



EPR

SpinFit Liquids

Simulating and fitting CW-EPR spectra of liquid samples

Innovation with Integrity

Introduction

SpinFit Liquids is a spectral simulation and fitting program for CW-EPR spectra of radicals in solution. SpinFit Liquids makes species identification easy by fitting a narrow set of parameters to the raw data with minimal input from the user. SpinFit Liquids comes with an extensive library of common radical spectra with corresponding fit parameters to allow for quick and easy identification. In liquids, the paramagnetic species are tumbling with a rate that depends on the viscosity of the solvent or the size of the species. The tumbling rate, i.e. rotational motion, determines the dynamic regime of the observed CW-EPR spectra. Simulations of spectra in different dynamic regimes require different theoretical descriptions that are available in SpinFit Liquids.

Bruker has brought ease-of-use and convenience to EPR with the patented SpinFit and SpinCount package that come standard with all Bruker EPR spectrometers using Xenon and Xepr and is optional with ESRStudio software. Samples can be accurately characterized without comparison to standard samples or separately measured calibration curves. With this, Bruker provides a simple and reliable solution that can be applied to a wide variety of scientific studies or process/quality control.

Features

- Simulation and fitting of radicals and transition metal species in liquid state
- An easy-to-use interface
- Spectra library of common species for radical identification
- Identification and quantification of individual species in complex mixtures
- Support of 1D- and 2D-datasets
- Automatic choice of dynamic regime
- Conveniently interfaced with SpinCount
- Incorporated into the spectrometer control software so researchers can quickly and easily identify paramagnetic species immediately after data collection

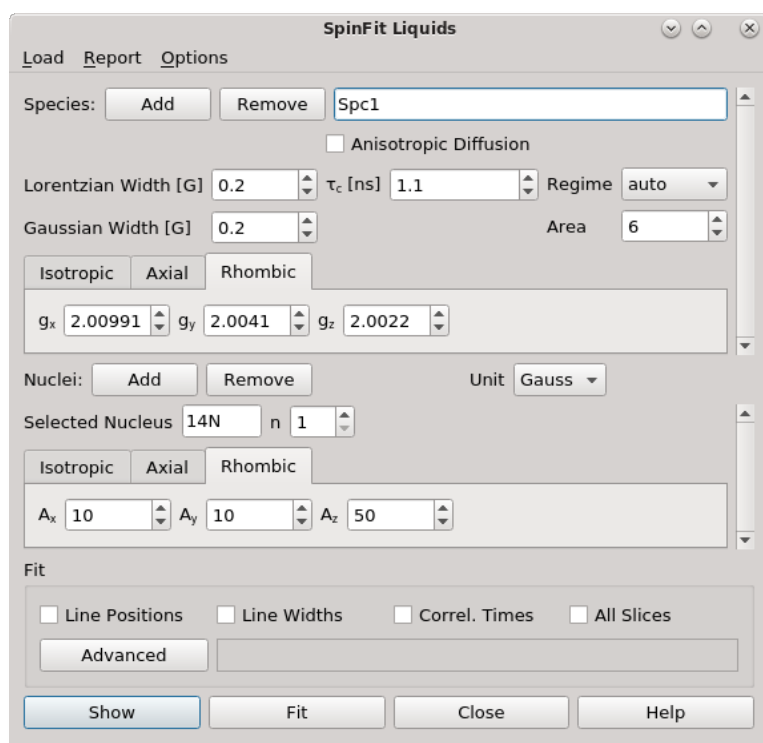


Figure 1

SpinFit Liquids User Interface

- Automatic or manual choice of dynamic regime
- Easy and precise simulation and fitting of spectra under different motional dynamic regimes

