

NMR Spectrum Simulation Software: for dynamic and static systems

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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.



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

- 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



gNMR 2006

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Department of Chemistry



WinDNMR-Pro 2009





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?

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Startseite	Spectra Simulation				
Software LinkByLink	Many molecules show temperature-dependent NMR spectra. The analysis of these spectra provides information about themodynamic data.				
Atari-Computer Spektrensimulation	GEMNMR and XNMR support the simulation of these spectra. I developed GEMNMR during my diploma thesis, XNMR during my PhD thesis in the <u>research group Kreiter</u> at the <u>Technical University of Kaiserslautern</u> , Germany.				
Private Projekte	Information on XNMR				
Sonstige Projekte	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				
<u>IT</u>	with Bruker NMR spectrometers. Some basic features of XNMR are:				
Chemie	Multiple datasets in multiple windows				
Kontakt	Lineshape analysis Stacked plots Scalable PostScript output Thermodynamic calculations				
	The ANSI C sources of XNMR are available for download.				
	Information on GEMNMR				
	The CENNIND elegences offluers runs under the CEN CLIL and supports the simulation of eveloping breadened NND exects				

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:

- <u>Atari version</u>
- PC version for GEM/3



Slow Exchange

• 2D-EXSY data analysis EXSYcalc mestrelab.com

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EXSY spectrum at mixing time = 0.025 s	Reference EXSY spectrum Mixing time = 0 s
A B A B	Diagonal peak A B
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- 1D-EXSY
- 1. selective inversion relaxation experiments CIFIT <u>www.chemistry.mcmaster.ca/bain/</u>
- M. Teresa Quiro's, Jesu's Angulo and Mari 'a Paz Mun^ooz. Chem. Commun., 2015, 51, 10222-10225. Kinetics of intramolecular chemical exchange by initial growth rates of spin saturation transfer difference experiments (SSTD NMR)