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Ligand-induced dynamical change of G-protein-coupled receptor revealed by neutron scattering UTSAB R. SHRESTHA, Wayne State University, DEBSINDHU BHOWMIK, EUGENE MAMONTOV, Oak Ridge National Laboratory, XIANG-QIANG CHU, Wayne State University — Light activation of the visual G-protein-coupled receptor rhodopsin leads to the significant change in protein conformation and structural fluctuations, which further activates the cognate G-protein (transducin) and initiates the biological signaling. In this work, we studied the rhodopsin activation dynamics using state-of-the-art neutron scattering technique. Our quasi-elastic neutron scattering (QENS) results revealed a broadly distributed relaxation rate of the hydrogen atom in rhodopsin on the picosecond to nanosecond timescale (beta-relaxation region), which is crucial for the protein function. Furthermore, the application of mode-coupling theory to the QENS analysis uncovers the subtle changes in rhodopsin dynamics due to the retinal cofactor. Comparing the dynamics of the ligand-free apoprotein, opsin versus the dark-state rhodopsin, removal of the retinal cofactor increases the relaxation time in the beta-relaxation region, which is due to the possible open conformation. Moreover, we utilized the concept of free-energy landscape to explain our results for the dark-state rhodopsin and opsin dynamics, which can be further applied to other GPCR systems to interpret various dynamic behaviors in ligand-bound and ligand-free protein.

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