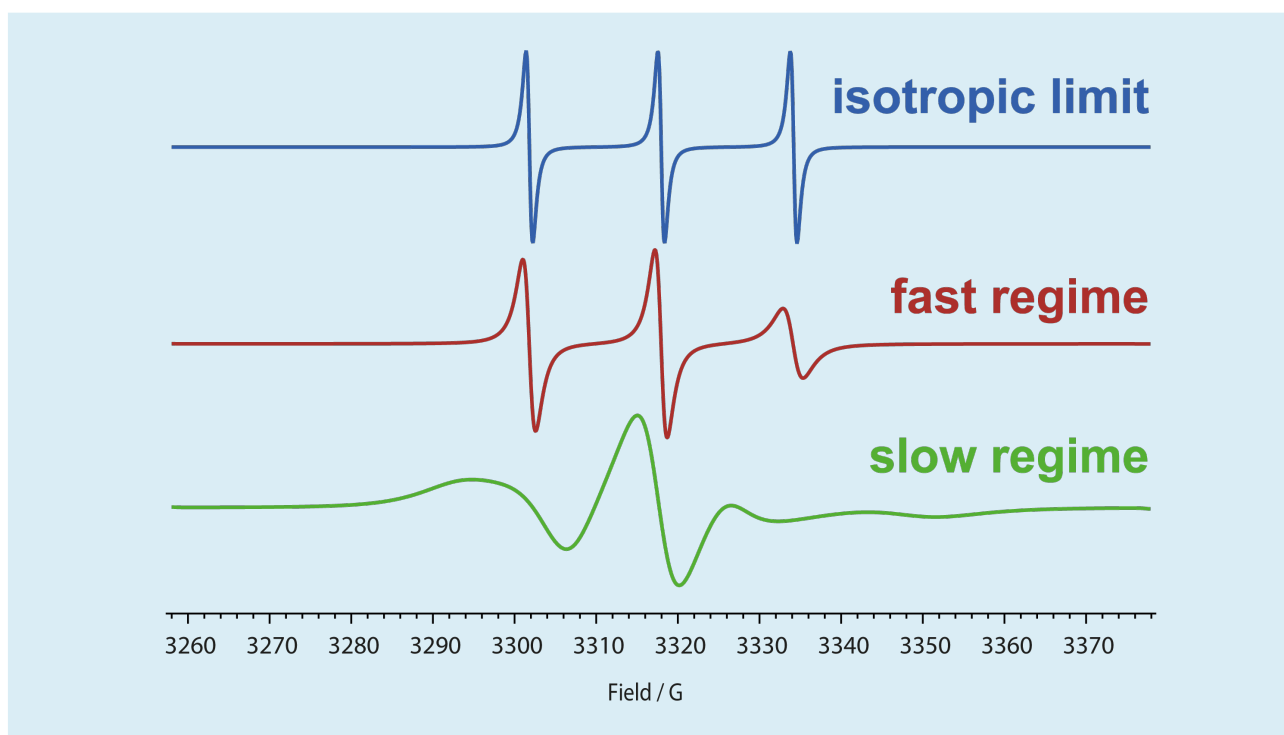


Figure 2

Nitroxide spectra under several dynamic regimes

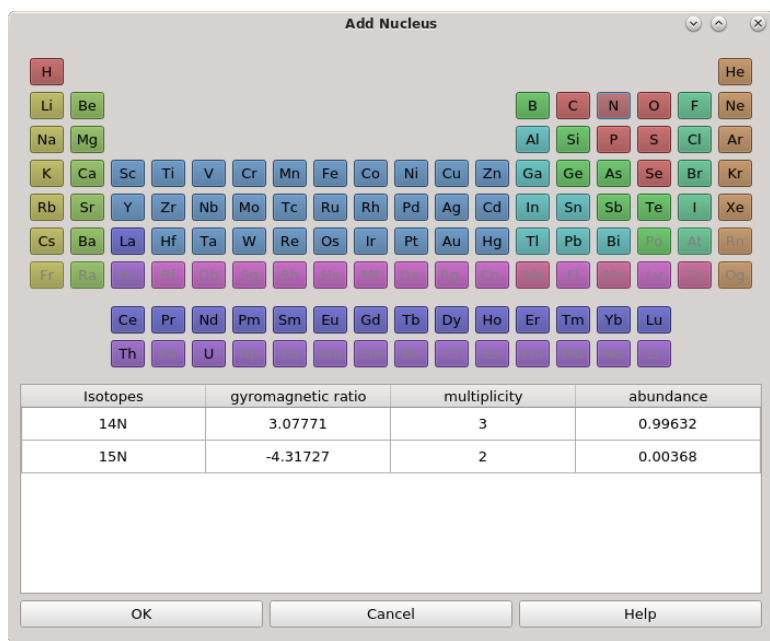


Figure 3
User friendly interface to select atoms and their isotopes from the periodic table of elements

