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P001	Midhun Kureekattil Madhu	Phosphorylation-Induced Allosteric Conformational Changes in a β2-adrenergic Receptor - Insights from Molecular Dynamics Simulations	Indian Institute of Science Education and Research Bhopal
P002	Yoshiki Hida	Analysis of membrane permeability of piracetam by using a variationally enhanced sampling and a free energy reaction route network method	Osaka Metropolitan University
P003	Takaharu Katsu	Comparison of β turn stabilities of L-Pro-Gly and D-Pro-Gly residues by using replica-exchange molecular dynamics simulations	Osaka Metropolitan University
P004	Riya Sharma	Cononsolvency in Triblock Copolymers: Insights from Molecular Dynamics Simulations	IIT KANPUR
P005	Yuki Mitsuta	Predicting the Biomembranes Permeability of Fentanyl and Its Analogues by Free Energy Reaction Route Network	Osaka Metropolitan University
P006	Teppei Yamada	Development of a secondary structure dependent protein backbone model for SPICA coarse-grained force field	Okayama University
P007	Yi-Chen Tsai	Integration of Structure-based Network Potentials with a Physics-based CG Model for Protein Folding Studies	National Cheng Kung University
P008	Donnifer Jr. Vailoces Reyes	In Silico Study and Synthesis Planning of α-Methyl β-Lactam- Chlorocatechol Derivatives as Potential Pseudomonas aeruginosa Penicillin-Binding Protein 3 (PBP3) Inhibitors	University of the Philippines Diliman
P009	James Peter Llego Lim	Investigating the Drug Resistance Mutations of HIV-1 Intasomes via Molecular Dynamics Simulations	University of the Philippines
P010	Jherome Brylle Woody Aresgado Santos	Molecular Dynamics Simulations on the Inhibitory Potentials of Dolutegravir derivatives Against HIV-1 Integrase	University of the Philippines Diliman
P011	Yusuke Miyazaki	Coarse-grained molecular dynamics study on lipid nanoparticles	Okayama University
P012	Fuga Watanabe	The Diffusivity of Intrinsically Disordered Proteins in Multicomponent Condensates	Keio University
P013	Kenta Shobu	Analysis of initial changes in the pore permeable to cations in channelrhodopsin-2	Keio University
P014	Ishioka Ryota	Analysis of dynamic properties of claudin-5 by MD simulation	Keio University
P015	Yui MATSUSHITA	How Multiple-domain Structures of TDP-43 Affects the Physical Properties of Membraneless Organelles Formed with RNA	Keio University
P016	Eiji Yamamoto	Mesoscale simulation of protein diffusion and localization in heterogeneous biological membranes	Keio University
P017	Saba - Ali	Enhancing Solubility and Binding of Oxyresveratrol through Inclusion Complexes with β-Cyclodextrins	Chulalongkorn University

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P018	Noriyuki Yasuda	Enhanced Solubility of 8-Bromobaicalein Through Inclusion Complexation With β-Cyclodextrins	Chulalongkorn University
P019	Nawanwat Chainuwong Pattaranggoon	Computational model for Lipid Binding Regions in Phospholipase (Ves a 1) From Vespa Venom	Chulalongkorn University
P020	Lipika - Oopkaew	CISPLATIN-LOADED CALCIUM CITRATE NANOPARTICLES AND THE QUANTUM MECHANICAL OF CISPLATIN-CITRATE COMPLEXES FOR LUNG CANCER TARGETED THERAPY	Chulalongkorn university
P021	Jia-Xian Yin	Investigation on the Binding Mechanism between CXCR3 and CXCL4L1	National Yang Ming Chiao Tung University
P022	Nalinee Kongkaew	Investigating the Binding Pathway of 2-Pralidoxime for Reactivating Organophosphate-Inhibited Human Acetylcholinesterase	Chulalongkorn University
P023	Shun Sakuraba	Free-energy calculation pipelines for biomolecules	National Institutes for Quantum Science and Technology
P025	Tuan Minh Do	Free-energy analysis of the effects of ATP on the Aβ(16-22) peptide fibrillation by all-atom molecular dynamics	Osaka University
P027	Chi Yuan Kao	Integrating RNA Synthesis and Bioluminescence Assay in a Platform to Evaluate Drug Efficacy against Nsp16/10 Complex	National Tsing Hua University
P028	Christopher Llynard Diasanta Ortiz	Frameshift-promoting PK induces a Rolled and Hyper-rotated 70S Ribosome	National Tsing Hua University
P029	Ahmed Mohamed Ragab	Accurate and efficient chemical similarity search tool and contact-distribution-matching method jointly identify FDA-approved drugs that modulate SARS-CoV2 -1PRF and suppress its replication	National Tsing Hua University
