

Elucidation of packing enhancement effect on the protein conformational stability

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At native state of protein, occluded surface and inner volume were investigated to have large portion in buried part of a protein¹). To consider the influence of occluded surface and inner volume to protein conformational stability and to describe hydrophobic interactions in buried part of a protein, packing-considered solvation energy model was developed. Packing-considered solvation energy model could discriminate the correctly folded forms in 25 native/decoy set more accurately than other solvation energy models²). This model could be suitable for accurate prediction of hydrophobic interaction to protein structure and could be useful for rational design of stable protein structure. Especially, stabilized mutants of five hydrolases and one lyase were designed *in silico* using homology modeling. Stabilization effects of packing enhancement in buried area were predicted by packing-considered solvation energy model, and were validated with experimental results in literatures. Such results would be useful for reducing the experimental efforts to obtain stable protein structure.

Reference

1. Fleming PJ, Richard FM "Protein packing: dependence on protein size, secondary structure and amino acid composition" (2000) *J. Mol. Biol.*, Vol 299, 487-498.
2. Juffer A, Eisenhaber F, Hubbard SJ, Walther D, and Argos P "Comparison of atomic solvation parameter sets"(1995) *Protein sci*, Vol 4, 2499-2509.