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High-Fidelity Understanding of Enzymes Through Integrative Computational and Experimental Data

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Understanding enzymes at the molecular level is crucial for enhancing their activity and functional specificity. A high-fidelity approach involves integrating computational methods—such as molecular dynamics simulations, quantum mechanical calculations, and machine learning techniques—with experimental data. This synergistic framework enables unprecedented insights into the structural and dynamic properties of enzymes, facilitating the rational design of improved activity and selectivity. Our work demonstrates how this integrative strategy advances the understanding of enzymatic mechanisms, paving the way for innovative approaches in enzyme engineering and biocatalysis