P030	Chih-Hui Lin	Using alternative conformations from MD simulations to develop new drugs targeting Omicron SARS-CoV-2 3CL protease by re-assembling chemical fragments of FDA-approved drugs.	National Tsing Hua University
P031	Zhang Yun Pei	Integrated Approach for Targeted Drug Discovery in Pancreatic Cancer: Combining Molecular Dynamics Simulations, Docking, and Free Energy Perturbation calculations	NTHU
P032	Yuan-Wei Ma	Integrating Molecular Dynamics Simulations, Fast Screening, and FEP/REST2 for Protein Stability Prediction: A Comprehensive Computational Approach	National Tsing Hua University
P033	Tong-You Lin	Integrating Protein Sequence, Structure, and Dynamic Features to Enhance Predictive Models for Pathogenicity of Single-Point Mutations	National Tsing-Hua University
P034	Fan Meng	The relationship between nanostructured bio-inspired materials surfaces and free energy barrier using coarse-grained molecular dynamics	Keio University

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P035	Meng-Chi Hsieh	The Possibility of Linker Rotation Induced CO2RR in MOF-253 Materials: The Comprehensive Discovery by Force Field and DFT Simulation	National Taiwan Normal University
P036	Chen-Cheng Liao	A Computational Perspective on Carbon-Carbon Bond Formation by Single Cu Atom on Pd(111) Surface for CO Electrochemical Reduction	National Taiwan Normal University
P037	Vy Thuy Nguyen	Interfacial Architectures Derived by Additives for High Yield Lithium Redox-Mediated Nitrogen Reduction to Ammonia	Chungnam National University
P039	Batjargal Sainbileg	Spin: an important factor in enhancing Oxygen Evolution Reaction - a case study on 2D Fe-MOF	National Taiwan University
P040	Hou-Jen Lai	Supported Iridium Clusters on TiO2: A Promising Catalyst for Methane Activation and Low-Temperature Steam Reforming of Methane	National Taiwan University of Science and Technology
P041	Chi-You Liu	Lowering the Overpotential via Excess Oxygen Molecules on Fe/C3N4 Nanotubes for Oxygen Reduction Reaction	NTNU
P042	Mangesh Bhendale	Molecular Insights on Mixed Micelles Formed by Ionic Surfactant and Nonionic Block Copolymer in Water Using Coarse-Grained Molecular Dynamics Simulations	Indian Institute of Technology Kanpur India
P043	SUDESHNA MADHUAL	Insights on Oxide Ion Transport In Yttria Doped Ceria from Molecular Dynamics Simulations	IIT Guwahati
P044	Akihiro Yamaguchi	All-atom molecular dynamics studies on the interfacial adhesion state of biodegradable polyesters and starch blends	Hitachi, Ltd.
P045	Takahiro Yokoyama	Self-assembled patterns of ABC triblock copolymers in confined nanoslit	Keio University
P046	Aindrila Indra	Understanding the Role of Polymers on the Nucleating Behavior of Water in Dilute Supercooled Solutions Using Molecular Dynamics Simulations	Indian Institute of Technology Kanpur
P047	Nanaka Yamamoto	Molecular dynamics study on the structures of the dry polymer brush composed of polyethylene or polyethylene glycol	University of Toyama
P048	Jiho Lee	Accurate Estimation of Room Temperature Li-Ion Conductivities in Argyrodite Li6PS5Cl Using Machine-Learned Potentials	Seoul National University
P049	Hirotaka Kishimoto	Hybrid molecular dynamics-Monte Carlo simulations: three-phase equilibrium analysis for methane hydrates	Keio University
P050	Mayu Hirose	A molecular dynamics study on the surface structure of alcohol-water mixture	University of Toyama
P051	Chou-Hsun Yang	Theoretical studies on ultrafast intramolecular triplet-triplet annihilation	Academia Sinica
P052	Kokoro Shikata	Revealing the hidden dynamics of confined water in acrylate polymers: Insights from hydrogen-bond lifetime analysis	Osaka University

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P054	Purun-hanul Kim	Exploring wet etching of GaN using molecular dynamics simulation with neural network potential	Seoul National University
P055	Riya Gupta	Role of Dimensionality on Excitonic and Polaronic properties of Heavy Pnictogen Chalcohalides from Many-body Perturbative Methods	Indian Institute of Technology Delhi
P056	Jaehoon Kim	Investigation of TaNx-Cu Interface Using Machine-Learned Potentials	Seoul National University
P057	Sangmin Oh	Atomistic simulation of silicon nitride etching by fluorocarbon using machine-learned potentials	Seoul National University
