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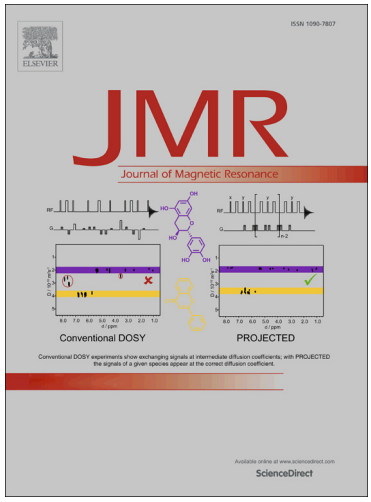

The determination of pair distance distribution by double electron-electron resonance: Regularization by the length of distance discretization with Monte Carlo calculations

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The determination of pair distance distribution by double electron-electron resonance: regularization by the length of distance discretization with Monte Carlo calculations

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Abstract

Pulsed double electron-electron resonance technique (DEER, or PELDOR) is applied to study conformations and aggregation of peptides, proteins, nucleic acids, and other macromolecules. For a pair of spin labels, experimental data allows for determination of their distance distribution function, $P(r)$. $P(r)$ is derived as a solution of a first-kind Fredholm integral equation, which is an ill-posed problem. Here, we suggest regularization by the increasing of distance discretization length, to its upper limit where numerical integration still provides agreement with experiment. This upper limit is found to be well above the lower limit for which the solution instability appears because of the ill-posed nature of the problem; so the solution indeed can be regularized in this way. For solving the integral equation, a Monte Carlo trials of $P(r)$ functions is employed. It has an obvious advantage of the fulfillment of the non-negativity constrain for $P(r)$. The approach is checked for model distance distributions and for experimental data taken from literature for doubly spin-labeled DNA and peptide antibiotics. For the case of overlapping broad and narrow distributions, "selective" regularization can be employed in which