

## Publications

### – English

- (1) “QM/MM Simulations of Vibrational Spectral in Bacteriorhodopsin and Channelrhodopsin-2” K. Welke, H. C. Watanabe, T. Wolter, and M. Elstner *Phys. Chem. Chem. Phys.* (2013) **15**, 6651-6659
- (2) “Towards an understanding of channelrhodopsin function: Simulations lead to novel insights of channel mechanism” H. C. Watanabe, K. Welke, D. J. Sindhikara, P. Hegemann, and M. Elstner *J. Mol. Biol.* (2013) **425**, 1795-1814
- (3) “Rotamer Decomposition and Protein Dynamics – Efficiently Analyzing Dihedral Populations from Molecular Dynamics” H. Watanabe, M. Elstner, and T. Steinbrecher *J. Comp. Chem.* (2013) **34**, 3, 198-205
- (4) “Structural model of channelrhodopsin” H. C. Watanabe, K. Welke, F. Schneider, S. Tsunoda, F. Zhang, K. Deisseroth, P. Hegemann, and M. Elstner, *J. Biol. Chem.* (2012) **287**, 10, 7456-7466
- (5) “Color Tuning in Binding Pocket models of the Channelrhodopsin” K. Welke, J. Fraehmcke, H. C. Watanabe, P. Hegemann, and M. Elstner, *J. Phys. Chem. B* (2011) **115**. 15119-15128
- (6) “Molecular Mechanism of long-range synergetic color tuning between multiple amino acid residues in conger rhodopsin” H. C. Watanabe, Y. Mori, T. Tada, S. Yokoyama, and T. Yamato *Biophysics* (2010) **6**, 67-78
- (7) “The theoretical modeling of O-intermediate structure of bacteriorhodopsin” H. C. Watanabe, T. Ishikura, T. Yamato *Proteins*, (2009) **75**, 1, 53-61
- (8) “Spectral tuning of Photoactive yellow protein” T. Yamato, T. Ishikura, T. Kakitani, K. Kawaguchi, and H. Watanabe *Photochem. Photobiol.* (2007) **83**, 323-327

### – Japanese

Prospects of FCS: Hiroshi Watanabe *Computation Center NEWS, Nagoya University* **6**, 4, 361-366