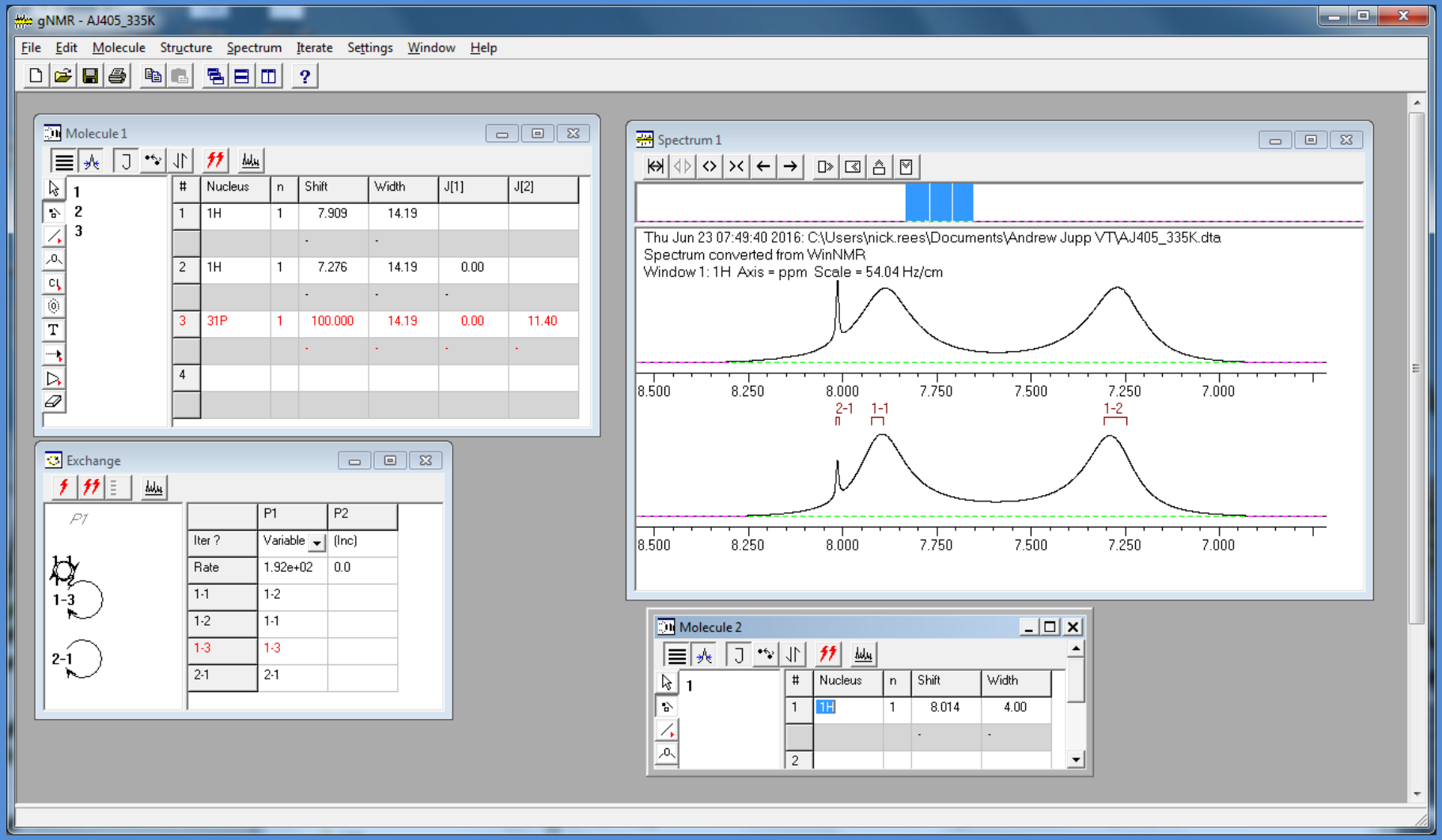
gNMR 2006



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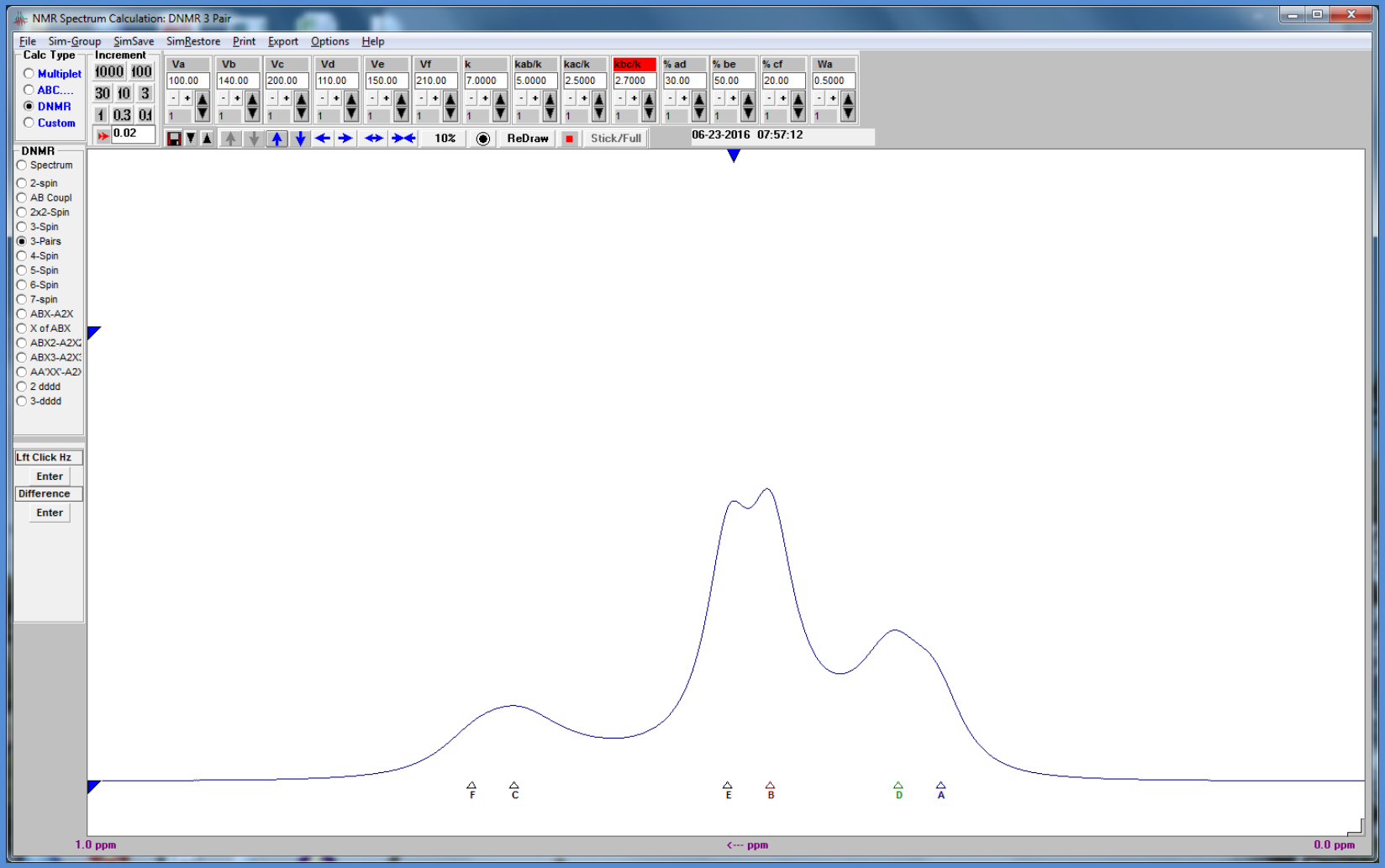
WinDNMR-Pro 2009



