Unraveling Proton Storage Site and Generic Proton Release Pathway in a Prototype Light-Driven Proton Pump Bacteriorhodopsin

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Understanding the mechanism of proton pumping in the simplest light-driven proton pump, bacteriorhodopsin (bR), is crucial to unveil the proton pumping function of even more complex proton pumps. Yet, despite decades of research various conflicting issues related to the location of excess proton and proton release pathways in bR are still not well understood. By applying state of the art computational techniques we unveil the precise location and chemical identity of the proton release group in addition to discovering the subsequent proton release pathways in bR. The proton release group as discovered from our study satisfies most available experimental results, specially the manifestation of continuum band in the obtained spectra and the associated anisotropic feature that has been experimentally observed only recently. Moreover, we disclose the molecular mechanism and pathway by which the stored proton, being stored in an ultra-strong centered H-bond, is released to the extracellular bulk. We believe that the insight obtained from our study can be utilized to understand the mechanism of ion pumping of other more complex membrane transporters.