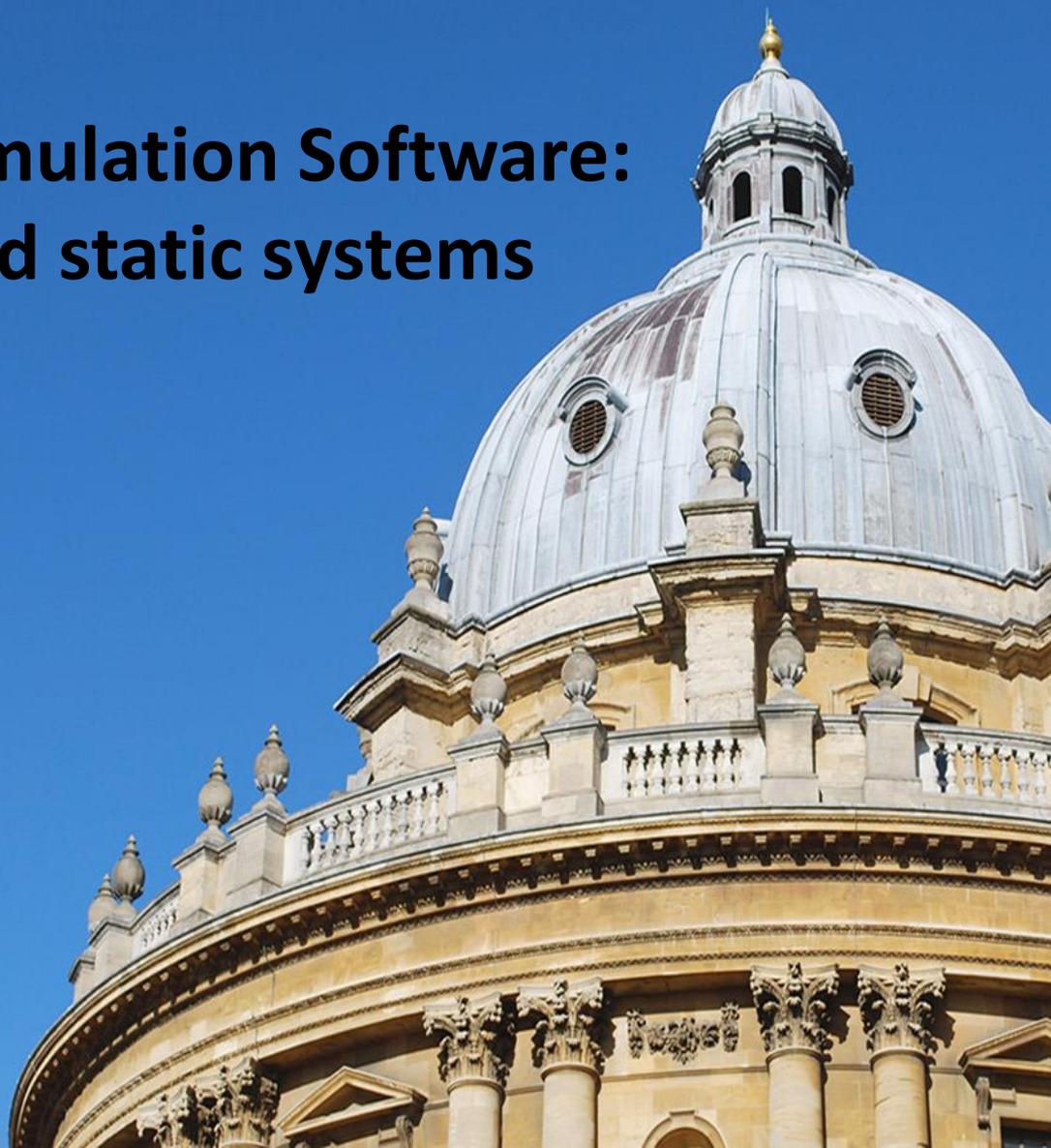


# NMR Spectrum Simulation Software: for dynamic and static systems

**Nick Rees**

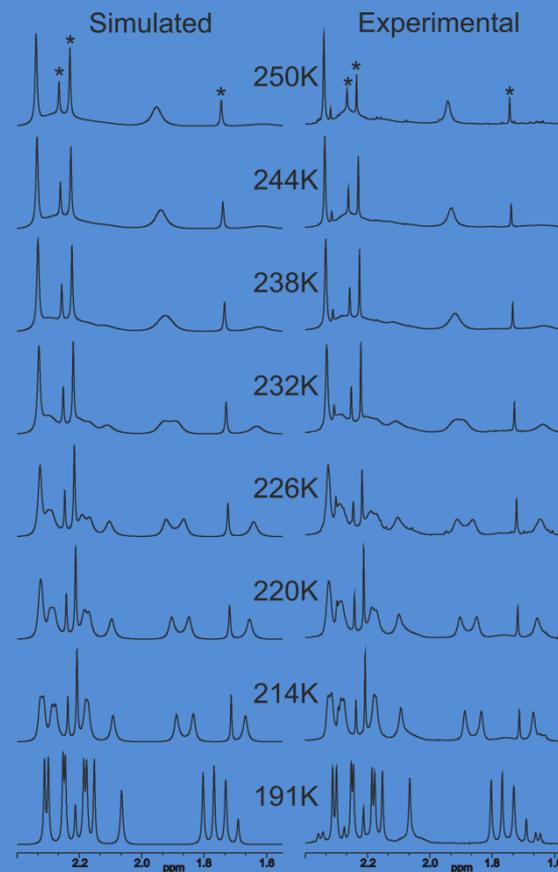


## Which computer programs:

- Simulate 1<sup>st</sup> and 2<sup>nd</sup> order NMR spectra based on input values of  $\delta$ , 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.

## 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?



## The packages I have used:

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

## Other packages I know of:

1. iNMR      [www.inmr.net](http://www.inmr.net)
