Dynamical View of Energy Coupling Mechanisms in Active Membrane Transporters

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Membrane transporters constitute the principal players in active exchange of materials across the cellular membrane in an energy-dependent manner. These complex proteins constitute highly sophisticated, fine-tuned molecular pumps that efficiently couple various sources of energy in the cell to vectorial transport of a wide range of molecules across the membrane, often against the electrochemical gradient. Substrate binding and translocation along the transport pathway in membrane transporters are closely coupled to numerous stepwise protein conformational changes of varying magnitude and nature that are induced by and/or coordinated with the energy-providing mechanisms. A detailed description of the mechanism of membrane transporters, therefore, relies on high-resolution methodologies that can describe the dynamics of the process at an atomic level. In this talk, latest results of molecular dynamics simulations performed on a number of atomic structures of membrane transporters and the molecular events involved in their function revealed by these simulations will be presented.