Structure and dynamics of chloride ion pumping rhodopsin revealed by time resolved SFX and atomic molecular dynamics simulations

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The chloride ion pumping rhodopsin was studied with the powerful X-ray lasers and supercomputers, to reveal the molecular mechanism of proteins. The chloride ion pumping rhodopsin (ClR) utilizes energies from light to actively transport Cl- ions through membranes. In this study, we report, for the first time, an atomic structure determined at room temperature using serial femtosecond X-ray Crystallography (SFX) method. The atomic structure determined using SFX method is very consistent with the structure solved at synchrotrons. Furthermore, using pump-probe method, time-resolved crystallography method was applied to determine structures at several time point after photoactivation. Extensive molecular dynamics simulations have been carried out to study the pathway of Cl- ions through the rhodopsin channel. By using all-atom molecular dynamics simulation method, the plausible pathways of Cl- ion were observed (Figure 1d,e). The residues that undergo substantial conformational changes during the ion transportation have been identified.

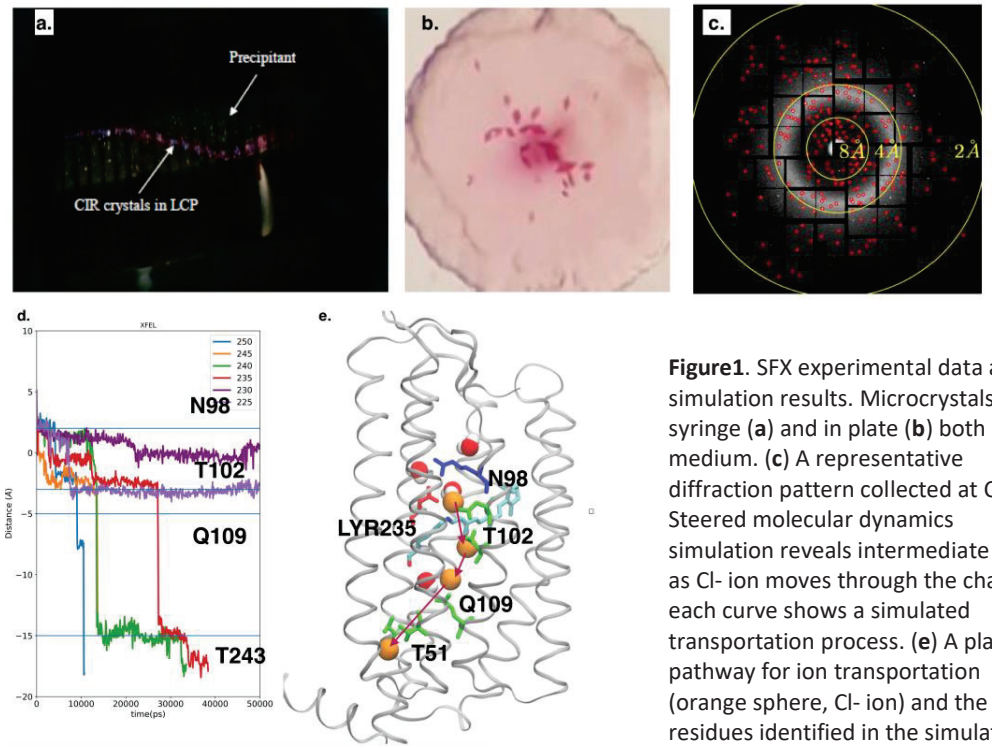

Figure1. SFX experimental data and simulation results. Microcrystals in syringe (**a**) and in plate (**b**) both in LCP medium. (**c**) A representative diffraction pattern collected at CXI. (**d**) Steered molecular dynamics simulation reveals intermediate states as Cl- ion moves through the channel, each curve shows a simulated transportation process. (**e**) A plausible pathway for ion transportation (orange sphere, Cl- ion) and the key residues identified in the simulations.

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