

Fragment molecular orbital study of hydration effects on enzyme-substrate complex of nylonoligomer hydrolase

Hiroyuki Ando¹, Yasuteru Shigeta*^{1,2}, Takeshi Baba¹, Chizuru Watanabe³,
Yuji Mochizuki⁴, and Masayoshi Nakano¹

¹ Graduate School of Engineering Science, Osaka University, Toyonaka 560-8531, Japan.

²CREST Project, Japan Science and Technology Agency, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

³Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan.

⁴Department of Chemistry, Faculty of Science, Rikkyo University, 3-34-1 Nishi-ikebukuro, Toshima-ku, Tokyo 171-8501, Japan.

Abstract

An enzyme NylB [1], which catalyzes the hydrolysis of the Ahx-linear dimer (ALD) into the aminohexanoic acid (Ahx), has attracted much attention from the viewpoint of a possible solution for environmental problems. We have performed the structural characteristics of NylB and its mutant by means of molecular dynamics simulation [2]. In order to design the highly active enzyme, it is important to know the detailed information of interaction between the enzyme and the substrate. In this study, we quantitatively analyzed the inter-fragment interaction energy (IFIE) difference between hydrated and dehydrated structures of NylB-ALD complex using the fragment molecular orbital (FMO) method [3,4], and found that the interaction energy between substrate and enzyme is about -220 kJ/mol for dehydrated and -360 kJ/mol for hydrated condition, respectively, indicating the hydration effects is of great importance for forming the enzyme-substrate complex.

References

- [1] S. Negoro, T. Ohki, N. Shibata, K. Sasa, H. Hayashi, H. Nakano, K. Yasuhira, D. Kato, M. Takeo, Y. Higuchi, *J. Mol. Biol.* **370**, 142-156 (2007).
- [2] T. Baba, K. Kamiya, T. Matsui, N. Shibata, Y. Higuchi, T. Kobayashi, S. Negoro, Y. Shigeta, *Chem. Phys. Lett.* **507**, 157-161 (2011).
- [3] Y. Mochizuki, K. Yamashita, K. Fukuzawa, K. Takematsu, H. Watanabe, N. Taguchi, Y. Okiyama, M. Tsuboi, T. Nakano, and S. Tanaka, *Chem. Phys. Lett.* **493**, 346-352 (2010).
- [4] S. Tanaka, C. Watanabe, and Y. Okiyama, *Chem. Phys. Lett.* **556**, 272-77 (2013).