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 fittting 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

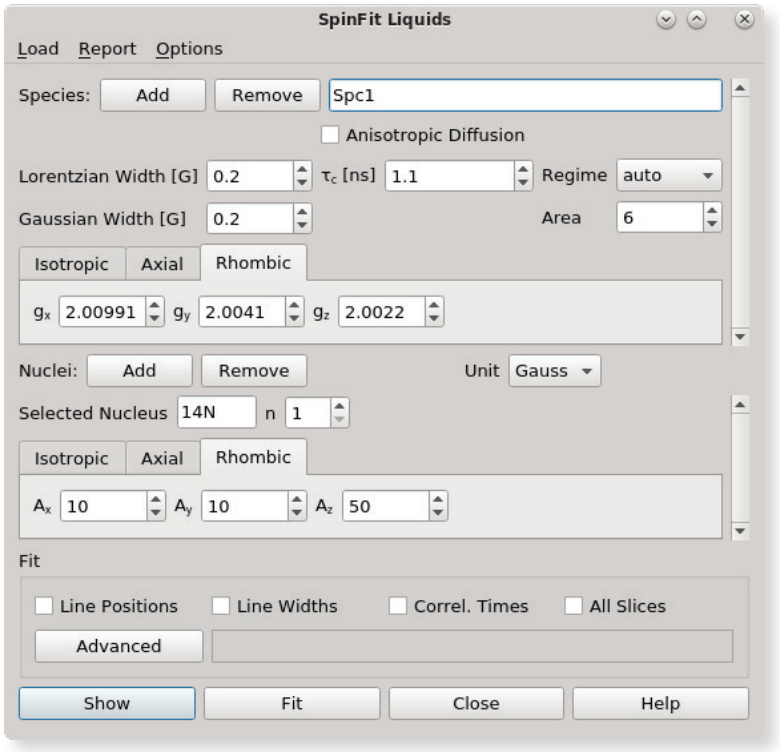

Figure 1
SpinFit Liquids User Interface

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

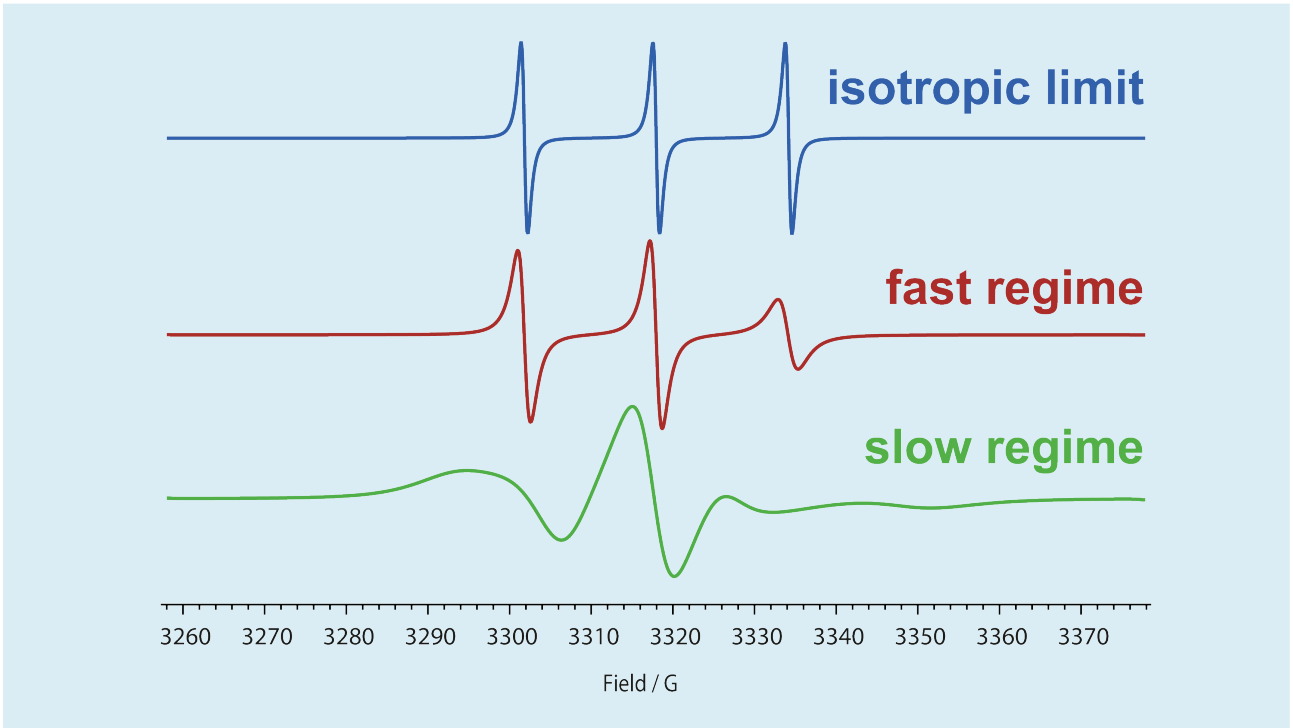

Figure 2
Nitroxide spectra under several dynamic regimes

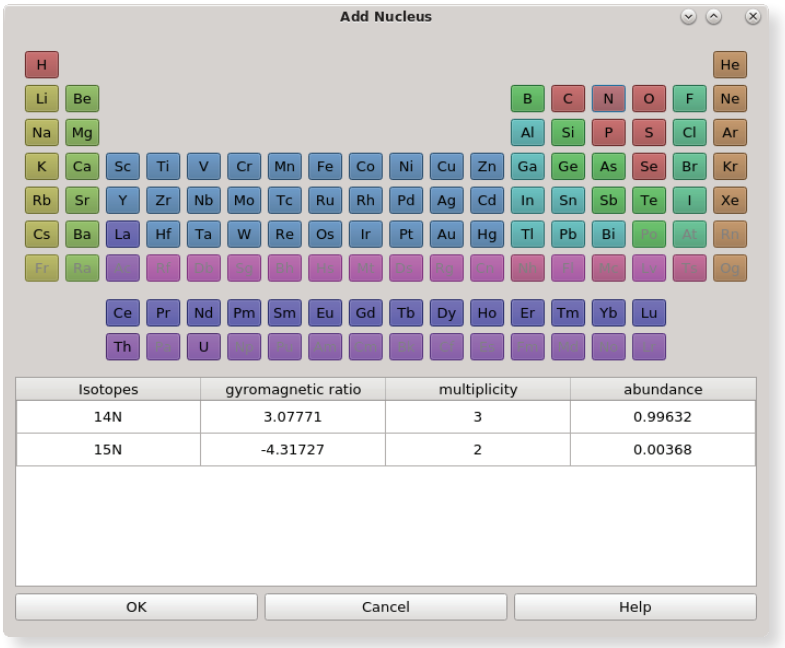

Figure 3
User friendly interface to select atoms and their isotopes from the periodic table of elements

