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Title: Unusual commonality in active site structural features of substrate promiscuous and specialist

enzymes

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Abstract:

Enzyme promiscuity is the ability of (some) enzymes to perform alternate reactions or catalyze non-cognate substrate(s). The latter is referred to as substrate promiscuity, widely studied for its biotechnological applications and understanding enzyme evolution. Insights into the structural basis of substrate promiscuity would greatly benefit the design and engineering of enzymes. Previous studies on some enzymes have suggested that flexibility, hydrophobicity, and active site protonation state could play an important role in enzyme promiscuity. However, it is not known yet whether substrate promiscuous enzymes have distinctive structural characteristics compared to specialist enzymes, which are specific for a substrate. In pursuit to address this, we have systematically compared substrate/catalytic binding site structural features of substrate promiscuous with those of specialist enzymes. For this, we have carefully constructed dataset of substrate promiscuous and specialist enzymes. On careful analysis, surprisingly, we found that substrate promiscuous and specialist enzymes are similar in various binding/catalytic site structural features such as flexibility, surface area, hydrophobicity, depth, and secondary structures. Recent studies have also alluded that promiscuity is widespread among enzymes. Based on these observations, we propose that substrate promiscuity could be defined as a continuum feature that varies from narrow (specialist) to broad range of substrate preferences. Moreover, diversity of conformational states of an enzyme accessible for ligand binding may possibly regulate its substrate preferences.

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