Structural and Functional Characteristics of TIM-Barrel as a Novel Scaffold for protein Design and Engineering

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Abstract—*During the last 25 years, many investigations have been carried out to understand the principles responsible for the folding and stability of the TIM-barrel fold. Recently the characteristics of TIM-barrel proteins have been reviewed in detail in terms of their structure, folding, function, and evolution. The TIM-barrel or (β/α)8-barrel fold is the most common enzyme fold in the protein data bank (PDB) database of known protein structures. It is seen in many different enzyme families catalysing completely unrelated reactions. Some of the most effective enzymes are TIM-barrel enzymes, for example TIM (triose phosphate isomerase) which catalyses an interconversion reaction in the glycosidic pathway. The (β/α)8-barrel fold is of particular interests for designing novel catalysts because it is the most common topology for enzymes and one of the most diverse superfolds. Recent efforts have been devoted to de novo-design symmetric and functional TIM-barrels which is ideal for enzyme design and protein engineering. In this study, we determined the structural and functional characteristics of a de novo-designed TIM-barrel for protein design and engineering purposes.*

Keywords*: TIM-barrel; (β/α)8-barrel; protein data bank; triose phasphate isomerase; superfolds; enzyme design.*