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**Exploring Protein Stability with Protein Language Models and Molecular Simulations**

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Enzyme-based biocatalysts are eco-friendly solutions for various industrial and green chemistry applications, including clean energy production and pollutant bioremediation. However, native enzymes often struggle under harsh conditions like extreme temperatures and pH, hindering large-scale use. Engineering enzymes to enhance their physicochemical properties and catalytic efficiency in suboptimal conditions is essential. Traditional protein engineering methods, such as directed evolution and mutagenesis, require extensive screening of sequence space. Recently developed artificial intelligence-based protein language models offer a promising approach for designing novel protein scaffolds. Our work demonstrates that these models significantly improve stability predictions with and without additional task-specific training. Coupling these predictions with molecular dynamics simulations deepens our understanding of the enzyme's structure-function relationships and aids in stability optimization with minimal screening, opening new pathways for advancing computational methods in protein stability prediction.