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A predictive model for methionine oxidation propensity in therapeutic protein

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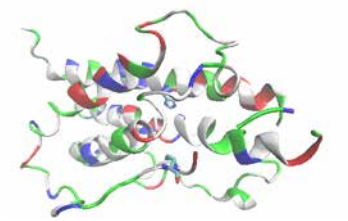
Methionine is one of the amino acids that are subjected to oxidation, and can subsequently lead to loss of molecular bioactivities or induce certain health conditions. Typically multiple methionine residues are present in protein molecules, and their oxidation characteristics can be dramatically different. The secondary structures, hydrophobicity, local chain flexibility, and solvent accessibility are all contributing factors to the oxidation propensity of these methionine residues. In this work, a predictive model has been developed to correlate the methionine residual oxidation propensities with their aforementioned properties. The model proteins used in this study, including monoclonal antibodies, growth hormone, interferons, etc., have all been investigated experimentally on their methionine oxidation propensity, and well resolved protein crystal structures documented in RCSB Protein Data Bank (PDB). The crystal structures of these proteins were optimized using QwikMD simulation program (UIUC) to produce well solvated structures. These properties of each methionine residue in the proteins, including hydrophobicity, local chain flexibility, and solvent accessibility, etc., were quantified and a mathematical model was developed to correlate them with the rank ordering of their oxidation propensities reported in literatures. The model, once further validated, provides a qualitative prediction tool to rank order methionine oxidation propensity in protein molecules that are complementary to experimental investigation approaches.



Biography

Anne Li is a Senior at Wootton High School with interest in Biological Chemistry. She takes an active role in the STEM field at her schools as the President of both Chemistry Club and Biology Club. Through her experience with the National Chemistry Olympiad and internship at the National Foundation for Cancer Research, she has been able to apply what she has learned in the classroom to help the mission to find a cure for cancer.

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