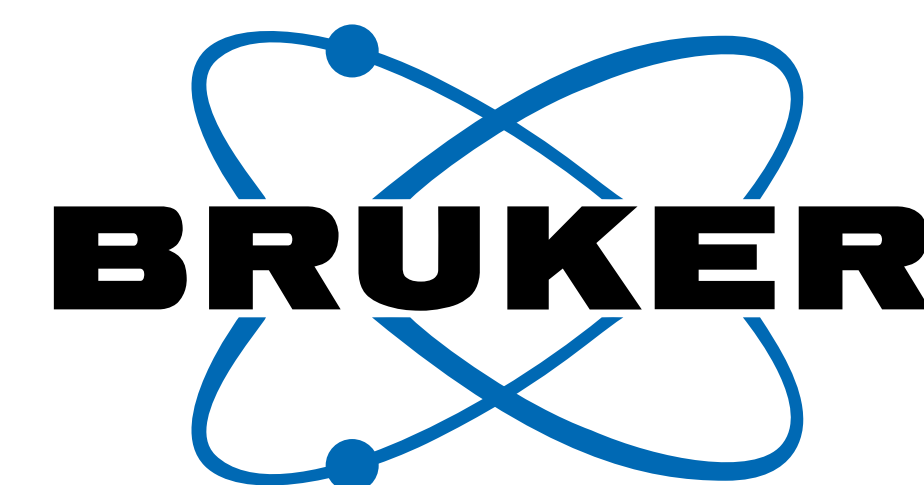


Screening DNP Polarizing Agents with EPR



The EMXnano Benchtop EPR Spectrometer

Built with a new generation of magnet system and a highly efficient microwave resonator, the EMXnano gives consistently accurate results and superior sensitivity. The EMXnano spectrometer enables researchers and students with limited EPR experience to use the power of EPR spectroscopy to characterize the DNP (Dynamic Nuclear Polarization) agents and their characteristics that are important for DNP enhancement. A full workflow for measuring, analyzing and quantifying DNP agents guides you through the entire procedure.



Measure Agents and their Properties with EPR

DNP can enhance the sensitivity of solid state NMR experiments by two to three orders of magnitude. The key to success in a DNP experiment is the paramagnetic enhancement agent. These DNP agents are typically dinitroxides. Nitroxides are stable radicals in which the unpaired electron is localized on an NO group in the molecule.

Properties of these DNP agents that are important for DNP efficiency are:

- Agent concentration
- Dipolar coupling between the nitroxides
- Exchange interaction between the nitroxides
- Electronic relaxation times of the nitroxides

These paramagnetic agents and their properties can be measured via EPR spectroscopy with the EMXnano. The Bruker patented SpinCount module facilitates quick and easy screening of DNP agents. Exchange interactions can be screened by room temperature measurements. Dipolar couplings can be estimated from analysis of low temperature measurements. Relaxation times can be estimated and compared from microwave power saturation characterized by the $P_{1/2}$ parameter at the same temperature as the solid-state DNP experiments.

- 1) Sauve C. et.al., *Angew. Chem. Int. Ed.*, 2013, 52, 10858
- 2) Matsuki Y. et.al., *Angew. Chem. Int. Ed.*, 2009, 48, 4996

