

8th ICRéDD International Symposium + Rising Star Program POSTER SESSION

PRESENTERS, POSTER NUMBERS AND POSTER TITLES

October 23rd, 2024

PRESENTER	No.	TITLE
Manussada Ratanasak	1	Exploring the Photolysis Mechanism of Propylene Oxide
Tsuyoshi Mita	2	Radical Diphosphination of Strained Small-Ring Molecules
Hikaru Matsumoto	3	Stabilization of Mono-P-Ligated Metal Complex on Polystyrene-Phosphine Monolith via Metal-Arene Interactions
Keisuke Kondo	4	Mechanochemical activation of lithium metal enabling rapid generation of organolithium species in air and their application to organic synthesis
Rikuro Takahashi	5	Studies for General Method of Silylenoid Generation from Silyl-Boronate Complex
Natsumi Hammyo	6	Synthesis of Oligosilane-Bridged Donor-Acceptor-Type Molecules
Priya Saha	7	Defluorinative Cross Couplings of Trifluoromethyl Arenes by Copper Photoredox Catalysis
Lian Duan	8	Integrative Study of Nitric Oxide Reductase: Conformational Changes, Proton Transfer Pathways, and Catalytic Mechanisms via QM/MM and MD Simulations
Hikaru Yamamoto	9	Investigation of novel alignment of n-conjugated acenes using crystalline molecular gear-box formed by triptycene and triadamantylphosphine
Ravindra Raut	10	Catalytic Asymmetric “Cracking” of Cyclopropanes

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PRESENTER	No.	TITLE
Natsuki Watanabe	11	Radial Distribution Function-based Data Sampling Method for Machine Learning Potential
Narendra Nath Pati	12	Strain-Based Template Free Synthetic Design for Subporphyrin
Kosaku Tanaka, III,	13	New Insights into Photoexcited Palladium Catalysis: Ketyl Radical Generation and Development of Organopalladium Reactions
Tavinder Singh	14	Amino Acid Synthesis Using the CO ₂ Radical Anion
Suvankar Debbarma	15	Solvent-Assisted, Visible-Light Induced, Photocatalyst-Free Aryl/Hydro-Carboxylation of Unactivated Alkenes Using the CO ₂ Radical Anion
Jintao He	16	Multi-omics analysis reveals intratumor heterogeneity in brain metastatic lung adenocarcinoma
Sota Kawamura	17	Mono-Selective Mechanochemical Nucleophilic Aromatic Substitution by <i>in Situ</i> Phase Transitions in Solids
Ken Hirose	18	Application of Virtual Ligand Strategy for Design of Boron-Based Lewis Acid Catalysts
Nowshin Farjana	19	Potential Intermediates in the Recycling Biosynthetic Pathway of Luminous Substrate in Firefly Squid Liver
Ayokanmi Joseph Aremu	20	Development of QSAR-ML Models and Quantum Chemical Analysis for Designing Diphenylamine Derivatives with Enhanced Antioxidant Properties

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PRESENTER	No.	TITLE
Zhi Jian Wang	21	Mechanically strengthening and morphogenesis of double network hydrogels via force-induced bond breaking and formation
Yuki Ide	22	Methods for Efficient Image Data Collection in Image-based Machine Learning Prediction System
Matthew Lowe	23	Mechanochemical Synthesis of Organosodiums
Borwornlak Toopradab	24	Design of Thioester-Based Inhibitors Targeting SARS-CoV-2 Main Protease Using QSAR and Machine Learning Models
Thanyada Rungrotmongkol	25	Unveiling the Antiviral Inhibitory Activity of Ebselen and Ebsulfur Derivatives on SARS-CoV-2 Using Machine Learning-Based QSAR, LB-PaCS-MD, and Experimental Assay
Yan Song	26	<i>Trans</i> -selective Carboxylative Radical Cyclization of 1,6-Dienes Induced by the CO ₂ Radical Anion
Shinichi Suda	27	Extension of Virtual Ligand Assisted Optimization (VLAO) Methods to 1,2-Bis(diphenylphosphino)ethane and Its Derivatives
Riho Somaki	28	Exploration of the Global Minimum and Conical Intersection with Bayesian Optimization
Yamato Ueno	29	In Silico Substrate Design to Facilitate Potential Side Reactions within the Reaction Path Network: Aryl Carboxylation of Alkenes
Yuma Nakamura	30	Exploration of Quantum-aided Ligand Generative Model for Rare Blood Diseases

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Satoshi Matsutani	31	Theoretical Studies on Asymmetric “Cracking” of Cyclopropanes
Soshi Ikuta	32	Development of an approximate calculation method for highly excited states in lanthanide systems
Shoya Kondo	33	Theoretical analysis of thin-layer film formation process based on the reaction path network: Reaction analysis of trimethylaluminium dimers on OH-terminated Si(001)
Akihiro Mutsuji	34	Theoretical analysis of intramolecular electron transfer reactions by an energy decomposition and extrapolation scheme and potential-crossing geometry optimization
Kiichi Ogata	35	Data set on Ce complexes and its application to machine learning
Ryunosuke Tomita	36	Molecular rotation-induced emission enhancement of NHC Cu(I) macrocyclic complex in crystalline media
Mahiro Takahashi	37	Mechanochemical Buchwald-Hartwig cross-coupling reactions of aromatic primary amines and their application to two-steps one-pot mechanochemical synthesis of unsymmetrical triaryl amines
Yohei Kojima	38	Proposal for an elementary reaction knowledge base for interpreting computational results of chemical reaction processes
Guotan Liu	39	Theoretical Calculation Study on Microscopic Mechanism and Mechanical Properties of Ti Surface Nitriding
Shijie Xu	40	Accurate and Fast Prediction of Protein pK _a by Protein Language Model

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Md Badiruzzaman	41	Gold Nanoparticle-Protein Conjugation Through N-Terminal Modification for Oriented Attachment
Hanyu Xiong	42	Successive Coupling Reactions on a Titanacyclopentene Complex
Shiyu Ma	43	Coupling of Cyclopentadienyl Ligand on Boronate substituted Titanacyclopentadienes
Kojiro Machi	44	A Framework for Reviewing Results of Automated Conversion of Structured Organic Synthesis Procedures from Literature
Md Sadikur Rahman Shuvo	45	Enhancing Enzymatic Breakdown of Polyethylene Terephthalate by Cutinase Tethering Hydrophobic Moiety at N-terminus
Lisa Connolly	46	Immobilization of Green Fluorescent Proteins Modified with an Alkyl Chain Groups at the N-Terminus Onto the Surface of Liposome
Yuya Maeda	47	N-terminal Modification of Antibodies Using Triazolecarbaldehyde Derivatives Containing a Fluorescent Dye
Mariko Kojima	48	Engineering of the active site of chitosanase to recognize hetero β -1,4-glycosidic linkage between GlcN and GlcNAc
Suh Young Yu	49	Stereospecific Establishment of bis- γ -Lactones via [2+2+1]-Cyclocarbonylation of Allenyl Glyoxylates
Aimin Zhang	50	The Aryne-based Synthesis of Dihydroquinolin-4-one and Chroman-4-imine Units through Regioselective Transformations of Sulfonylamides and Sulfinylamides
Jihye Lee	51	Kinetic Resolution of N-tosyl Tetrahydroquinolones through Noyori ATH
Hibiki Hatano	52	Development of a Highly Efficient Synthetic Route for Imidodiphosphorimidate (IDPi)