Approaches to structure and dynamics of biological systems by electron-paramagnetic-resonance spectroscopy

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Propositions

1. The presence of extra copper signals in the EPR spectrum of a crystal of a type-2 copper protein needs not hamper the determination of the complete g-tensor, provided that enough is known about the crystallographic properties of the crystal.
   See Chapter 2

2. The rotation-correlation times of spin labels at different surface sites of proteins provide a better ranking of the spin-label mobility than the lineshape analysis according to the Hubbell method.
   See Chapter 3

3. Whether the lipids are in the gel phase or in the liquid-crystalline phase determines the aggregation of WALP peptides in a lipid bilayer.
   See Chapter 4

4. The 5-pulse RIDME sequence is the only pulsed EPR method that allows to precisely determine the distance between a nitroxide spin label and a paramagnetic species with large spectral anisotropy.
   See Chapter 5

5. Hubbell and coworkers propose a lineshape analysis of EPR spectra to characterize the mobility of spin labels in relation to the secondary structure of proteins. When using this method, the errors in both the reciprocal second moment and the reciprocal central line width should be taken into consideration.
   Isas, J. M.; Langen, R.; Haigler, H. T.; Hubbell, W. L. *Biochemistry* **2002,** *41* (5), 1464-1473

6. Despite new developments in pulsed techniques, the classical power saturation method is still the most convenient technique to determine the longitudinal relaxation time of paramagnetic centers in EPR.
   Castner, T. G. *Physical Review* **1959,** *115* (6), 1506-1515.
   Schweiger, A.; Jeschke, G. *Principles of Pulse Electron Paramagnetic Resonance;* Oxford University Press: 2001.

7. The theoretical analysis of the resonance Raman spectra of different isotopomers of spheroidene in the Rhodobacter sphaeroides reaction center (RC) indicates that the RC contains spheroidene in more than one configuration. Resonance Raman experiments as a function of the temperature can be used to investigate this inference.
   Wirtz, A. C.; van Hemert, M. C.; Lugtenburg, J.; Frank, H. A.; Groenen, E. J. J. *Biophys. J.* **2007**, *93*, 981-991.

8. The plasma membrane has a strongly compartmentalized structure, but a more detailed model of its organization and of the role it plays in cell signaling is needed. To achieve this, the dynamic properties of single proteins as well as of protein complex formation should be studied.
   Edidin M. *Curr. Opin. Struct. Biol.* **1997,** 7, 528– 532.
   Lommerse P. H. M., Spaink H. P. and Schmidt T. *BBA* **2004,** 1664, 119-131.

9. The use of the spin label methanethiosulfonate in site-directed spin labeling is a double-edged sword. On the one hand, this paramagnetic probe is small, commercially available and easy to attach to proteins; on the other hand, its long linker may negatively affect the results of experiments performed to study mobility and structure of spin-labeled proteins.