Imaging protein statistical substate occupancy in a spectrum-function phase space

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Hemeprotein ligand rebinding studies reveal varying IR absorbance and rebinding function across a cryogenic ensemble. Since IR-active vibrations and rebinding barriers couple to structural coordinates, spectral and functional heterogeneity arise from conformational heterogeneity. Modeling rebinding data as a spectrally resolved superposition of first order rate processes and employing maximum entropy regularization, protein heterogeneity is imaged as ensemble occupancy of a spectrum-function phase space. Simulations indicate that the method used to solve the associated numerical inverse problem of Fredholm type is robust. Results from myoglobin rebinding carbonmonoxide are discussed, and a structural interpretation is suggested.