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Rhodopsin Activation in Membranes Studied by Solid-State NMR Spectroscopy XIAOLIN XU, Department of Physics, University of Arizona, ANDREY STRUTS, Department of Chemistry and Biochemistry, University of Arizona;Laboratory of Biomolecular NMR, St Petersburg State University, MICHAEL BROWN, Department of Physics;Department of Chemistry and Biochemistry, University of Arizona — Crystal structures of rhodopsin are available, yet the activation mechanism remains unknown. We introduced site-specific ^{2}H labels into various methyl groups of the retinal cofactor and incorporated rhodopsin into membrane bilayers. Solid-state ^{2}H NMR experiments were conducted for selectively deuterated retinal bound to rhodopsin in aligned samples in the active Meta-II state. The degree of alignment was tested by ^{31}P NMR spectroscopy of the lipids. Solid-state ^{2}H NMR lineshapes of the aligned samples were simulated by a static uniaxial distribution, which revealed the bond orientations of retinal methyl groups and mosaic spread [1]. Comparison with solid-state ^{2}H NMR spectra predicted by X-ray results enabled the proposed structures for active Meta-II to be tested. Moreover, the dynamics of retinal were investigated by spin-lattice and quadrupolar-order relaxation measurements. Our generalized model-free method yields mean-squared amplitudes and correlation times of retinal bound to rhodopsin [2] as a basis for molecular dynamics (MD) simulations. Our broad aim is to establish how the local fluctuations of the ligand initiate the structural changes of rhodopsin to understand the activation mechanisms of GPCRs in general. [1] A.V. Struts et al. 2011, *NSMB* **18**, 392. [2] X. Xu et al. 2014, *eMagRes* **3**, 275.

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