UCBSHIFT 2.0

Tech ID: 34123 / UC Case 2025-170-0

PATENT STATUS

Patent Pending

BRIEF DESCRIPTION

The identification of chemical shifts is a foundational step in determining a protein's three-dimensional structure via Nuclear Magnetic Resonance (NMR) spectroscopy. Current computational methods often struggle with accuracy and efficiency, particularly in handling the complex influence of protein side chains on shift values. UCBShift 2.0, a technology by UC Berkeley researchers, addresses this critical bottleneck by providing a highly accurate chemical shifts identifier. This innovation is a computational tool that includes a sequence transfer predictor for initial protein analysis, a novel machine learning module to predict side chain shifts, and a regressor that combines these outputs to produce a highly accurate predicted chemical shift for the entire protein. By specifically leveraging augmented feature extraction that includes side chain information, UCBShift 2.0 achieves greater predictive power and speed compared to existing methods, streamlining the time-consuming process of protein structure determination.

SUGGESTED USES

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Accelerating Protein Structure Determination: Expediting the initial stage of NMR-based protein structure studies by quickly and accurately assigning chemical shifts.

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High-Throughput Analysis: Enabling the rapid computational analysis of large libraries of protein sequences to predict their potential NMR characteristics.

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Validation of Experimental Data: Serving as a cross-validation tool for researchers to check the quality and accuracy of their experimentally determined chemical shift assignments.

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Drug Discovery and Design: Assisting in the analysis of protein-ligand interactions by providing reliable baseline chemical shifts.

ADVANTAGES

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Superior Accuracy: Incorporates augmented feature extraction specifically including side chains into the machine learning module, leading to more accurate shift predictions than conventional methods.

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Computational Efficiency: The sequential and modular design, including a dedicated sequence transfer predictor and regressor, offers a faster alternative to computationally intensive *ab initio* or quantum mechanical calculations.

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Handles Complex Structures: Improved capability in predicting shifts for challenging and conformationally flexible regions of a protein due to the enhanced feature set.

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INVENTORS

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OTHER INFORMATION

CATEGORIZED AS

» **Biotechnology**

» Bioinformatics

» **Computer**

» Software

» **Research Tools**

» Bioinformatics

RELATED CASES

2025-170-0

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Streamlined Workflow: Simplifies the data processing step for researchers working with NMR data, allowing them to focus on downstream structural analysis.

RELATED MATERIALS

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