Tertiary Structure and Active Sites Conformations in Forms I and II RuBisCO

William J. Lin, Scott T. Hansen, Nicholas Boekelheide
Colby College, Department of Chemistry, Waterville, Maine 04901

A slow catalytic rate and poor substrate discrimination are contrasted by the essential biological role of the ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO) enzyme¹. There are two major forms of catalytically active RuBisCO. Despite a highly conserved active site, the two forms exhibit distinct tertiary structures and sequence heterogeneity. The structure-function relationship between enzyme structure and a proposed trade-off between substrate specificity and catalytic rate²,³ is an area of focus in studies to improve RuBisCO’s catalytic efficiency. Here we present results from molecular dynamics simulations of both forms of the activated RuBisCO enzyme. We present results of molecular dynamics simulations of activated form I and II RuBisCO enzymes and identify the inter- and intramolecular interactions that occur through thermal fluctuations.

![Figure 1](image)

Figure 1 (left). The apparent negative correlation between substrate specificity and rate of catalysis²,³ in RuBisCO across species and forms. Full citations with poster. (Right). The tertiary structures of the two forms of RuBisCO, the hexadecamer form I (top) and the

References: