

Global Optimization by Conformational Space Annealing and its Applications to Various Biological Systems

Jooyoung Lee

Center for In Silico Protein Science and School of Computational Sciences
Korea Institute for Advanced Study
207-43 Cheongnyangni 2-dong, Dongdaemun-gu,
Seoul 130-722, Korea
E-mail: jlee@kias.re.kr
Web-page: <http://lee.kias.re.kr>

One of the fundamental goals of modern sciences is to understand the nature of life, and deciphering the protein structure and its working mechanism lies at the very heart of this agenda. Due to the tremendous success of many genome projects, the number of available protein sequences reached over 5.3 million as of 2007, but less than 1% of these protein structures are known. Reliable and accurate protein structure prediction using only the sequence information is greatly in demand, but it remains as an unsolved problem even after many years of efforts. We intend to establish a successful protein modeling method that is solely based on direct application of principles excluding human interference in modeling steps. This should be contrasted to the common conception in the field that human expertise accumulated by many years of protein modeling is the most important asset for accurate protein structure prediction. In this talk we will discuss recent progresses of our efforts in protein structure prediction. It appears that our newly proposed method, which is based on the direct and rigorous optimization of relevant score functions, can provide significant improvement for 3D modeling of proteins in the category of High-Accuracy Template-Based Modeling. Applications of highly accurate proteins 3D models to various biological systems will be discussed.

Acknowledgments: Computation was carried out using KIAS Supercomputers (Center for Advanced Computation) and this work was supported by Korea Science and Engineering Foundation (KOSEF) and Korea government (MEST) by the grant number: 2009-0063610.

References

- [1] Keehyoung Joo, Jinwoo Lee, Sunjoong Lee, Joo-Hyun Seo, Sung Jong Lee, and Jooyoung Lee, *Proteins* **69**, 83-89 Suppl. 8 (2007).
- [2] Keehyoung Joo, Jinwoo Lee, Ilsoo Kim, Sung Jong Lee and Jooyoung Lee, *Biophys. J.* **95**, 4813-4819 (2008).
- [3] Keehyoung Joo, Jinwoo Lee, Joo-Hyun Seo, Kyoungrim Lee, Byung-Gee Kim, Jooyoung Lee, *Proteins* **75**, 1010-1023 (2009) .
- [4] Elmar Krieger, Keehyoung Joo, Jinwoo Lee, Jooyoung Lee , Srivatsan Raman, James Thompson, Mike Tyka, David Baker, and Kevin Karplus, *Proteins* **77**, 114-122 Suppl. 9 (2009).
- [5] Mina Oh, Keehyoung Joo, Jooyoung Lee, *Proteins* **77**, 152-156 Suppl. 9 (2009).
- [6] Jae-Sung Woo, Jae-Hong Lim, Ho-Chul Shin, Min-Kang Suh, Bonsu Ku, Kwang-Hoon Lee, Keehyoung Joo, Howard Robinson, Jooyoung Lee, Sam-Yong Park, Nam-Chul Ha and Byung-Ha Oh, *Cell* **136**, 85-96 (2009).
- [7] Keehyoung Joo, Juyong Lee, Sangjin Sim, Sun Young Lee, Kiho Lee, Seungryong Heo, In-Ho Lee, Sung Jong Lee Jooyoung Lee, *Proteins* (2013).
- [8] Young Kwan Kim, Mi-Jeong Kwak, Bonsu Ku, Hye-Young Suh, Keehyoung Joo, Jooyoung Lee, Jae U. Jung and Byung-Ha Oh, *Acta Crystallography, D* **69**, 1587-1597 (2013)