

PROTEIN SURFACE PROPERTIES PERTAINING TO PROTON TRANSFER IN CYTOCHROME C OXIDASE

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Cytochrome c oxidase (COX) is a proton pump, which utilizes free energy of oxygen reduction for creation of mitochondrial proton gradient. The details of molecular mechanism of proton translocation by the enzyme are unknown. Molecular dynamics simulation of cytochrome c oxidase solvated in water has been utilized to study proton transfer along and in the vicinity of the surface of the enzyme. Using computer analysis we are able to quantify the time scales of both the surface and bulk water hydrogen bond network critical for proton transfer. The application of graph theory makes it possible to survey the protein surface for specific proton transfer pathways leading to a proton channel in COX. Results and conclusions are presented in detail. The obtained data provide evidence that proton transport is dominated by the surface processes, as recently suggested on phenomenological grounds in Ref [1].

Reference:

[1] Y. Georgievskii, E.S. Medvedev and A.A. Stuchebrukhov, *Biophys. J* (2000), to be published.