2. SpinEvolution      [spinevolution.com](http://spinevolution.com)
3. XNMR      [www.seimet.de/en/simulation.html](http://www.seimet.de/en/simulation.html)

# gNMR 2006

gNMR - AJ405\_335K

File Edit Molecule Structure Spectrum Iterate Settings Window Help

Molecule 1

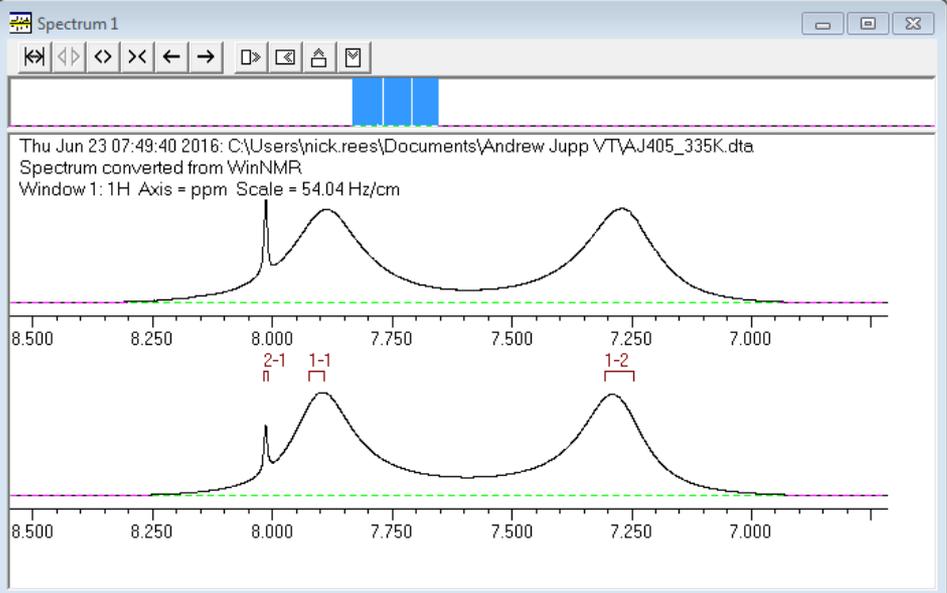
#	Nucleus	n	Shift	Width	J[1]	J[2]
1	1H	1	7.909	14.19		
2	1H	1	7.276	14.19	0.00	
3	31P	1	100.000	14.19	0.00	11.40
4						

Exchange

Iter ?	Variable (Inc)	P1	P2
Rate	1.92e+02	0.0	
1-1	1-2		
1-2	1-1		
1-3	1-3		
2-1	2-1		