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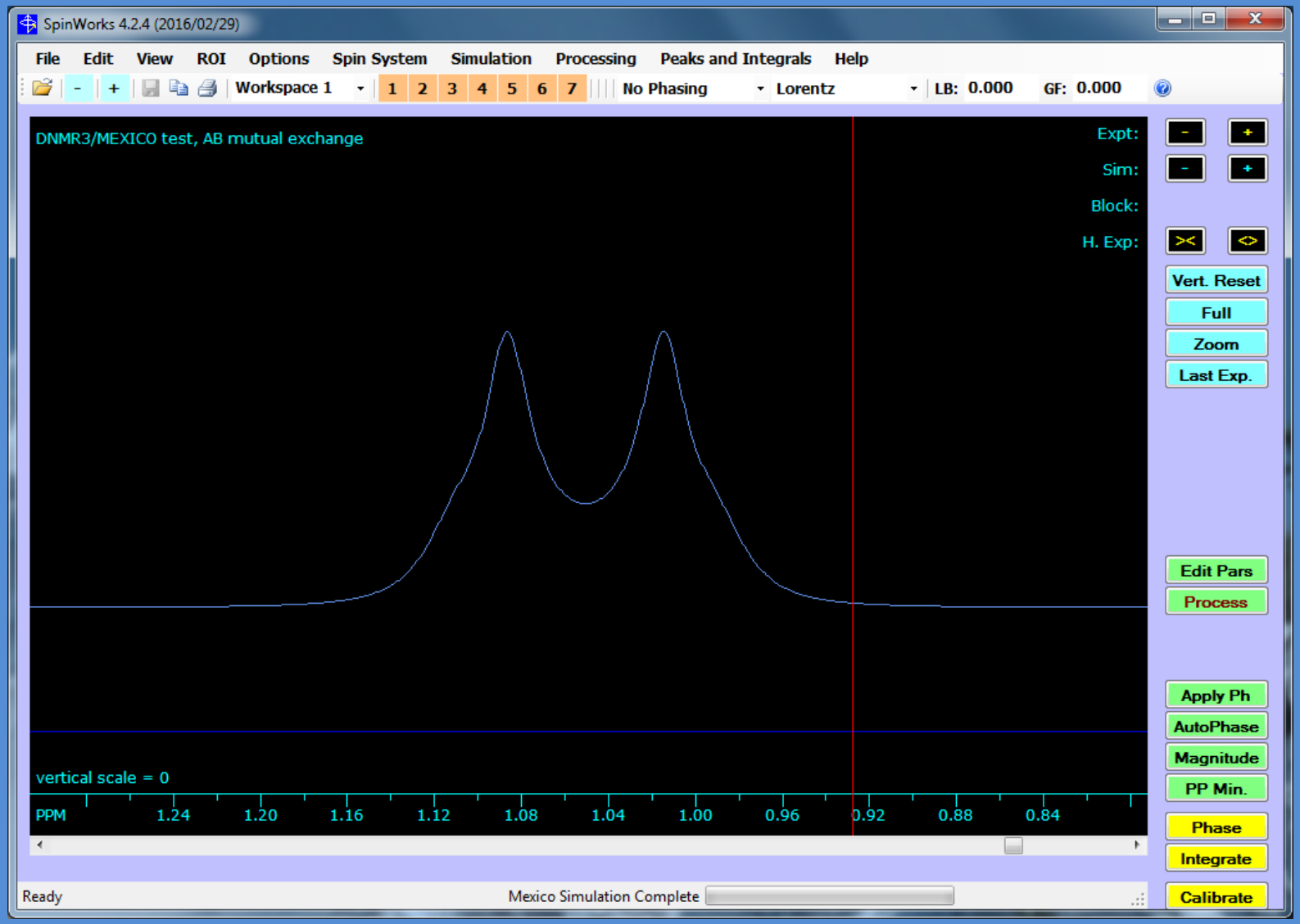
Spinwork (Mexico & DNMR3) 2016



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