Inventory of Anti-Catalytic Residue Multimeters

To this end, we propose here a deep learning-based solution, called SCREEN, for the accurate prediction of catalytic residues in enzymes.

Here, we review the data on the catalytic residues of 648 enzymes, as annotated in the Mechanism and Catalytic Site Atlas (M-CSA), and compare our results with those in previous studies.

In our group, we have developed a consensus based or meta-approach (CSmetaPred) to predict catalytic residues that combines four well-known catalytic residue prediction methods (CRPred, ...

We combined a 97 contrastive learning framework on PLM per-token embeddings with a rationally designed hierarchical 98 pair scheme to create a sequence-based catalytic residue predictor that is ...

We introduce a computational method to predict and annotate the catalytic residues of a protein using only its sequence information. An annotation of an enzyme"s catalytic residues describes their ...

We present an analysis of the residues directly involved in catalysis in 178 enzyme active sites.

In order to improve ranking of catalytic residues and their prediction accuracy, we have developed a meta-approach based method CSmetaPred. In this approach, residues are ranked based on the ...

To address these challenges, we developed Squidly, a sequence-only tool that leverages contrastive representation learning with a biology-informed, rationally designed pairing scheme to ...

Our guideline provides a practical roadmap for identifying true catalysts, eliminating impurity-driven errors, and ensuring reliable research outcomes. Designed primarily for handling ...

To find the best threshold that can optimally classify each residue as catalytic or non-catalytic, predictions were made for each test data at a given threshold and the averaged performance ...

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