ASI 杉田理論生物化学研究室

誌 上 発 表 Publications

[雑誌]

(原著論文) ＊印は査読制度がある論文誌

Re S., Miyashita N., Yamaguchi Y., and Sugita Y.: "Structural Diversity and Changes in Conformational Equilibria of Biantennary Complex-Type N-Glycans in Water Revealed by Replica-Exchange Molecular Dynamics Simulation", Biophys. J. **101**, No. 10, pp. L44–L46 (2011). ＊

Imai T., Miyashita N., Sugita Y., Andriy K., Hirata F., and Kidera A.: "Functionality Mapping on Internal Surfaces of Multidrug Transporter AcrB Based on Molecular Theory of Solvation: Implications for Drug Efflux Pathway", J. Phys. Chem. B **115**, No. 25, pp. 8288–8295 (2011). ＊

Shibata N., Sato H., Sakaki S., and Sugita Y.: "Theoretical Study of Magnesium Fluoride in Aqueous Solution", J. Phys. Chem. B **115**, No. 35, pp. 10553–10559 (2011). ＊

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Ogushi F., Ishitsuka R., Kobayashi T., and Sugita Y.: "Rapid flip-flop motions of diacylglycerol and ceramide in phospholipid bilayers", Chem. Phys. Lett. **522**, 96–102 (2012). ＊

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Ogushi F., Ishitsuka R., Kobayashi T., and Sugita Y.: "Flip-flop motions of ceramides, diacylglycerols, and cholesterols in phospholipid bilayer systems", ISSP/SOFT2010, (Institute of solid state physics, the Univ. of Tokyo), Kashiwa, Aug.–Aug. (2010).

Pisliakov A. and Sugita Y.: "Computer Simulations Reveal Proton Transfer Pathways in Nitric Oxide Reductase", Frontiers in the Simulation of Macromolecules, Los Angeles, USA, Nov. (2010).

Pisliakov A. and Sugita Y.: "Water dynamics and proton transfer in nitric oxide reductase: Insights from computer simulations", 2nd Cold Spring Harbor Asia conference on Membrane Proteins: Structure and Function, (Cold Spring Harbor), Suzhou, China, May (2011).

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