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Project description

Building on existing assignments covering 35% of the membrane spanning part, The applicant will extend the assignments of outer membrane protein G sufficiently as a prerequisite and then calculate a structure of this porin within its native lipids. In the application of solid-state NMR to membrane proteins the assignment problem is very severe because of signal overlap and the reduced selection of amino acids in the membrane-spanning portion. To combat this, two different approaches may be envisaged in solid-state NMR. One involves selectively labelled samples, the other including proton chemical shifts into structure determination concepts. The latter approach will be tested by Anup Chowdhury, whereas the applicant will take profit from recently prepared samples of OmpG, with 1,3- and 2-glycerol labelling pattern within a restricted set of amino acids, while the others remain largely unlabelled. The samples are termed, for example, 2- or 1,3-TEMPQANDS; 2- or 1,3-SHLYGWAF or the like, depending on the labelling pattern. We have obtained a first set of spectra which look very good – and resolved, giving the applicant the opportunity to assign most of the critical parts of the protein and collect long range constraints. As a major part of the project, the applicant will collect all data already existing and design new experiments and strategies to end up with a well-refined structure. In this context, the effects of paramagnetic solutes in the aqueous phase will be tested, and – if possible – also in the

lipid bilayer. In the course of the structure calculations, new strategies will be explored incorporating such data. The student is expected to work in the NMR group in Berlin preparing samples and applying NMR techniques, and to stay in close interaction with the groups in Göttingen (Grubmüller) for structure calculations and in Utrecht (Baldus) and Toulouse (Milon) for individual measurements. Results will be compared with the studies on other porins in the groups in Toulouse and Utrecht.