

High-Throughput Mutational Scanning via Alchemistry and HPC

In our recent study, "**High Throughput Mutational Scanning of a Protein via Alchemistry on a High-Performance Computing Resource**," we explored how **advanced computational methods** can assess the effects of mutations in dihydrofolate reductase (DHFR), particularly in the context of antibiotic resistance.

Key Tools & Theories Used:

- **Alchemical Free Energy Calculations:** We employed these precise computational techniques to estimate binding energies and assess the molecular fitness of various DHFR mutants.
- **Deep Mutational Scanning:** This approach allowed us to generate a comprehensive computational library of DHFR variants, facilitating a high-throughput analysis of potential mutations.
- **High-Performance Computing (HPC):** Leveraging HPC resources enabled us to perform extensive simulations and analyses, which are essential for handling the computational demands of alchemical free energy calculations.

Our findings demonstrate the feasibility of integrating **alchemical free energy calculations with deep mutational scanning**, providing a robust framework for predicting the impacts of mutations on protein function. This approach holds significant potential for **understanding antibiotic resistance mechanisms** and guiding the design of more effective therapeutic strategies.

 Read more: [DOI Link](#)

#AlchemicalCalculations #DeepMutationalScanning #HighPerformanceComputing
#AntibioticResistance #ComputationalBiology #Biochemistry #Research