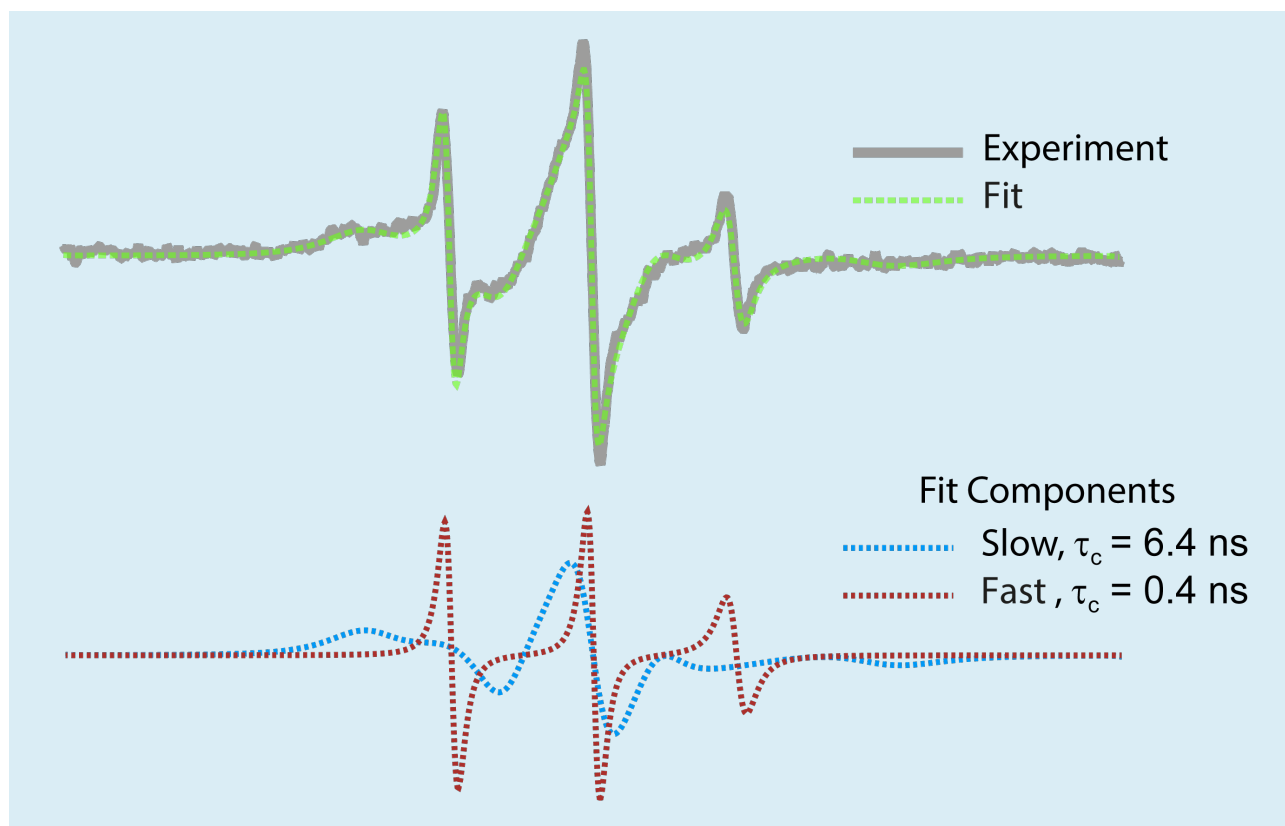
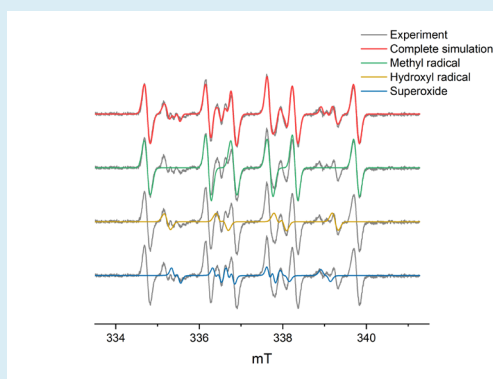


Figure 4

Two-component spectra of spin-labeled protein

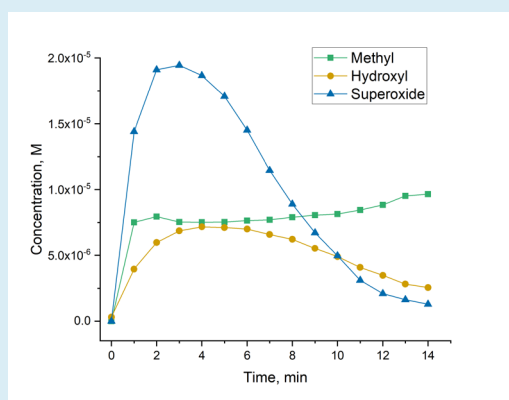
- Resolving and identifying multiple components and species
- Fitting of the rotational correlation time to gain insight into motional dynamics
- Determining labelling efficiency by combining SpinFit Liquids with the SpinCount module

