Heat Dissipation from the Catalytic Center of Human Heart Lactate Dehydrogenase

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We examine if the rate promoting vibration of lactate dehydrogenase (hLDH) is a preferred axis of thermal energy transfer. It seems plausible that such a mechanistically important motion is also a favored direction of energy transfer, but no previous study has directly addressed this question. It is possible that the promoting vibration, while catalytically important, has no different thermal properties than any other axis in the protein. Resolution of this issue is important for two reasons: First, if energy is transferred along this axis in a preferred fashion, it shows that the protein is engineered in a way that transfers excess thermal energy into a motion that is coupled to the chemical step. Second, the discovery of a preferred direction of thermal transfer provides a potential route to experimental verification of the promoting vibration concept. Our computational experiments are specifically designed to mimic potential laser experiment with the deposition of thermal energy in an active site chromophore with subsequent measurement of temperature at various points in the protein.