Hunting for recondite proton translocation inside Cytochrome c Oxidase

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During the final phase of respiration, cytochrome c oxidase (CcO) catalyzes the reduction of oxygen to water to fuel the proton pumping through the membrane[1]. According to the crystal structures of CcO, two proton transfer channels exists D and K channels. In the crystal structure, the D channel is filled with water molecules and hydrophilic residues but for the K-channel no such information is available[2]. The proton translocation mechanism and communication between D and K channel is investigated by a combination of classical molecular dynamics simulations of different protonation states. Excess protons are placed at entrance and final residues of the channels, Asp132-Glu101, Glu286-Tyr288 and in addition to that water molecules are modeled as hydronium ions. The overlap of hydrogen-bonded networks based on geometrical criteria between different protonation states and correlation between residues ni the two channels gives insight into possible communication pathways.

References:

[1] Collman J.P., Devaraj N.K., Decréau R.A., Yang Y., Yan Y.L, Ebina W., Eberspacher T.A., Chidsey C.E.D., A Cytochrome c Oxidase Model Catalyzes Oxygen to Water Reduction Under Rate-Limiting Electron Flux, Science 16 March 2007: 315 (5818), 1565-1568.

[2] Iwata S., Ostermeier C., Ludwig B. Michael H., Structure at 2.8 Å resolution of cytochrome c oxidase from Paracoccus denitrificans ,Nature 376, 660 - 669 (24 August 2002)