Quantum chemical analysis of the hydrogen bond interactions in secondary structures of proteins with Negative Fragmentation Approach

Yu Takano[1,2], Hiroko X. Kondo[1,3], and Haruki Nakamura[2]

[1] *Graduate School of Information Sciences, Hiroshima City University, Hiroshima 731-3194 Japan*

[2] *Institute for Protein Research, Osaka University, Suita 565-0871 Japan*

[3] *Faculty of Engineering, Kitami Institute of Technology, Kitami, 090-8507, Japan*

Hydrogen bond (H-bond) is one of the major factors that build the macromolecular structures of proteins, nucleic acids and their complexes. In particular, pair-wise H-bonds in protein backbones are essential to form their characteristic three-dimensional (3D) structures based on their ordered secondary structures, α-helices and β-sheets. Therefore, their structural energies should be correctly computed for analyses and predictions of protein 3D structures.

In this study, we have investigated the hydrogen bond interactions in secondary structures, α-helices, β-sheets, and turns by precise DFT calculations, followed by a negative fragmentation approach to extract a local interaction between molecular fragments [1–3]. Our computation showed that the reduced H-bond energy in α-helix originated from the depolarizations of both the H-bond donor and acceptor groups, due to the repulsive interactions with the neighboring polar peptide groups in the α-helix backbone [1].

References

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