Exploring Keratinases for Efficient Keratin Recovery

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Abstract:
Keratin from human hair represents a high-value biomaterial with broad biomedical potential. Although ionic liquids (ILs) and keratinases have individually been utilized to enhance keratin hydrolysis, their synergistic application for sustainable extraction is still largely unexplored. In this work, the structural stability of two keratinases—one from *Stenotrophomonas maltophilia* and the other from *Bacillus subtilis* —was examined using molecular models generated by AlphaFold2. All-atom molecular dynamics simulations of 200 ns duration were conducted in aqueous medium and in six selected ILs known for effective keratin dissolution. Keratinases stability was assessed through root mean square deviation (RMSD) and root mean square fluctuation (RMSF) analyses. The *S. maltophilia* keratinase maintained stability in water as well as in two ILs, namely 1-allyl-3-methylimidazolium chloride ([AMIM]Cl) and 1-butyl-3-methylimidazolium bromide ([BMIM]Br), whereas the *B. subtilis* keratinase remained stable only in [AMIM]Cl. These computational insights highlight the potential of integrating ILs with keratinases for environmentally responsible and efficient recovery of keratin from human hair waste, thereby contributing to sustainable biomaterial valorization strategies.