P058	Sajjan Sheoran	Emergence of Cubic Ordered Persistent Spin Textures in Expanded Brillouin Zone Regions	Indian Institute of Technology Delhi
P059	Ankita Phutela	Strain-driven topological quantum phase transition in (pseudo)-cubic Cs/MA/FA (mixed)-halide perovskites	Indian Institute of Technology Delhi
P060	Kojiro Suzuki	Effect of the chemical structure of surfactants on the stability of concentrated O/W emulsions: A dissipative particle dynamics study	Keio University
P061	Shota Goto	Non-Gaussianity and dynamic heterogeneity in ring polymer melts	Osaka University
P062	Yuchi Kao	Simulating Adsorption and Activation of Molecules in Zirconium-Based Metal-Organic Frameworks with QM/MM Methods	National Taiwan University
P063	Yen-Yung Wu	Zeolite nanosheets as organic solvent reverse osmosis (OSRO) membranes for ethanol/water separation	National Taiwan University
P064	Takahiro Ikeda	Self-assembly and viscosity of the amphiphilic hard cubes under shear	Kyoto Institute of Technology
P065	Teppei Matsumura	Free-energy analysis of adsorption onto solid-liquid interfaces with all-atom MD simulation and a solvation theory	Osaka University
P066	Hsiu Feng Lu	The Optical Property of the TADF-based NIR-II Semiconducting Polymer Dots: A DFT Study	Academia Sinica
P067	Dinesh Kumar Dhanthala Chittibabu	Electrocatalytic Mechanism of N2 Reduction Reaction by single atom catalyst TM-BP	Chung Yuan Christian University
P068	Liang-Yao Huang	Molecular Dynamics Simulation Study on the Role of Cysteine in the Nucleation of CO2 Hydrates	National Taiwan University
P069	Shun Imamura	Anomalous heat transfer of water in a nanochannel by molecular dynamics simulation	Keio University
P070	Youxuan Chen	Molecular-Simulation-Driven Improvement of the BJH Method for Accurate Pore Size Analysis	National Central University
P071	Hsuan Chu Chen	Application of Flat Histogram Monte Carlo Method for Binary Mixture Adsorption in Porous Materials	National Taiwan University
P072	Shang-Wei Lin	Probing the MOF Self-assembly with Molecular Dynamics Simulation	Fu Jen Catholic University

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P073	Ken Sasaki	Coarse-grained molecular simulation for mechanical properties of composites with polymer-tethered nanoparticles	Keio-university
P074	Fumiki Takano	Tracking the melting process of polymer lamellar structures by local order parameters	Kogakuin University
P075	Kenshin Mukae	Molecular dynamics simulation of small molecules dissolved in polymer	Osaka University
P076	Nam Hoang Truong	Designing of electrochemical nitrogen reduction reaction catalysts: A first-principles study	Chungnam National University
P077	Phuong Minh Nguyen	Computational Design of MoX2 (X= S, Se, and Te) based Electrocatalysts for Ammonia Production	Chungnam National University
P078	Phan Thi Yen Nhi	First-principles investigation to improve the electrochemical properties and stability of spinel structures cathodes for lithium-ion batteries	Chungnam National University
P079	YINGXIAO XI	Development of a cat-GRRM/MC/MD method to study crosslinking processes and physical properties: Role of molecular catalysts	TOHOKU University
P080	Yuuki Ishiwatari	Analysis of the molecular structure dependence on the critical packing parameter using machine learning and molecular simulation	Keio University
P081	Sourabh Singha	Computational workflow for investigating hydrogen permeation rate in novel hydrogen storage materials	IIT Bombay
P082	Ying-Li Hu	Electroreduction of CO2 to Hydrocarbons on Disordered Copper-Based Alloys: A DFT study	National Taiwan University of Science and Technology
P083	Mei-Ru Lai	The Role of Aggregative Solvation Structures in Localized High-Concentration Electrolytes for Enhancing Electrochemical Performance of Lithium Metal Battery	National Taiwan University of Science and Technology
P084	Shi-Hong Xu	A DFT study on Suppressing O2 formation in Ni-rich NCM811 Cathode Material by S and Cl doping towards improved electrochemical stability	National Taiwan University of Science and Technology
P085	Shih-Huang Pan	Characterizing the Impact of Mg-Doped Li Metal Anode and Electrolyte Additives for Stabilizing Solid-Electrolyte Interface: A Theoretical Study	National Taiwan University of Science and Technology
