Title:	To Study the Evolutionary Origin of Specificity in Triosephosphate Isomerase (TIM) and to Extract Protein-Ligand Interaction Features Using Canonical Correspondence Analysis (CCA)
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Abstract:	Recent studies have shown that enzymes can catalyze alternate reaction or substrate/s apart from their physiologically relevant activity. This ability of enzyme is referred to as enzyme promiscuity. Usually, promiscuous activities have low catalytic efficiency and specificity. However, these can become important under any genotype/environment perturbations. Jensen has hypothesised that in ancestral enzymes showed broad specificity (generalist) and these become specialized during evolution. Based on this, we studied whether ancestral enzymes exhibit low catalytic efficiency or have weak substrate affinity. For this, we used core glycolytic enzyme Trios-phosphate isomerase (TIM). We generated phylogenetic tree of TIM enzymes and overlay with known experimental kinetic parameters. We observed that catalytic efficiencies are similar in enzymes from both ancestral and recently evolved enzymes. However, binding affinity of ancestral enzymes is weaker in comparison to modern enzymes. In the second project, we have used statistical methods to identify recurring patterns in protein sequences and compounds that can assist in understanding ligand-protein interactions. We have used canonical correspondence analysis (CCA) method with proteins represented as 6-mers string kernels and ligands expressed as atomic signatures. Based on preliminary analysis of 92 ligands, it can be suggested that CCA could be helpful in identifying important features of protein-ligand interactions. Further, this could be used in prediction of ligand binding sites.
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