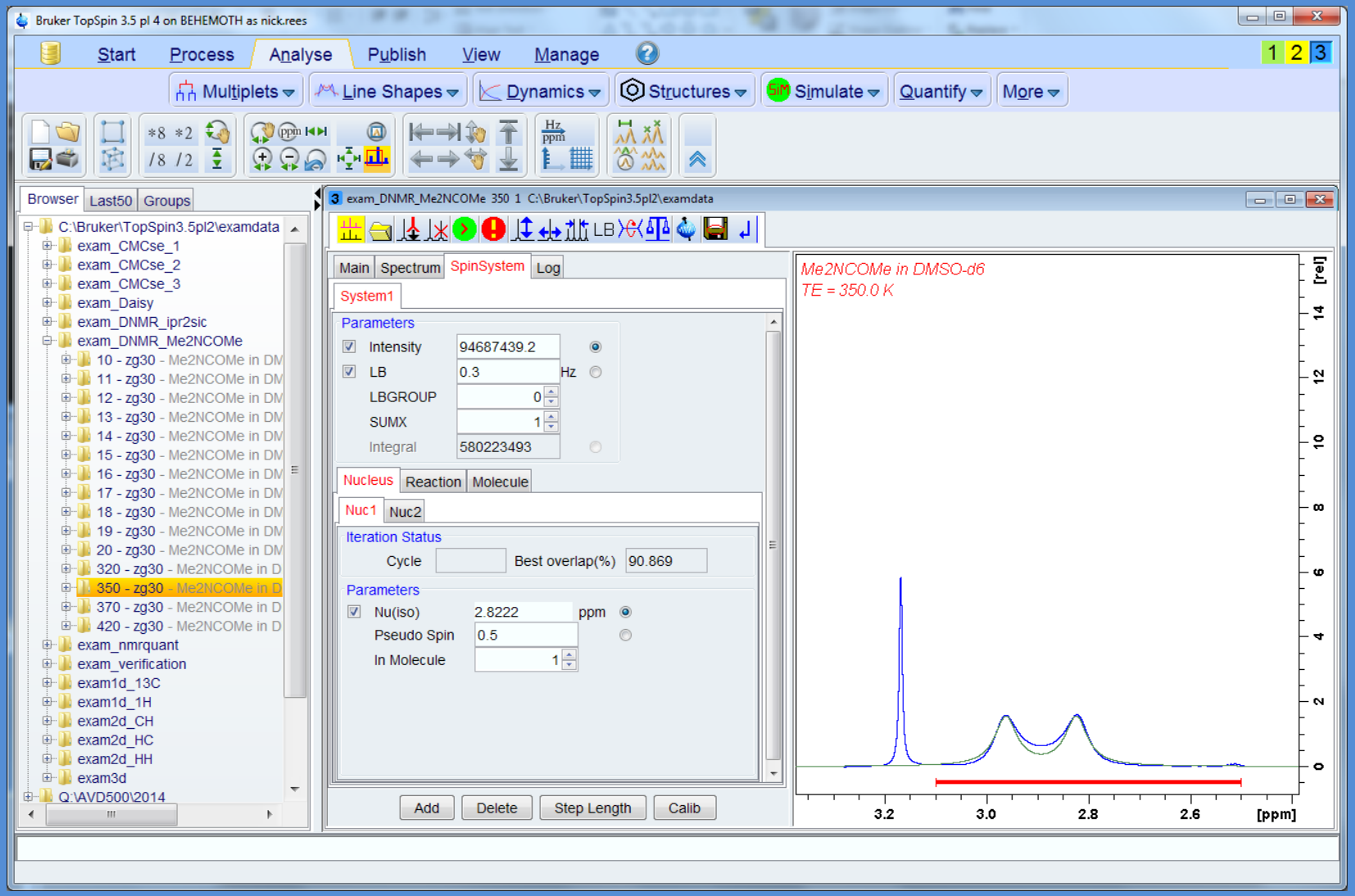
Topspin (DNMR) 2007



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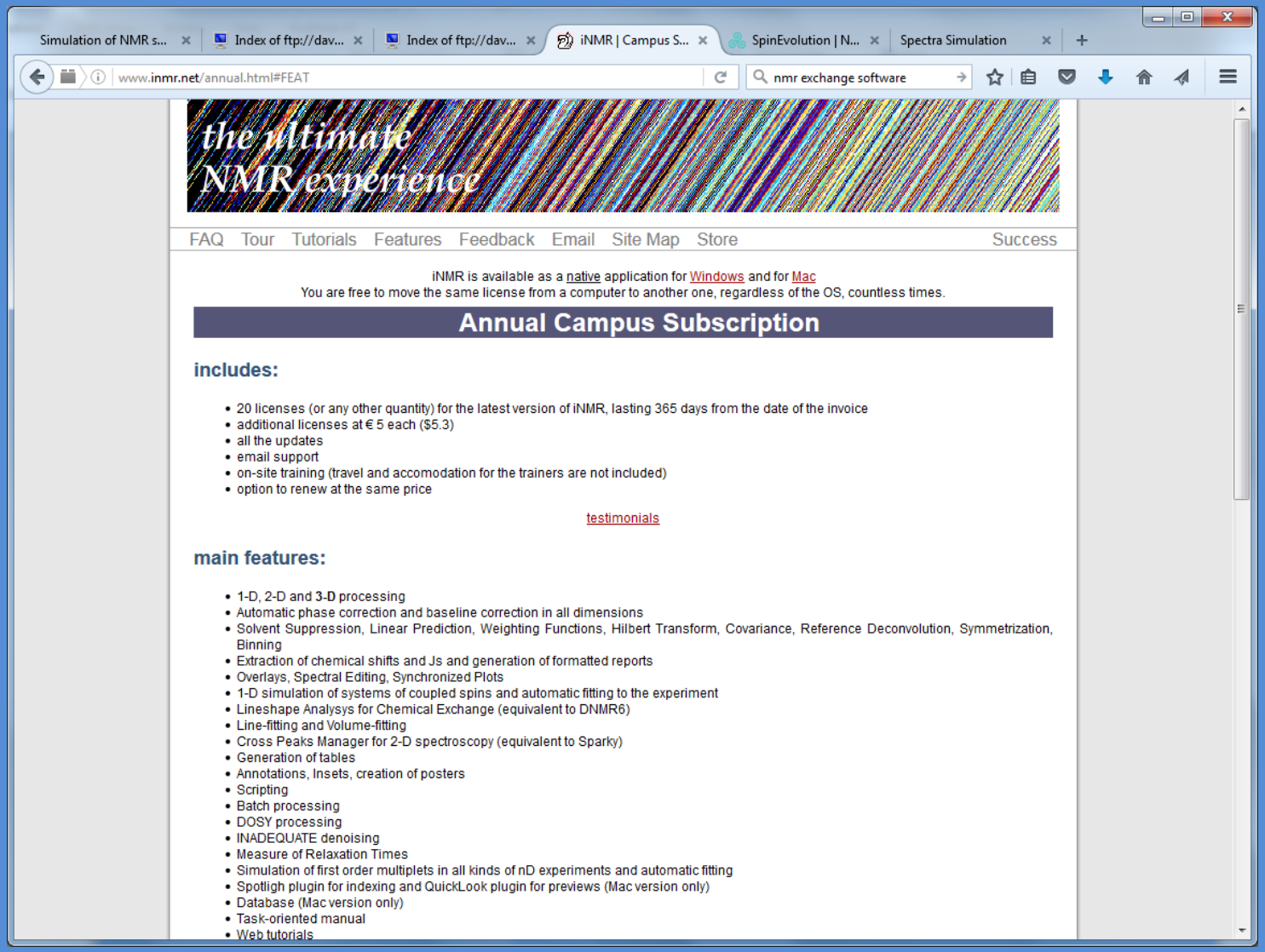