P086	Li Han Wang	New Insights into Interfacial Properties of the Argyrodite Li6PS5Cl and Magnesium Compounds by First-Principles Calculations	National Taiwan University of Science and Technology
P087	Muhammad Ruslan Novianto	Structural Stability of Zeolitic Ices Augmented by the Inclusion of Hydrogen Molecules	Brawijaya University
P088	Satoki Ishiai	Unsupervised learning method using graph neural network for ice interface molecular dynamics simulation	Keio University
P089	Grzegorz Lazarski	Tool assisted development of glycosaminoglycan (GAG) parameters for the SPICA forcefield	Jagiellonian University / Okayama University

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P091	yano kentaro	Graph neural networks for structural classification of glass-forming liquids: Unveiling the prediction framework	osaka university
P092	Kai-Yuan Kuan	Predictions of Selectivity and Kinetic Isotope Effects for Reactions with Nonclassical Dynamics from Trajectories with Machine-Learned Forces	Academia Sinica
P093	Takeo Sudo	Quantitative classification of self-assembly of amphiphilic molecules by combining molecular simulation and machine learning	Keio University
P094	Jerwin Collado Quirante	In Silico Design and AI-Guided Synthesis of Cytidine Derivatives as Potential Inhibitor of SARS-CoV-2 RNA-Dependent RNA polymerase (RdRp)	University of the Philippines Diliman
P095	Venkata Siva Krishna Sanagavarapu	Petascale Brownian dynamics simulations of highly resolved polymer chains with hydrodynamic interactions using modern GPUs	Indian Institute of Technology Kanpur
P096	Zong Rong Ye	Transformer Based Compound Protein Interaction Model via 2D Representations	NTNU
P097	Liu Cheng Han	Molecular Dynamic Modeling DNA aptamer interact with target drug.	National Chung Cheng University
P098	Hsu-Kai Cheng	Predicting Potential Energies of Chemically Complex Alloys with Quantum Machine Learning	Academia Sinica
P099	Ying-Cheng Chen	Capturing the potential energy surface of large molecular clusters: deep learning of SchNet for 1 to 4-body interactions	Academia Sinica
P100	Huu Trong Phan	A neural network potential assisted first-principle exploration of the structure of mono-saccharides	National Tsing Hua University
P101	Seungwon Jeong	Force Field dependent structural and dynamical properties in lithium/ionic liquid electrolytes	Pohang University of Science and Technology (POSTECH)
P102	ĐỒNG CAO HIEU	Exploring energy landscape of neutral and protonated di-, tri- and tetra-glycine with assistance of neural network potentials	NTU
P103	Jia-Lin Chang	Theoretical study of the photoelectron spectra of the dimer of methylketene	Nationtal Taichung University of Education
P104	Hao Yu Kuo	Theoretical Investigations on the Mechanism of Decomposition of Hyponitrite Molecules	National Yang Ming Chiao Tung University
P105	Shubham Kumar	Low-energy electron attachment to citric acid: A mixed electronic structure and quantum dynamics study	Indian Institute of Technology Guwahati
P106	Masaki Hiratsuka	Vibrational Spectra of Water Molecules in Clathrate Hydrates with Machine Learning Force Field	Kogakuin University

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P107	Taichi Inagaki	Hybrid Monte Carlo Method with Potential Scaling for Canonical Multimodal Distributions and Relaxation Processes	Keio University
P108	Yuya Matsubara	Development of a solution statistical mechanics theory describing the molecular permeation through lipid membrane	Osaka University
P109	Kazuya Okita	Diffusion theory of molecular liquids based on the energy representation solution theory and application to solvation dynamics	Osaka University
P110	Yun-Chu Chou	A generic rotamer model to explain the temperature dependence of BSA protein fluorescence	Tamkang University
P111	Yuka Hamada	Free energy analysis of cosolvent effects on molecular association	Osaka Graduate School
P112	Ting-Yi Wei	Kinetics of human Cofilin1 and Ubiquitin dynamics modeling using VMD (Visual molecular dynamics)	National Chung Cheng University
P113	Yoshifumi Nishimura	Species-selective Quantum Chemical Nanoreactor: Accelerated Sampling of Complex Chemical Processes	Waseda University
P114	Théo P. Gonçalves	Aromaticity-Active Ligands in Catalysis	King Abdullah University of Science and Technology
P115	Brataraj Ghosh	Base Pair Compositional Variability Influences DNA Structural Stability and Hydration Dynamics	Academia Sinica