CCS International Symposium 2020

12th Symposium on Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences

October 6, 2020

https://www.ccs.tsukuba.ac.jp/sympo20201006en/

Parallel Session 5: Life Science and Chemistry

Time: 16:20 – 17:37 (JST)

Place: https://zoom.us/j/93547549001

Convenor: Mitsuo Shoji (CCS, University of Tsukuba)

Time (5 + 2 min. each)	**Speaker (Affiliation)**	**Title**
16:20 – 16:27	Ryuhei Harada (Univ. of Tsukuba)	Developments of Computational Methods for Drug Design Based on PaCS-MD
16:27 – 16:34	Hiroaki Saito (Hokuriku University)	In silico molecular design of transmembrane peptide induces lipid flipping
16:34 – 16:41	Norifumi Yamamoto (Chiba Institute of Technology)	Theoretical Study on the Aggregation-Induced Emission
16:41 – 16:48	Kazutomo Kawaguchi (Kanazawa University)	Resting membrane potential and ion distribution by all-atom molecular dynamics simulations
16:48 – 16:55	Hiroaki Kumada (Univ. of Tsukuba)	Development of a core technologies for multi-modal treatment planning system with the high-speed and high-precision Monte Carlo dose calculation engine
16:55 – 17:02	Mitsuo Shoji (Univ. of Tsukuba)	Theoretical elucidations of chemical reactions by using large-scale molecular simulations
17:02 – 17:09	Yuki Nagata (Max Planck Institute for Polymer Research)	Accessing the accuracy of density functional theory through structure and dynamics of the water–air interface
17:09 – 17:16	Megumi Oya (Juntendo University)	Automatic target segmentation for whole breast irradiation using the 3D-UNet and

		its gradient-weighted class activation mapping analysis
17:16 – 17:23	Yasuteru Shigeta (Univ. of Tsukuba)	Theoretical studies on membrane permeability using molecular dynamics simulations
17:23 – 17:30	Hiroko Kondo (Kitami Institute of Technology)	Molecular dynamics study of an effect of mutations on the structure of the anti-HIV neutralizing antibody PG16
17:30 – 17:37	Hiromitsu Shimoyama (Kitasato University)	Atomistic Detailed Free-energy Landscape of Intrinsically Disordered Protein studied by Multi-scale Divide-and-conquer Molecular Dynamics Simulation