iNMR 2016



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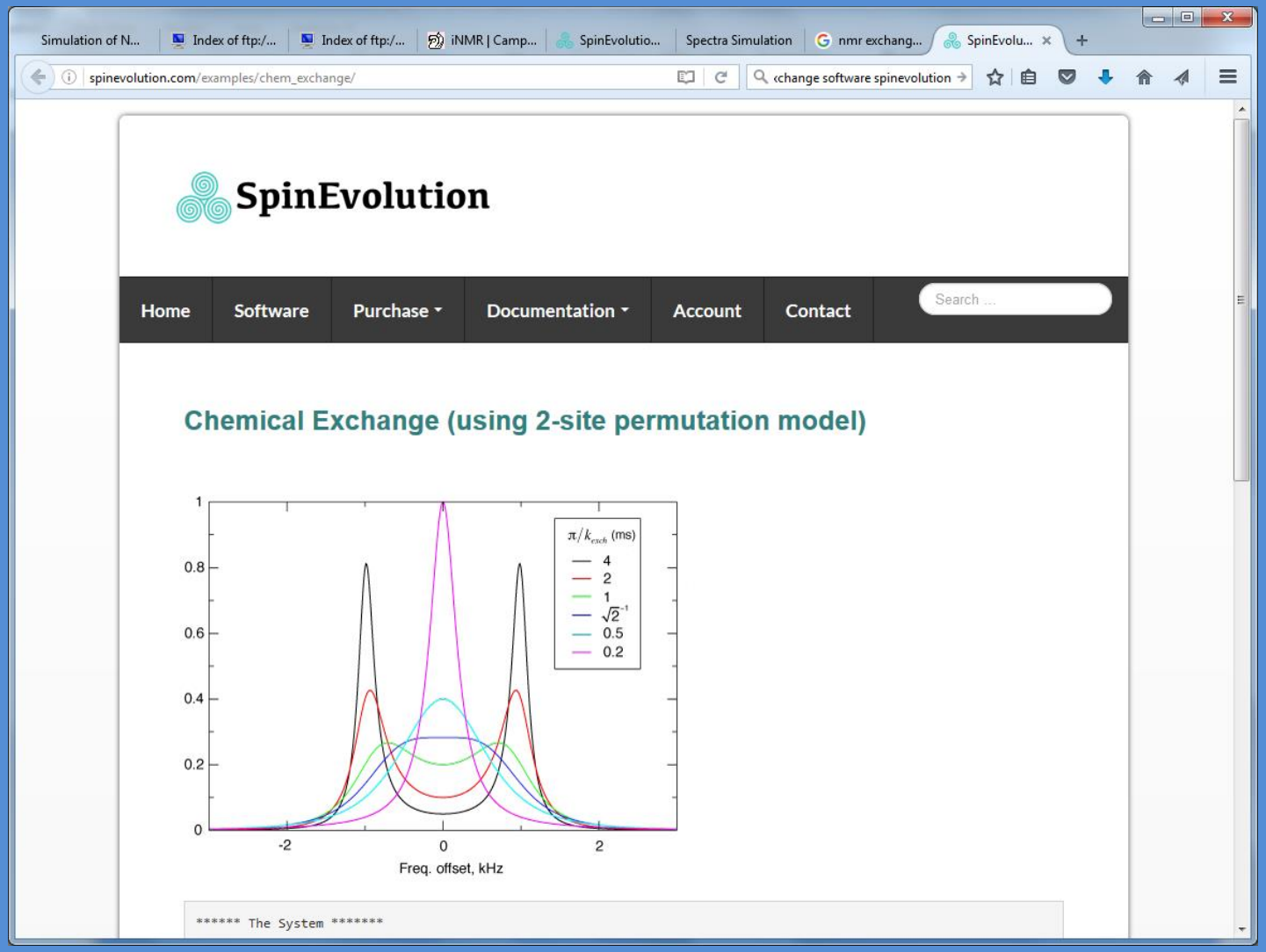
SpinEvolution 2016



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