

Abstract Submitted  
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**Proton-Pumping Mechanism in Complex I of Mitochondria Membrane** DAVNEET KAUR, Queens College CUNY — Mitochondria are the powerhouses of animal cells and also many bacteria. Complex I is the first enzyme in the mitochondrial respiratory chain, the process leading to storage of energy in the form of Adenosine Triphosphate (ATP). The structure of the enzyme was recently resolved and its functionality was correlated to the motion of a helical protein structure. However, the actual mechanism of the electron assisted proton-pumping of Complex I has remained mysterious because the electron ( $e^-$ ) and proton ( $H^+$ ) pathways are well separated by a distance of up to 15 nm making the direct interaction of these charges negligible. We model the helix assisted indirect coupling between the electron and proton pathways as a non-uniformly charged piston oscillating between the coupled sites of a 3 site series system. The energy conversion is determined by single  $e^-$  and  $H^+$  transport events. The piston oscillates between that central proton and electron sites and modulates their energy, while the coupling with other sites is weak and negligible. We show that with realistic values of parameters, this structure allows for proton pumping against the potential gradient.

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