

SpinWorks Installation Guide

SpinWorks is buggy and inconsistent but is the only free program that has DNMR3. This installation guide is based on having Windows 7 64 bit OS but should work on other Windows versions.

- Download SpinWorks 3.1.8.1 from the link at <http://home.cc.umanitoba.ca/~wolowiec/spinworks/>
- Unzip and run setup. Use the default location and confirm that the program installed correctly if asked. You can then delete installation programs.
- Run SpinWorks and agree to create c:\Temp if asked.
- Open Edit -> Edit Start-up Options and change External Module Path to "C:\Program Files (x86)\SpinWorks_3" then click OK.

To test DNMR3 and familiarize yourself with its operation set up and run an AB<>BA mutual exchange simulation:

- Set Simulation -> Simulation Mode to DNMR3/Mexico
- Open Spin System -> Edit Chemical Shifts...

Set Group 1 fields to: 1 a H 1/2 500

and Group 2 fields to: 1 b H 1/2 550

NOTE: You must use Hz for the shift option, ppm works for NUMMRIT but does not work for DNMR3. If you use ppm to enter shifts, you need to click on Hz to convert shifts to Hz before run DNMR3 simulation.

- Open Spin System -> Edit Scalar (J) Couplings...

Set the one listed value to J(1,2)

- Open Spin System -> Edit Simulation Options and DNMR Parameters

Set RC(1,2) to 5 (this is confusingly k(1,2) in other parts of the program)

Set the first 2 fields of Permutation Vector 2 to: 2 1

Mutual Exchange should be checked, no need to set Population of Sites for mutual exchange.

- To run DNMR3 simulations

Click Simulation -> Run DNMR3 Simulation (or, click on Simulate button at far lower right then click on DNMR3 in popup window).

- After confirming that you see a simulated AB pattern, change the rate constant from 5 to 20 and observe that the lines broaden. Then try 50, 100, 500 and 1000 to observe coalescence into a singlet.

This value is RC(1,2) in Spin System -> Edit Simulation Options and DNMR Parameters, OR k(1,2) in the Simulate popup window.