The activation pathway of human rhodopsin in comparison to bovine rhodopsin

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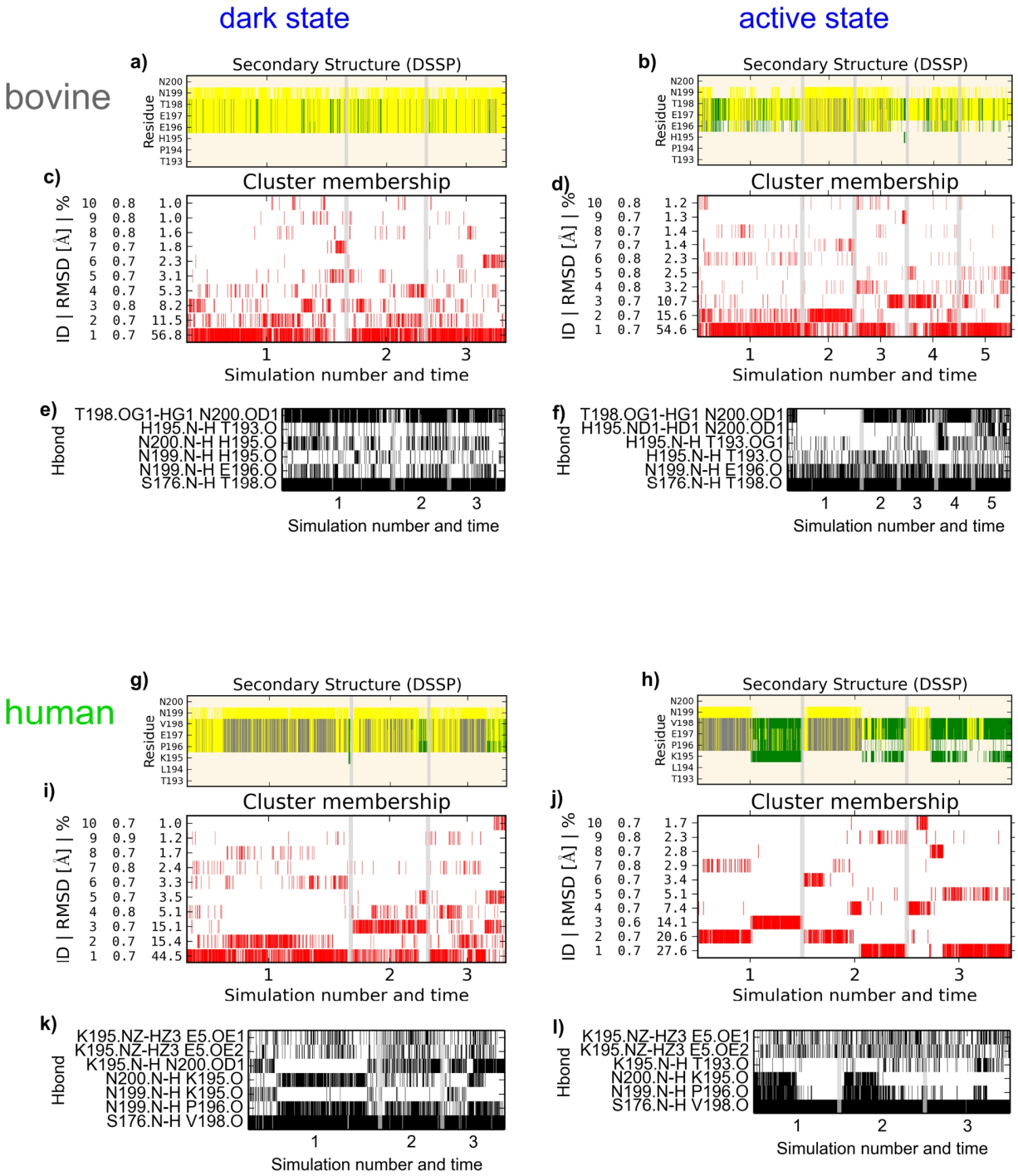

SI Figure 1. Secondary structure, cluster analysis and hydrogen bonding of the T_5E_2C-region in MD simulations.

a, b, g, h) The secondary structure analysis by DSSP (W. Kabsch, C. Sander, Biopolymers 1983, 22, 2577–2637.) shows differences in the composition of secondary structure elements comparing bovine and human rhodopsin. In bRho turn structures (*yellow*) are prevalent whereas in hRho we observe the T_5E_2C-region (highlighted in *pale blue*) to bend (*green*) and 3_{10}-helix (*grey*) structures. **c, d, i, j)** The cluster analysis shows a large homogeneity for inactive/active bRho and inactive hRho. The three largest clusters together contain 76.5% (dark state bovine), 80.9% (active state bovine), 75.0% (dark state human) and 62.3% (active state human) of the clustered structures. However, in active state hRho transitions between the three largest clusters are very rare and much less frequent than in dark/active state bRho or dark state hRho. This indicates the formation of T_5E_2C sub-states in active state hRho simulations. The cluster analysis was performed (after aligning the trajectories on the transmembrane helices) with the GROMACS tool g_cluster using the gromos cluster method with a cut-of of 0.8 Å. **e, f, k, l)** Hydrogen bonding observed between the T_5E_2C-region and proximal receptor residues. In hRho a hydrogen bond between E5 and K195 is observed, which is absent in bRho. However, in bRho a backbone-backbone hydrogen bond is prevalent between E196 and T198 whereas in active hRho the interaction between P196 and V198 is eventually lost. Hydrogen bond analysis was performed with the GROMACS tool g_hbond using cut-of angle between acceptor-donor-hydrogen of 30° and a distance cut-of between acceptor-donor of 3.6 Å.