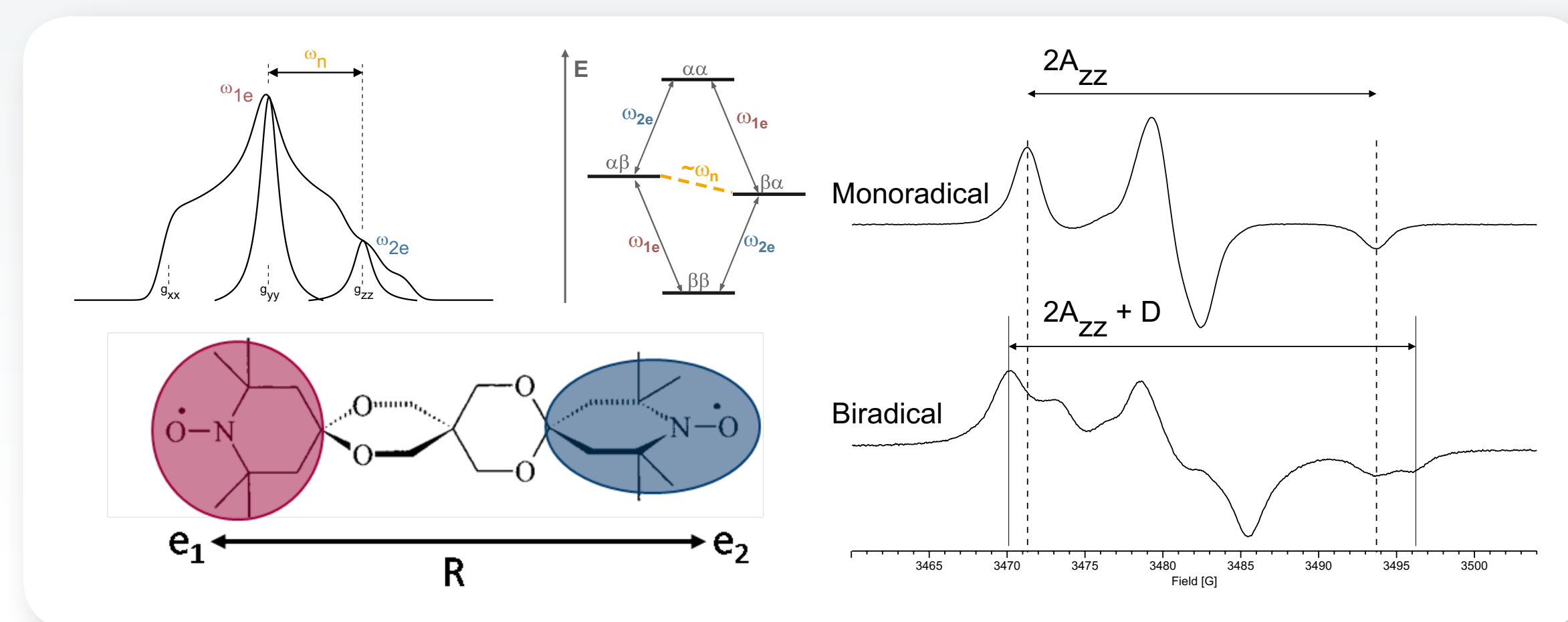


Fig. 1 The low temperature EPR spectra of TEMPOL (monoradical) and bTbK (biradical). Analysis of the biradical features allows the determination of the electron-electron dipolar coupling (right).