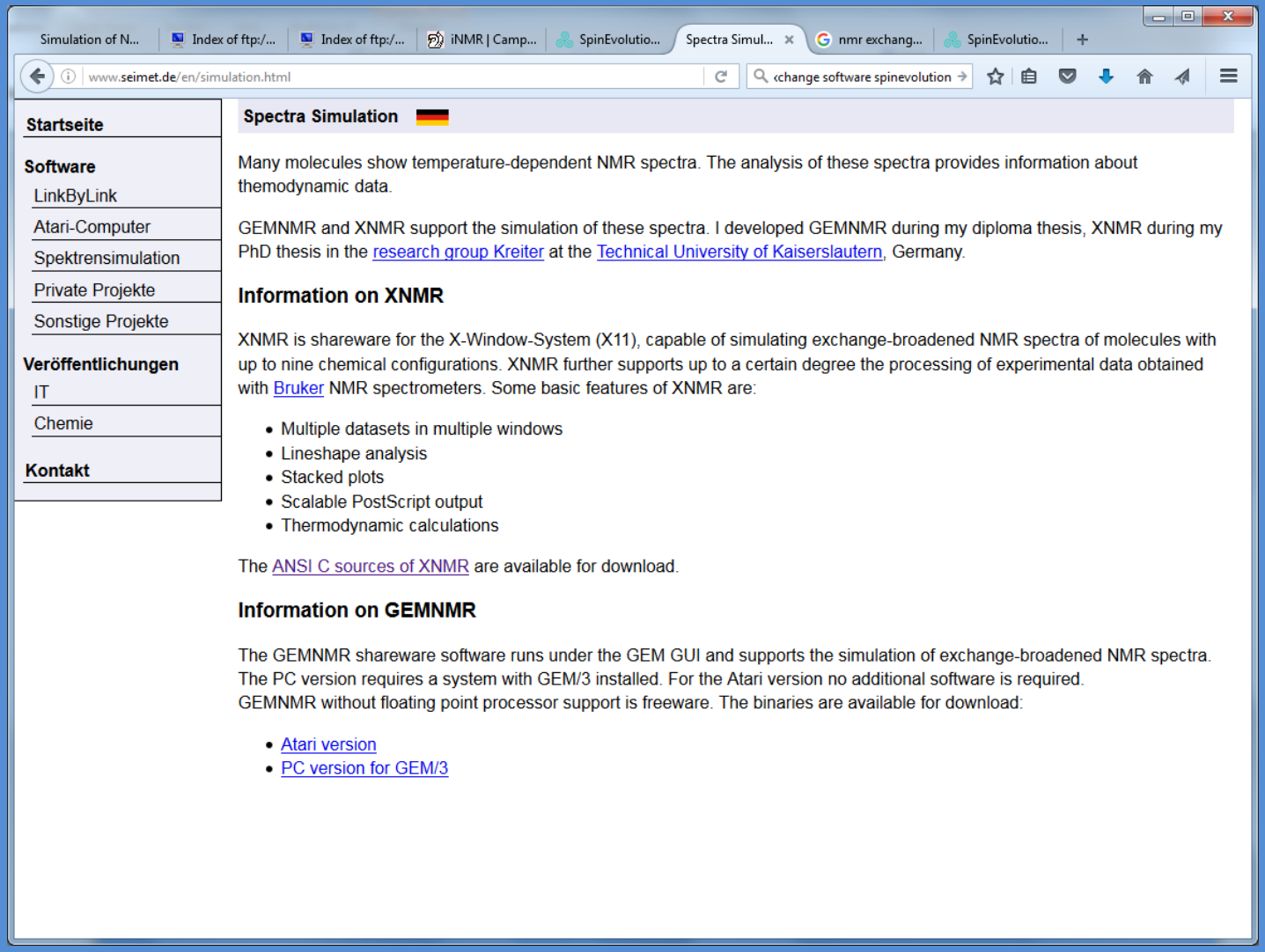
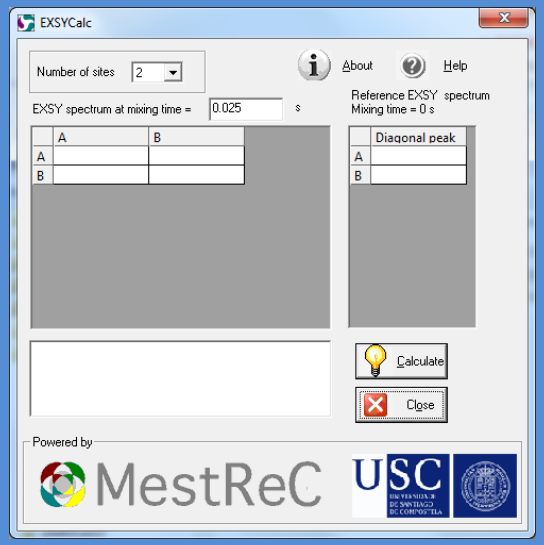
XNMR ?



Slow Exchange

- 2D-EXSY data analysis

  EXSYcalc mestrelab.com



- 1D-EXSY

1. selective inversion relaxation experiments CIFIT
   www.chemistry.mcmaster.ca/bain/
2. M. Teresa Quiro´s, Jesu´s Angulo and Marı´a Paz Mun˜oz. Chem. Commun., 2015, 51, 10222-10225. Kinetics of intramolecular chemical exchange by initial growth rates of spin saturation transfer difference experiments (SSTD NMR)