

Innovative Protein Surface Analysis: A High-Resolution Approach for Structural Insights

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Abstract Text : Protein surface analysis is essential for understanding molecular interactions, binding sites, and functional regions in structural biology. While artificial intelligence and machine learning have gained prominence in computational biology, there remains a critical need for human-interpretable, transparent, and easily implementable methods that do not rely on black-box algorithms.

Here, we present a novel computational approach for high-resolution protein surface analysis, designed to be fully interpretable and accessible to researchers without requiring expertise in AI. Our workflow is implemented in Python, using widely available libraries, ensuring ease of adoption and reproducibility. Unlike AI-driven approaches, our method provides clear, step-by-step results that researchers can directly visualize, validate, and interpret. Case studies demonstrate its applicability in analyzing protein binding sites and membrane interfaces, where surface properties are crucial for biological function.

This approach bridges the gap between structural biology and surface analysis, offering a robust, user-friendly tool for exploring protein surfaces with high precision. It is particularly valuable for applications in drug design, protein engineering, and biomolecular interaction studies, where transparency and interpretability are as important as accuracy.

Bibliography :

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