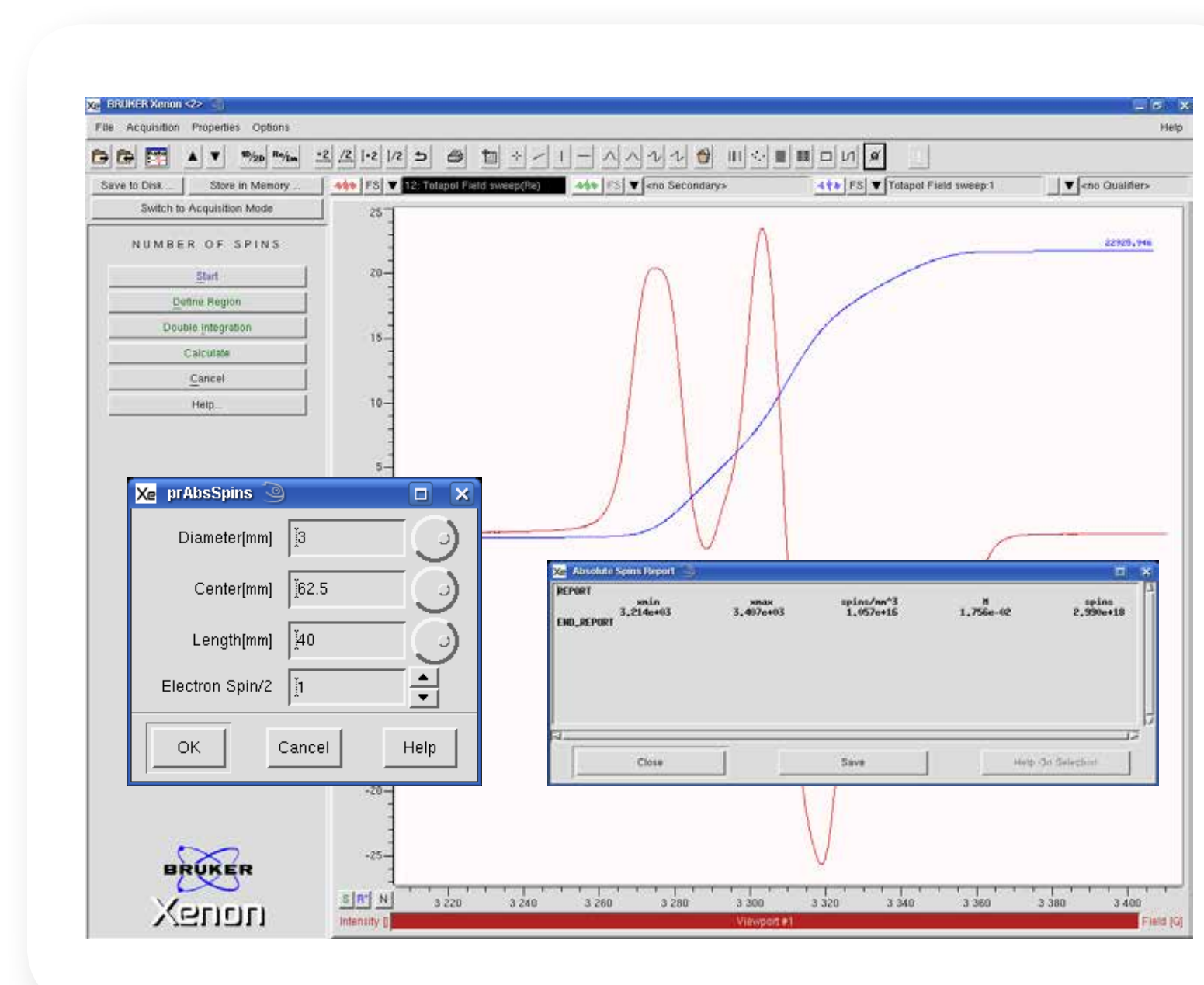


Fig. 2 The Totapol concentration can be quickly and accurately determined from the EPR spectrum using the SpinCount module.

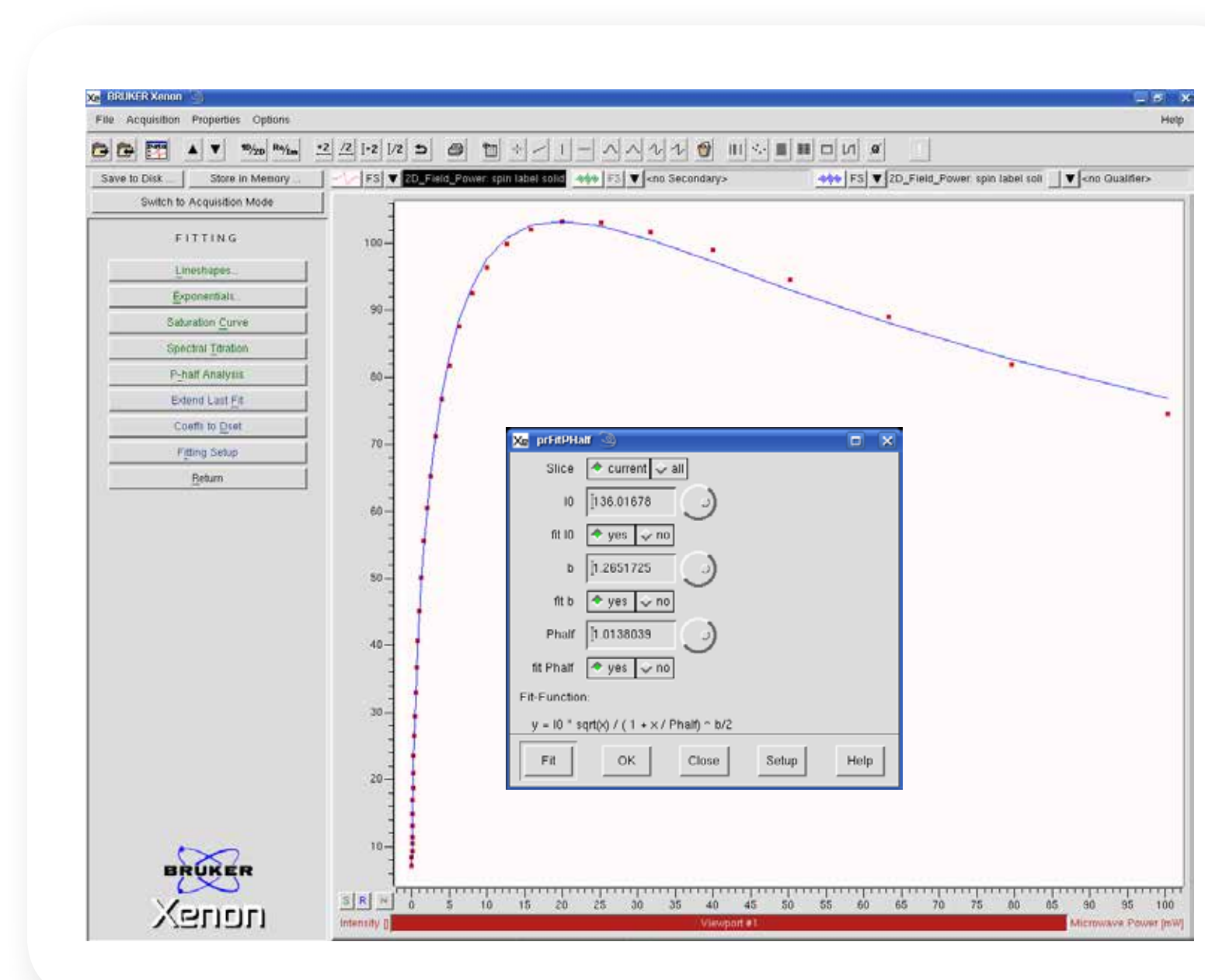


Fig. 3 By fitting the microwave power saturation data the $P_{1/2}$ value can be determined providing insight into the electron relaxation times. For the DNP agent Amupol the 2D Power vs Field data the $P_{1/2}$ was determined to be 0.53 mW.