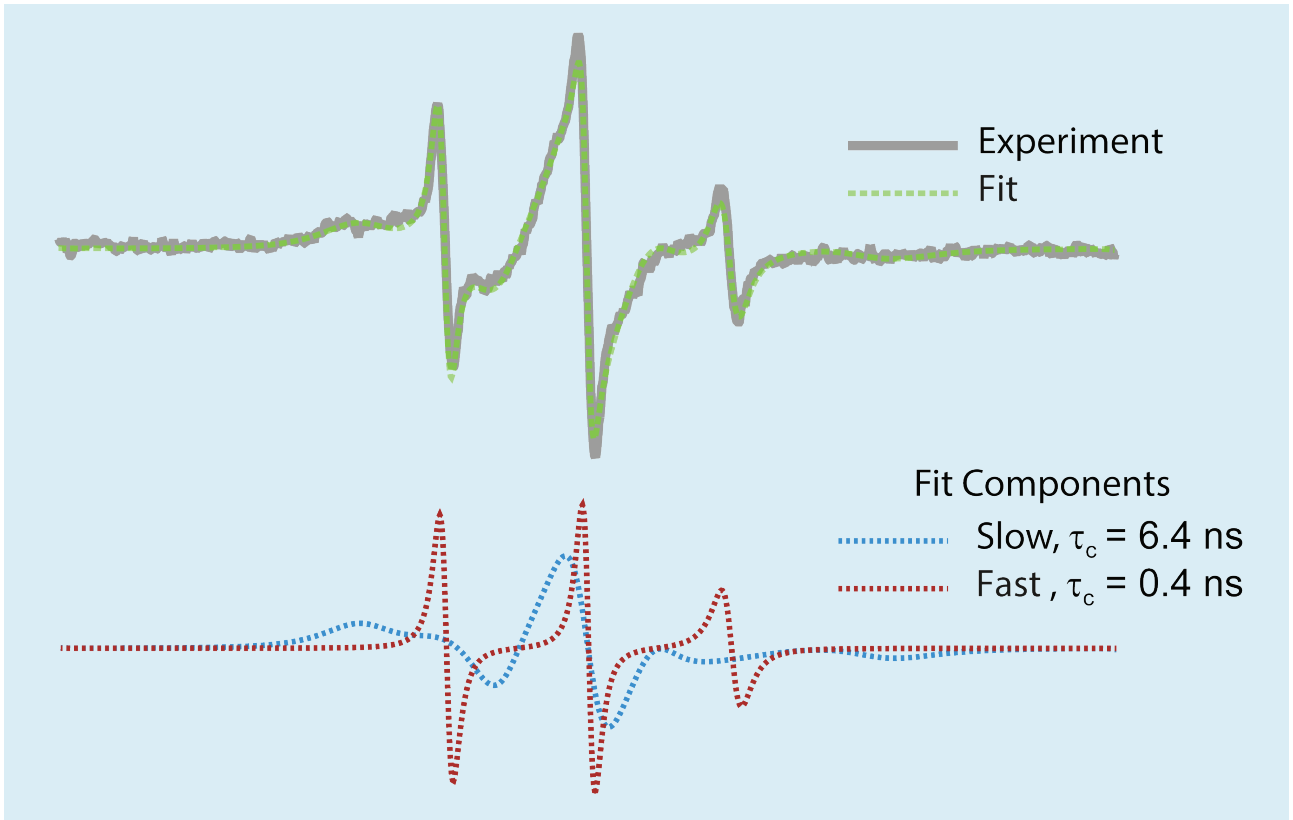

Figure 4
Two-component spectra of spin-labeled protein

- 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

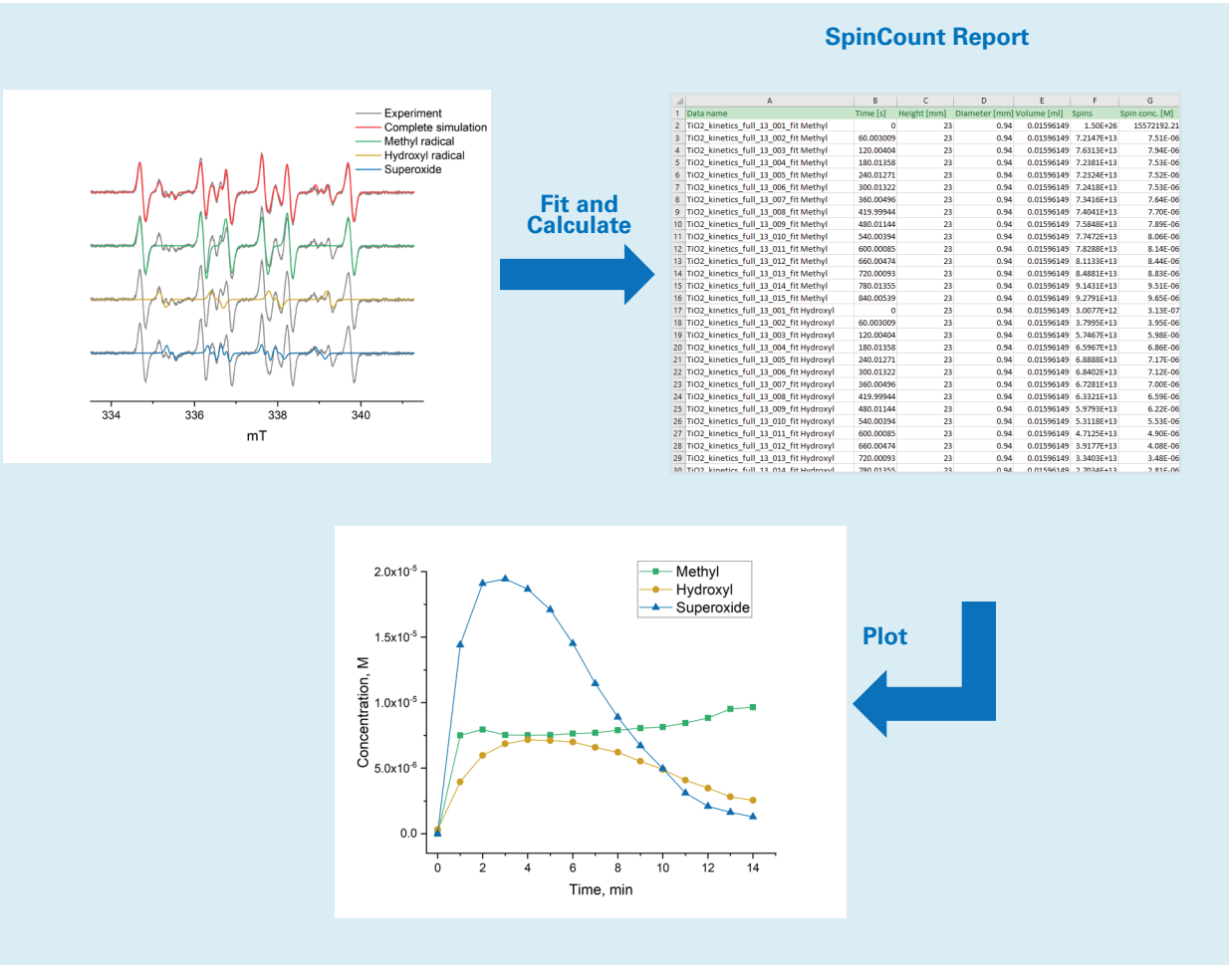

Figure 5

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
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Online information
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