Spectrum 1

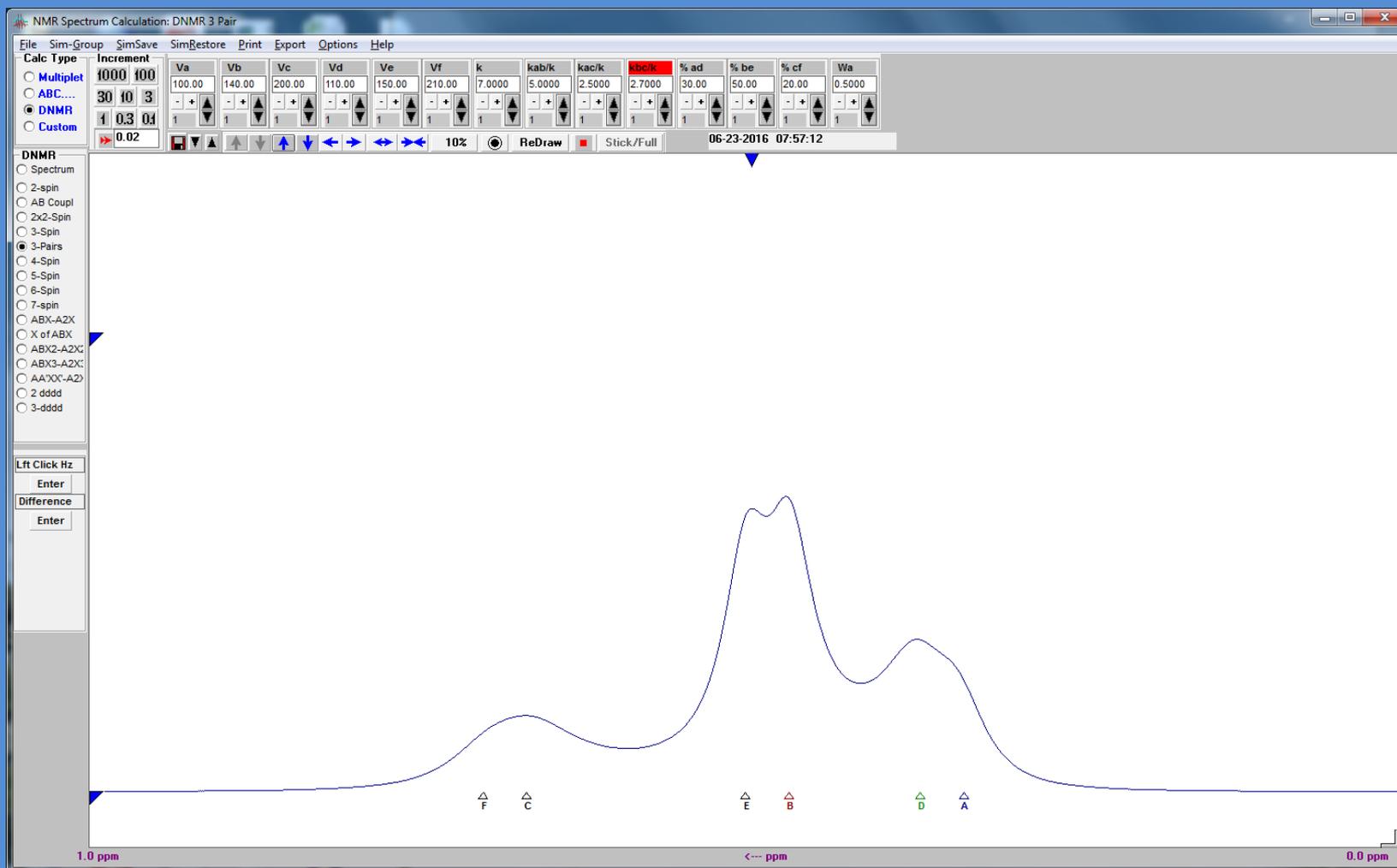
Thu Jun 23 07:49:40 2016: C:\Users\nick.rees\Documents\Andrew Jupp VT\AJ405\_335K.dta  
Spectrum converted from WinNMR  
Window 1: 1H Axis = ppm Scale = 54.04 Hz/cm



