MATHEMATICAL FORMALIZATION OF PROTEIN EVOLUTION BASED UPON GEOMETRIC CONSTRAINTS

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The consideration of molecular evolution has broadly based implications in both genetic divergence and molecular structure-function relatedness. The tertiary structure of proteins, particularly enzymes, has been employed to study evolutionary divergence. The contribution of thermodynamically favored three-dimensional structure assumptions and geometries are considered to limit the expression of large numbers of protein systems. Constraints upon these arrays may be interpreted in terms of Cauchy sequences whereby the muliplicity of possible tertiary geometries is limited to the sequence. In the case of divergent proteins, the subset of allowed thermodynamic foldings would be described as a bounded Cauchy sequence because of the relative lack of divergence in the basic protein backbone structure as expressed in the primary and secondary structure of the protein molecule. Thus, discussion of series of proteins related by tertiary structure homology in terms of Cauchy sequence theory might provide a mathematical description and analysis of such evolutionary patterns.

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