MAR05-2004-003057

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Protein structure determination via EPR of endogenous and introduced electron spins

GARY GERFEN, Albert Einstein College of Medicine of Yeshiva University

Electron Paramagnetic Resonance (EPR) probes the environment of unpaired electron spins. Short range structural information (within 10 Ångströms) can be obtained by determining the identity, number and location of nuclei coupled to the electron spin(s). EPR-based experiments designed to achieve these measurements include continuous wave (CW) EPR, 1-dimensional pulsed techniques (Electron Spin Echo Envelope Modulation or ESEEM), 2-dimensional pulsed techniques (Hyperfine Sublevel Correlation or HYSCORE), double resonance spectroscopy (Electron Nuclear Double Resonance or ENDOR), and High Frequency EPR (HFEPR). These experiments are typically performed on "endogenous" electrons spins localized on metal ions, substrate radicals or amino acid radicals in or near enzyme active sites. Long range structural information (10–50 Ångströms) can be obtained by measuring the dipolar interaction between two or more electron spins using CW and pulsed (Double Electron-Electron Resonance or DEER) techniques. The electron spins for these measurements are typically "introduced" into the system under study using site directed spin labeling (SDSL). This technique expands the applicability of EPR to macromolecules that do not contain an endogenous electron spin, and allows long range structure determination in large molecular weight samples without the requirement of single crystals. Examples of all of these EPR-based techniques will be presented as applied to a variety of protein systems, including Prostaglandin H Synthase, PI 3-Kinase, Prion protein and models, and ribonucleotide reductase.