SpinCount Report



Fit and Calculate

A	B	C	D	E	F	G
Data name	Time [s]	Height [mm]	Diameter [mm]	Volume [ml]	Spins	Spin conc. [M]
1 TiO2_kinetics_full_13_001_fit Methyl	0	23	0.94	0.01596149	1.50E+26	15572192.21
3 TiO2_kinetics_full_13_002_fit Methyl	60.003009	23	0.94	0.01596149	7.2147E+13	7.51E-06
4 TiO2_kinetics_full_13_003_fit Methyl	120.00404	23	0.94	0.01596149	7.6313E+13	7.94E-06
5 TiO2_kinetics_full_13_004_fit Methyl	180.01358	23	0.94	0.01596149	7.2381E+13	7.53E-06
6 TiO2_kinetics_full_13_005_fit Methyl	240.01271	23	0.94	0.01596149	7.2324E+13	7.52E-06
7 TiO2_kinetics_full_13_006_fit Methyl	300.01222	23	0.94	0.01596149	7.2418E+13	7.53E-06
8 TiO2_kinetics_full_13_007_fit Methyl	360.00496	23	0.94	0.01596149	7.3416E+13	7.44E-06
9 TiO2_kinetics_full_13_008_fit Methyl	419.99944	23	0.94	0.01596149	7.4044E+13	7.70E-06
10 TiO2_kinetics_full_13_009_fit Methyl	480.01144	23	0.94	0.01596149	7.5848E+13	7.89E-06
11 TiO2_kinetics_full_13_010_fit Methyl	540.00394	23	0.94	0.01596149	7.7472E+13	8.06E-06
12 TiO2_kinetics_full_13_011_fit Methyl	600.00085	23	0.94	0.01596149	7.8288E+13	8.14E-06
13 TiO2_kinetics_full_13_012_fit Methyl	660.00474	23	0.94	0.01596149	8.1133E+13	8.44E-06
14 TiO2_kinetics_full_13_013_fit Methyl	720.00093	23	0.94	0.01596149	8.4881E+13	8.83E-06
15 TiO2_kinetics_full_13_014_fit Methyl	780.01355	23	0.94	0.01596149	9.1431E+13	9.51E-06
16 TiO2_kinetics_full_13_015_fit Methyl	840.00539	23	0.94	0.01596149	9.2791E+13	9.65E-06
17 TiO2_kinetics_full_13_001_fit Hydroxyl	0	23	0.94	0.01596149	3.0077E+12	3.13E-07
18 TiO2_kinetics_full_13_002_fit Hydroxyl	60.003009	23	0.94	0.01596149	3.7995E+13	3.95E-06
19 TiO2_kinetics_full_13_003_fit Hydroxyl	120.00404	23	0.94	0.01596149	5.7467E+13	5.98E-06
20 TiO2_kinetics_full_13_004_fit Hydroxyl	180.01358	23	0.94	0.01596149	6.5967E+13	6.86E-06
21 TiO2_kinetics_full_13_005_fit Hydroxyl	240.01271	23	0.94	0.01596149	6.8886E+13	7.17E-06
22 TiO2_kinetics_full_13_006_fit Hydroxyl	300.01222	23	0.94	0.01596149	6.8402E+13	7.12E-06
23 TiO2_kinetics_full_13_007_fit Hydroxyl	360.00496	23	0.94	0.01596149	6.7281E+13	7.00E-06
24 TiO2_kinetics_full_13_008_fit Hydroxyl	419.99944	23	0.94	0.01596149	6.3321E+13	6.59E-06
25 TiO2_kinetics_full_13_009_fit Hydroxyl	480.01144	23	0.94	0.01596149	5.9793E+13	6.22E-06
26 TiO2_kinetics_full_13_010_fit Hydroxyl	540.00394	23	0.94	0.01596149	5.3118E+13	5.53E-06
27 TiO2_kinetics_full_13_011_fit Hydroxyl	600.00085	23	0.94	0.01596149	4.7125E+13	4.90E-06
28 TiO2_kinetics_full_13_012_fit Hydroxyl	660.00474	23	0.94	0.01596149	3.9177E+13	4.08E-06
29 TiO2_kinetics_full_13_013_fit Hydroxyl	720.00093	23	0.94	0.01596149	3.3401E+13	3.48E-06
30 TiO2_kinetics_full_13_014_fit Superoxide	780.01355	23	0.94	0.01596149	3.7801E+13	3.91E-06



Plot

Figure 5

Multi-component spectrum with a mixture of three spin-trapped radicals

- A library of commonly encountered radical species to facilitate analysis
- Support for 1D and 2D datasets
- Deconvolution of overlapping spectra to measure individual concentrations
- Quantitative analysis with high precision, even with low signal-to-noise

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Customer Support
<https://www.bruker.com/en/services/support.html>

Online information
bruker.com/