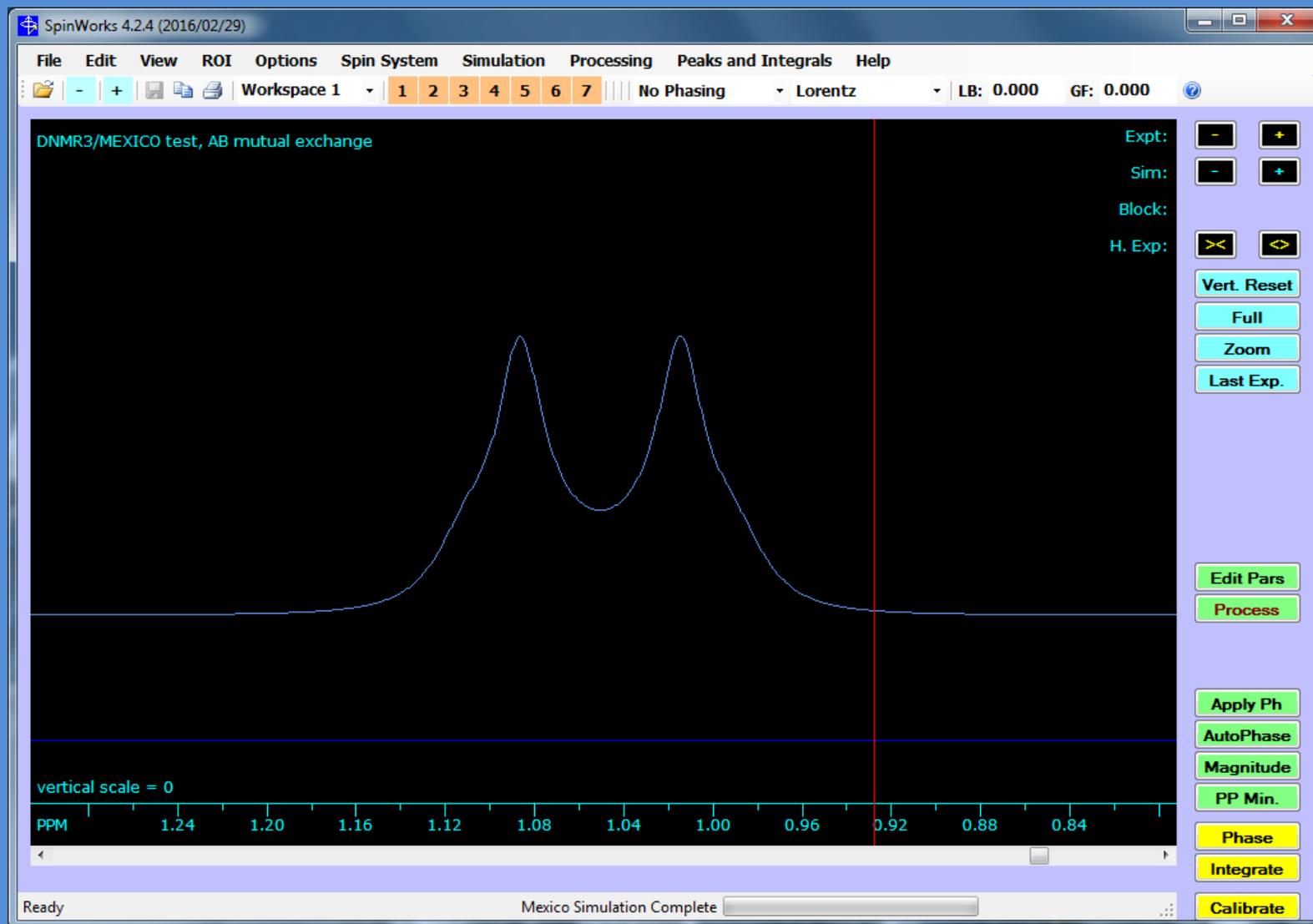
Molecule 2

#	Nucleus	n	Shift	Width
1	1H	1	8.014	4.00
2				

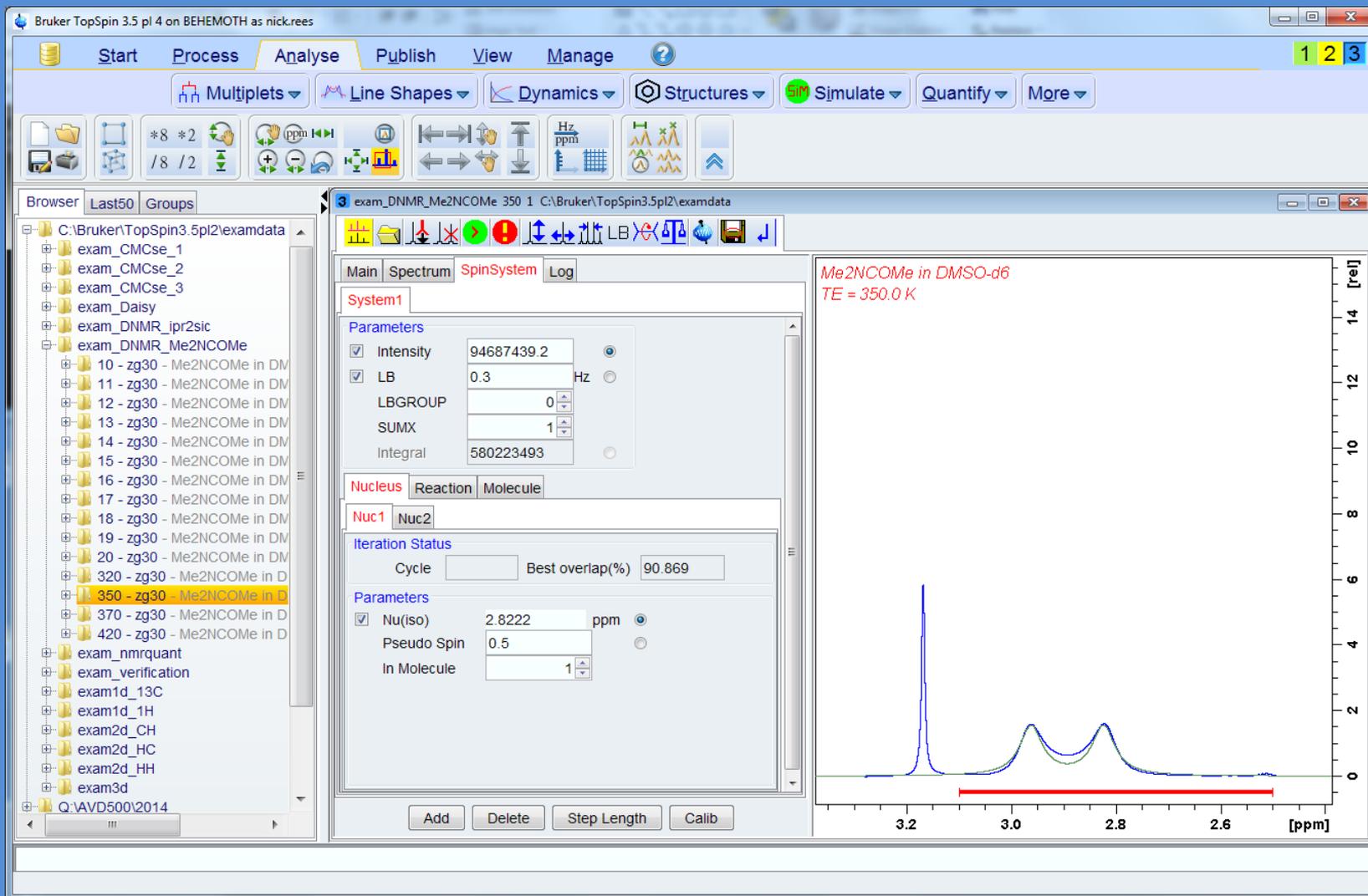
# WinDNMR-Pro 2009



# Spinwork (Mexico & DNMR3) 2016



# Topspin (DNMR) 2007



3 exam\_DNMR\_Me2NCOMe 350 1 C:\Bruker\TopSpin3.5pl2\examdata

Main | Spectrum | SpinSystem | Log

System1

Parameters

<input checked="" type="checkbox"/> Intensity	94687439.2	<input type="radio"/>
<input checked="" type="checkbox"/> LB	0.3	Hz <input type="radio"/>
LBGROUP	0	
SUMX	1	
Integral	580223493	<input type="radio"/>

Nucleus | Reaction | Molecule

Nuc1 | Nuc2

Iteration Status

Cycle		Best overlap(%)	90.869
-------	--	-----------------	--------

Parameters

<input checked="" type="checkbox"/> Nu(iso)	2.8222	ppm <input type="radio"/>
Pseudo Spin	0.5	<input type="radio"/>
In Molecule	1	

