

## EPR-based modelling of membrane protein structures

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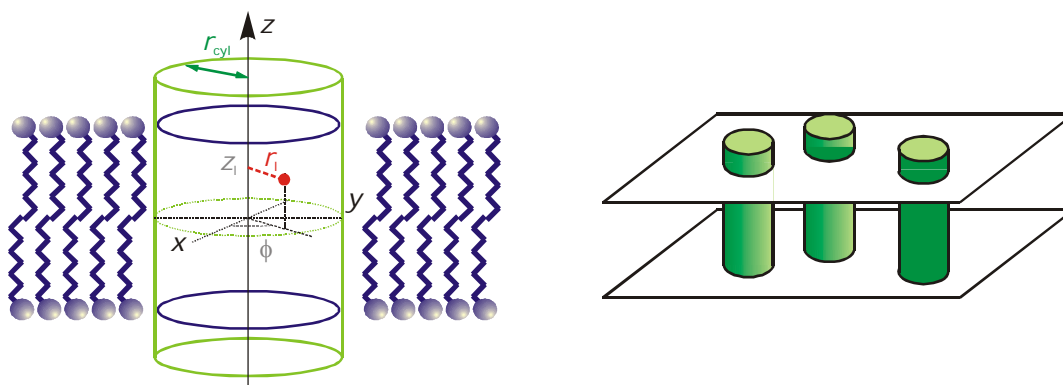
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Crystallization of membrane proteins is still a formidable challenge. Although high-resolution and solid-state NMR are now emerging as prospective alternative techniques for structure determination with atomistic resolution, it is hard to predict up to which size of a membrane protein these approaches will work. Furthermore, structures obtained by NMR techniques and, in particular, crystal diffraction may be missing information on the conformational distribution, which is often related to function.

The combination of site-directed spin labelling with application of a variety of EPR techniques to singly and doubly labelled mutants can thus provide information on structures in this important class of proteins which is complementary to information from other techniques. To enhance the impact of such studies, we have to find ways to translate the information from EPR experiments as fully as possible to a picture of structure and structural dynamics. Further method development of pulsed EPR techniques for spin-labelled membrane proteins should be guided by requirements of structural modelling.



This contribution presents first steps into this direction. On the example of plant light-harvesting complex IIb we illustrate how the combination of measurements of distance *distributions* with established approaches for modelling protein loops can provide a picture for conformational switching of a domain. We also introduce the cylinder model of a membrane protein which guides approximate determination of the position of a single label by DEER and <sup>31</sup>P ENDOR measurements.