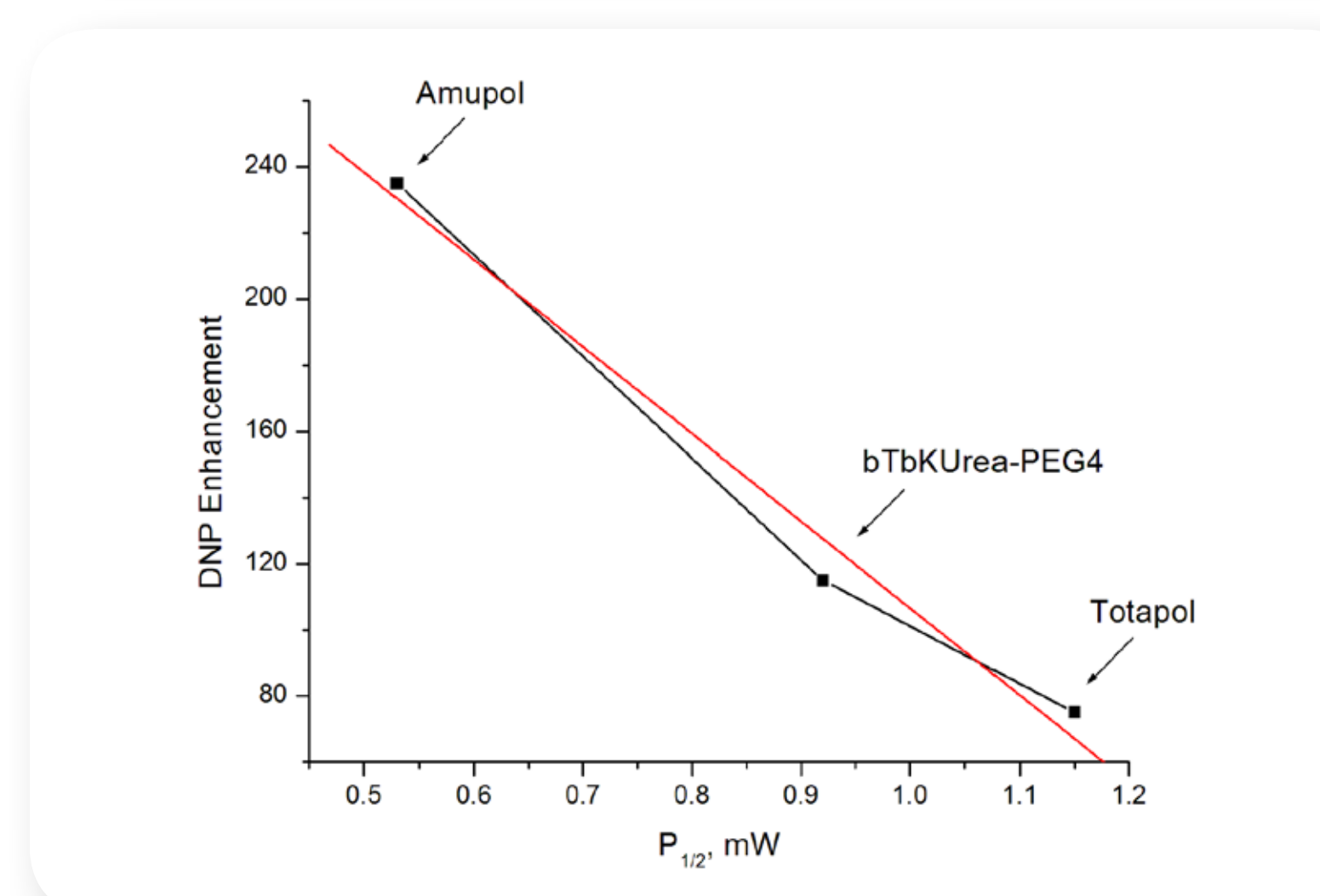


Fig. 4 The $P_{1/2}$ value determined by EPR measurements at 110K correlates well with the DNP enhancements observed.

Summary

- State-of-the-art benchtop EPR spectrometer
- Superior sensitivity
- Fast, accurate concentration determinations
- Easy-to-use software
- $P_{1/2}$ determination for analysis of T_{1e} and T_{2e}
- Variable sample temperature from 100 K to 300 K