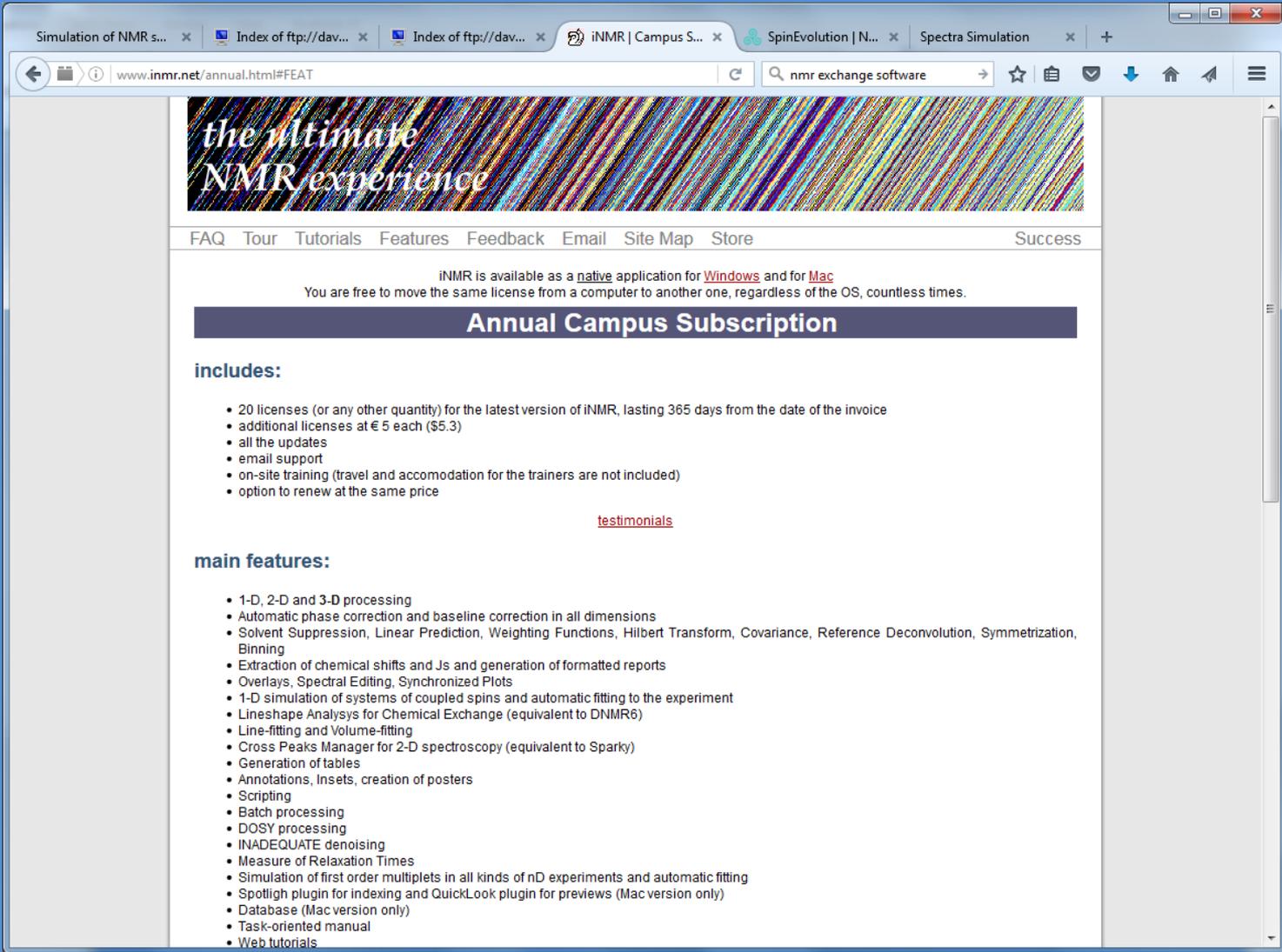
Add | Delete | Step Length | Calib

Me2NCOMe in DMSO-d6  
TE = 350.0 K

3.2 3.0 2.8 2.6 [ppm]

14 [rel]

# iNMR 2016



Simulation of NMR s... x Index of ftp://dav... x Index of ftp://dav... x iNMR | Campus S... x SpinEvolution | N... x Spectra Simulation x +

www.inmr.net/annual.html#FEAT

nmr exchange software

*the ultimate NMR experience*

FAQ Tour Tutorials Features Feedback Email Site Map Store Success

iNMR is available as a [native](#) application for [Windows](#) and for [Mac](#).  
