

CCS International Symposium 2021

**13th Symposium on Discovery, Fusion, Creation of New Knowledge
by Multidisciplinary Computational Sciences**

October 8, 2021

<https://www.ccs.tsukuba.ac.jp/sympo20211008en/>

Parallel Session 5: Life Science, Chemistry, Biology

Time: 16:15 – 17:11 (JST)

Place: <https://us02web.zoom.us/j/89031283499>

Convenor: HARADA Ryuhei (CCS, University of Tsukuba)

Time (5 + 2 min. each)	Speaker (Affiliation)	Title
16:15 – 16:22	SHOJI Mitsuo (Univ. of Tsukuba)	Theoretical Elucidations of Chemical Reactions by Using Large-scale Molecular Simulations
16:22 – 16:29	KUMADA Hiroaki (Univ. of Tsukuba)	Research of Realization for Comprehensive Dose Estimation System for Various Radiotherapy with PHITS, a High Accuracy Monte Carlo Code
16:29 – 16:36	OYA Megumi (RIKEN)	Investigation of Clinical Target Volume Segmentation for Whole Breast Irradiation Using Three-dimensional Convolutional Neural Networks with Gradient-Weighted Class Activation Mapping
16:36 – 16:43	SHIGETA Yasuteru (Univ. of Tsukuba)	Drug Repositioning for Covid-19 Main Protease
16:43 – 16:50	WATANABE Hiroshi (Keio University)	Proton Transfer Dynamics in Bulk Phase Using Adaptive QM/MM Method

16:50 – 16:57	INAGAKI Yuji (Univ. of Tsukuba)	The Phylogenetic Position of a Microeukaryote Strain SRT706 as Inferred from a 300-gene Analyses
16:57 – 17:04	TSUJIMURA Masaki (The Univ. of Tokyo)	Protonation State of the Key Residue Asp234 in Light-gated Anion Channelrhodopsin GtACR1
17:04 – 17:11	HARADA Ryuhei (Univ. of Tsukuba)	Developments of Computational Methods for Drug Design Based on Parallel Cascade Selection Molecular Dynamics (PaCS-MD) and its Applications