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Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome JEFFREY NOEL, Center for Theoretical Biological Physics Rice University, JORGE CHAHINE, VITOR LEITE, Universidade Estadual Paulista, Rio Preto, Brazil, PAUL WHITFORD, Physics Dept Northeastern Univ — To reveal the molecular determinants of biological function, one seeks to characterize the interactions that are formed in conformational and chemical transition states. In other words, what interactions govern the molecule's energy landscape? To accomplish this, it is necessary to determine which degrees of freedom can unambiguously identify each transition state. Here, we perform simulations of large-scale aminoacyl-tRNA (aa-tRNA) rearrangements during accommodation on the ribosome and project the dynamics along experimentally-accessible atomic distances. From this analysis, we obtain evidence for which coordinates capture the correct number of barrier-crossing events and accurately indicate when the aa-tRNA is on a transition path. While a currently-used coordinate in single-molecule experiments performs poorly, this study implicates alternative coordinates along which rearrangements are accurately described as diffusive movements across a one-dimensional free-energy profile. From this, we provide the theoretical foundation required for single-molecule techniques to uncover the energy landscape governing aa-tRNA selection by the ribosome. More details can be found at doi:10.1529/biophysj.106.090944.

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