You are free to move the same license from a computer to another one, regardless of the OS, countless times.

## Annual Campus Subscription

**includes:**

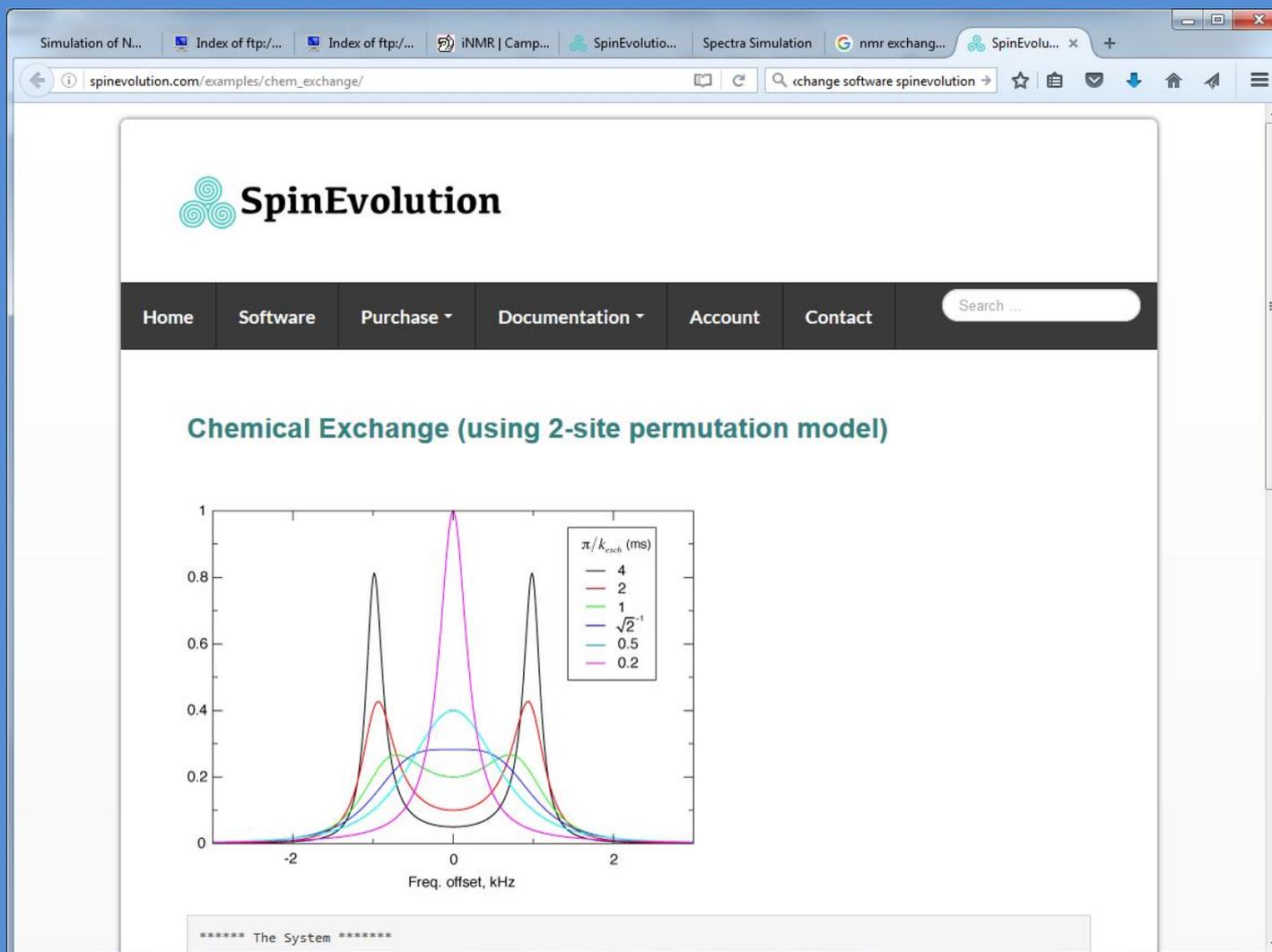
- 20 licenses (or any other quantity) for the latest version of iNMR, lasting 365 days from the date of the invoice
- additional licenses at € 5 each (\$5.3)
- all the updates
- email support
- on-site training (travel and accommodation for the trainers are not included)
- option to renew at the same price

