

Description of Additional Supplementary Files

Title: Supplementary Data 1

Description: Sequences of oligonucleotides used for mutation in the expression vectors of OxIT.

Title: Supplementary Movie 1

Description: The first 600 ns trajectory of OxIT starting from the occluded conformation, which remained in the occluded state, is shown. The representation is the same as Fig. 4e, except all water molecules are shown in the CPK color.

Title: Supplementary Movie 2

Description: The first 500 ns trajectory of OxIT starting from the occluded conformation with a transition to the outward-open state is shown. The representation is the same as Fig. 4f, except all water molecules are shown in the CPK color.