Development of thermostable CiP(Coprinus cinereus peroxidase) through in-silico design

김수진, 이정아, 김용환[1,*], 송봉근
한국화학연구원; [1]광운대학교
(metalkim@kw.ac.kr*)

Recently, there have developed many programs in the area of computational protein design. The B-factors of protein crystal structures reflect the fluctuation of atoms about their average positions. This computational approach is useful for analyzing the dynamic properties of proteins. The Rosetta Design server identifies low energy amino acid sequences for target protein structures. This software searches for amino acid sequences that pack well, bury their hydrophobic atoms and satisfy the hydrogen bonding potential of polar atoms. In this study, we devise new method to predict amino acid residue that raise thermal stability of peroxidase (recombinant CiP) utilizing two computational protein designs, Rosetta Design and B-factor profile. We found two amino acid sequences, Q70 and Q146, and those having high B-factor value expected to contribute thermal stability of protein. Starting from these points, we researched low energy amino acid sequence using Rosetta Design. As a result, our method predicted Q70L and Q147L in rCiP and these point mutations showed more thermally stable property than that from original sequence. In the future, we will test about the relationship between these sequence and thermal stability of rCiP.