[testimonials](#)

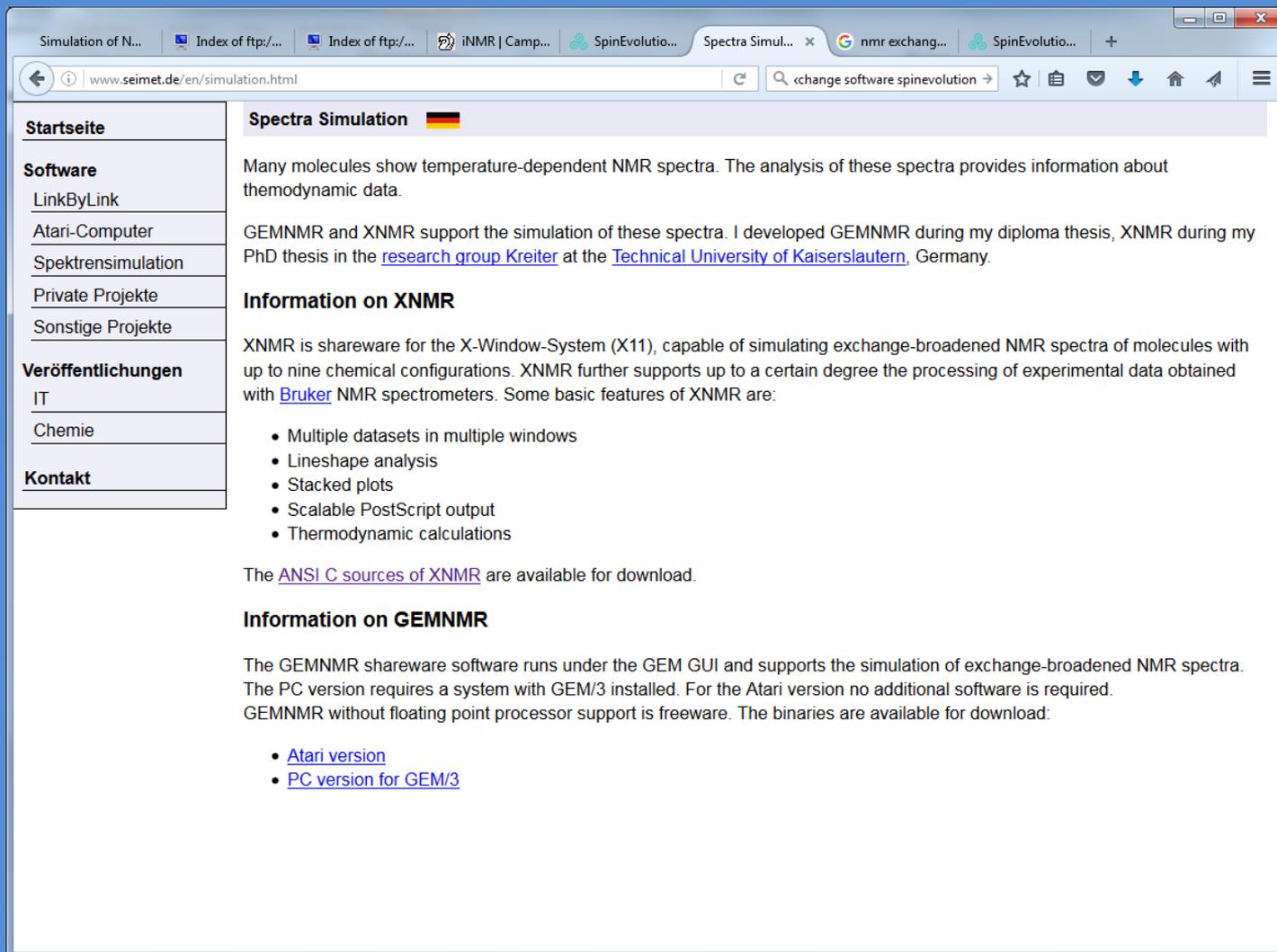
**main features:**

- 1-D, 2-D and 3-D processing
- Automatic phase correction and baseline correction in all dimensions
- Solvent Suppression, Linear Prediction, Weighting Functions, Hilbert Transform, Covariance, Reference Deconvolution, Symmetrization, Binning
- Extraction of chemical shifts and Js and generation of formatted reports
- Overlays, Spectral Editing, Synchronized Plots
- 1-D simulation of systems of coupled spins and automatic fitting to the experiment
- Lineshape Analysis for Chemical Exchange (equivalent to DNMR6)
- Line-fitting and Volume-fitting
- Cross Peaks Manager for 2-D spectroscopy (equivalent to Sparky)
- Generation of tables
- Annotations, Insets, creation of posters
- Scripting
- Batch processing
- DOSY processing
- INADEQUATE denoising
- Measure of Relaxation Times
- Simulation of first order multiplets in all kinds of nD experiments and automatic fitting
- Spotlight plugin for indexing and QuickLook plugin for previews (Mac version only)
- Database (Mac version only)
- Task-oriented manual
- Web tutorials

# SpinEvolution 2016



# XNMR ?



Simulation of N... Index of ftp/... Index of ftp/... iNMR | Camp... SpinEvolutio... Spectra Simul... x nmr exchang... SpinEvolutio... +

www.seimet.de/en/simulation.html

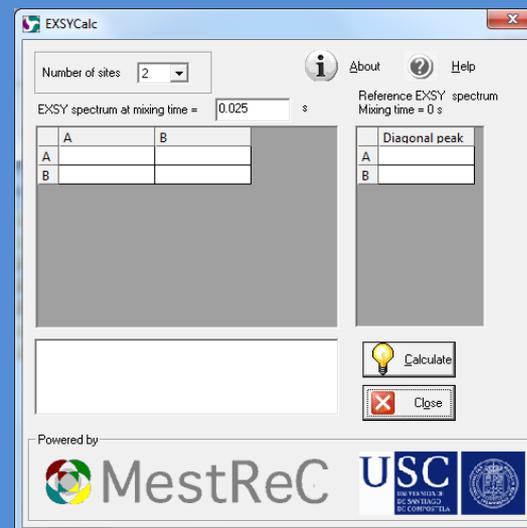
← xchange software spinevolution → ☆ 📁 📧 🏠 🔍 ☰

<b>Startseite</b>	<b>Spectra Simulation</b> 
<b>Software</b>	Many molecules show temperature-dependent NMR spectra. The analysis of these spectra provides information about thermodynamic data.
LinkByLink	
Atari-Computer	GEMNMR and XNMR support the simulation of these spectra. I developed GEMNMR during my diploma thesis, XNMR during my PhD thesis in the <a href="#">research group Kreiter</a> at the <a href="#">Technical University of Kaiserslautern</a> , Germany.
Spektrensimulation	
Private Projekte	
Sonstige Projekte	
<b>Veröffentlichungen</b>	<b>Information on XNMR</b>
IT	XNMR is shareware for the X-Window-System (X11), capable of simulating exchange-broadened NMR spectra of molecules with up to nine chemical configurations. XNMR further supports up to a certain degree the processing of experimental data obtained with <a href="#">Bruker</a> NMR spectrometers. Some basic features of XNMR are:
Chemie	<ul style="list-style-type: none"><li>• Multiple datasets in multiple windows</li><li>• Lineshape analysis</li><li>• Stacked plots</li><li>• Scalable PostScript output</li><li>• Thermodynamic calculations</li></ul>
<b>Kontakt</b>	The <a href="#">ANSI C sources of XNMR</a> are available for download.
	<b>Information on GEMNMR</b>
	The GEMNMR shareware software runs under the GEM GUI and supports the simulation of exchange-broadened NMR spectra. The PC version requires a system with GEM/3 installed. For the Atari version no additional software is required. GEMNMR without floating point processor support is freeware. The binaries are available for download:
	<ul style="list-style-type: none"><li>• <a href="#">Atari version</a></li><li>• <a href="#">PC version for GEM/3</a></li></ul>

# Slow Exchange

- 2D-EXSY data analysis

EXSYcalc [mestrelab.com](http://mestrelab.com)



- 1D-EXSY

1. selective inversion relaxation experiments CIFIT

[www.chemistry.mcmaster.ca/bain/](http://www.chemistry.mcmaster.ca/bain/)

2. M. Teresa Quiro's, Jesu's Angulo and Mari'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)