Accepted Manuscript

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PII: S0005-2736(15)00438-1

DOI: doi: 10.1016/j.bbamem.2015.12.032

Reference: BBAMEM 82091

To appear in: BBA - Biomembranes

Received date: 1 November 2015 Revised date: 24 December 2015 Accepted date: 29 December 2015



Please cite this article as: Takaharu Mori, Naoyuki Miyashita, Wonpil Im, Michael Feig, Yuji Sugita, Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms, *BBA - Biomembranes* (2016), doi: 10.1016/j.bbamem.2015.12.032

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ACCEPTED MANUSCRIPT

Molecular Dynamics Simulations of Biological Membranes and Membrane Proteins Using Enhanced Conformational Sampling Algorithms

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Keywords

Generalized Born (GB) model, generalized-ensemble algorithm, replica-exchange molecular dynamics (REMD), replica-exchange umbrella sampling (REUS), surface-tension REMD, replica exchange with solute tempering (REST).

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