



Conformational Sub-States and Transient Heterogeneity in Enzyme Function

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Message from the Guest Editors

This Special Issue of Catalysts will illustrate how experimental and computational methodologies provide evidence on the functional importance of transiently-populated enzyme sub-states that define conformational heterogeneity in enzymes. Studies will highlight the role of enzyme motions/dynamics at different time and length scales in detailed enzyme mechanisms, and the changes in conformational populations as the enzyme cycles through the reaction coordinates. Conformational studies inform on the mechanistic and structural importance of atomic flexibility in enzymes, and how that information can be leveraged towards the development of new catalysts. We are also interested in highlighting how enzyme technology is impacting a wide variety of fields from medicine to chemical industry.

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