Molecular Dynamic Analysis on the Regional Fluctuations of a Hyperthermophilic Methylglyoxal Synthase

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Methylglyoxal synthase (MGS) converts dihydroxyacetone phosphate to methylglyoxal, which is a precursor to 1,2-propanediol, for industrial uses such as antifreeze and substrates to polymers. A novel, hyperthermophilic methylglyoxal synthase has been characterized to this end, with temperature optimum at 80°C and 59% residual activity at 95°C. The hyperthermophilic MGS was subjected to a comparison to a thermophilic MGS and a mesophilic MGS via molecular dynamic analysis. The structural analysis showed that the hyperthermophile structure was more rigid than those of the thermophilic and mesophilic MGSs, as represented by a lower overall root-mean-square-deviation (RMSD) value. Distinct regions within the mesophilic and thermophilic MGSs were found to have high residual fluctuations, whereas specific hydrogen bonds and salt bridges between secondary structures could stabilize the regions in the hyperthermophilic enzyme. The analytical approach and the information on specific interactions for regional stabilization can be exploited to further engineer the MGSs for various applications.