

## Publications

- [1] Y. Mizuhara, M. Takano, “Biased Brownian motion of KIF1A and the role of tubulin’s C-terminal tail studied by molecular dynamics simulation”, *Int. J. Mol. Sci.*, **22**, 1547(10 pages) (2021).
- [2] H. Sato, M. Sugishima, M. Tsukaguchi, T. Masuko, M. Iijima, M. Takano, Y. Omata, K. Hirabayashi, K. Wada, Y. Hisaeda, K. Yamamoto, “Crystal structures of hydroxymethylbilane synthase complexed with a substrate analog: A single substrate-binding site for four consecutive condensation steps”, *Biochem. J.*, **478**, 1023-1042 (2021).

## Presentations

- [1] J. Ohnuki, M. Takano, “Electrostatic ratcheting mechanism of peptide synthesis by nonribosomal molecular machine”, The 58th Annual Meeting of Biophysical Society of Japan, Online, Sept. 2020.
- [2] Y. Taguchi, Y. Mizuhara, J. Ohnuki, M. Takano, “Role of C-terminal tail of tubulin in microtubule kinesin binding”, 58th Annual Meeting of Biophysical Society of Japan, Online, Sept. 2020.
- [3] 大貫隼, 高野光則, “誘電アロステリーによるアクチン繊維の脱重合機構”, 第1回生体分子シミュレーション・モデリング研究会, オンライン開催, 2021年3月.

## Research Summary

- We conducted the coarse-grained and the all-atom molecular dynamics simulations of KIF1A-microtubule system, and elucidated the physical mechanism behind the biased Brownian motion of the molecular motor and the role of the C-terminal tail of the tubulin.
- We conducted the all-atom molecular dynamics simulation of heme-precursor synthase using the newly-solved structure, and provided an insight into the physical mechanism of the successive reaction mechanism.
- We conducted the all-atom molecular dynamics simulation of peptide synthesis by a non-ribosomal molecular machine using the newly-solved structure, and provided an insight into the physical mechanism of the successive reaction mechanism.
- We analyzed the piezoelectric allostery and the dielectric allostery involved in the regulatory mechanism of the actin filaments.