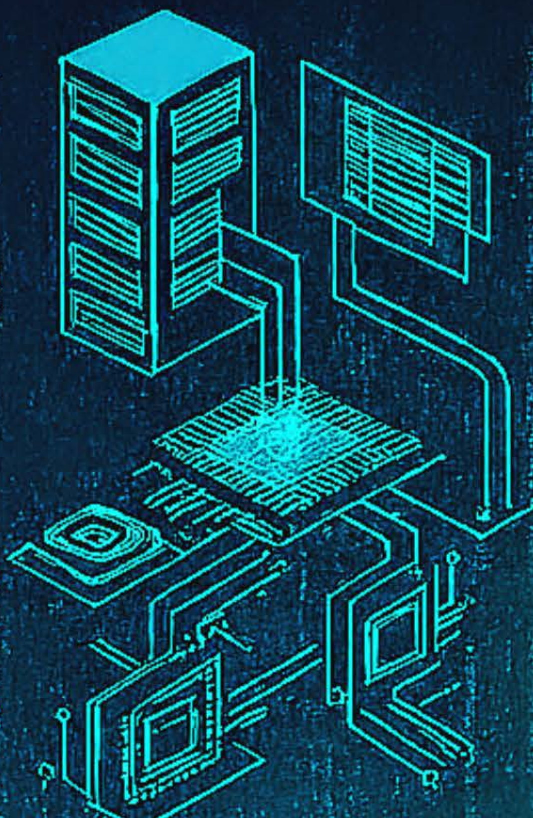
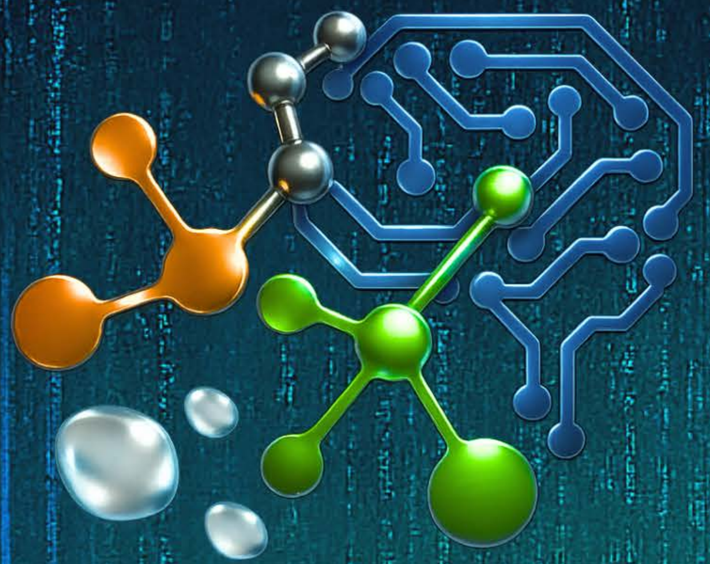
7th Conference on Advanced Organic Synthesis (CAOS-7)

&

Digitalization-driven Transformative Organic Synthesis 5th in Taiwan (Digi-TOS-5 in Taiwan)

JOINT INTERNATIONAL SYMPOSIUM





January 9 – 11, 2026

National Yang Ming Chiao Tung University
Hsinchu, Taiwan

7th Conference on Advanced Organic Synthesis
(CAOS-7)
&
Digitalization-driven Transformative Organic Synthesis 5th in Taiwan
(Digi-TOS-5 in Taiwan)

JOINT INTERNATIONAL SYMPOSIUM

CAOS-7/Digi-TOS-5
January 9 – 11, 2026
SB-210
National Yang Ming Chiao Tung University
Hsinchu, Taiwan

Organizing Committee of International Symposium DigiTOS-5/CAOS-7:
Prof. Tomoko Yajima (Ochanomizu University),
Prof. Yoshito Tobe (National Yang Ming Chiao Tung University)
Prof. Ilhyong Ryu (National Yang Ming Chiao Tung University)

Local Organizing Committee
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Yoshito Tobe
Wen-Sheng Chung
K.-K. Tony Mong
Chung-Ming Sun
Shih-Ching Chuang
Yen-Ju Cheng
Yen-Ku Wu
Yi-Lin Wu

Supports
Department of Applied Chemistry, NYCU
Center for Emergent Functional Matter Science, NYCU
Transformative Research Area (A): “Digitalized Organic Synthesis for Advanced and Precise Molecule Constructions”
Japan Society for the Promotion of Science

WELCOME

It is my great pleasure to welcome you to the Taiwan–Japan joint symposium combining Digi-TOS-5 (Digitalization-driven Transformative Organic Synthesis in Taiwan) and CAOS-7 (the 7th Conference on Advanced Organic Synthesis), held from January 9 to 11, 2026, at the Department of Applied Chemistry, National Yang Ming Chiao Tung University (NYCU), Taiwan. On behalf of the Department, I sincerely thank all speakers and participants for their enthusiastic participation. The symposium program highlights cutting-edge developments in organic synthesis, with particular emphasis on digitalization-enabled methodologies and sustainable synthetic strategies. We anticipate that the scientific exchanges will foster meaningful discussions, inspire new ideas, and further strengthen collaborative networks between Taiwan and Japan.

Sincerely yours,

Yen-Ju Cheng, Chairman, Department of Applied Chemistry, NYCU

PREFACE

I am delighted to welcome you to a Taiwan-Japan joint symposium of Digi-TOS-5 in Taiwan (Digitalization-driven Transformative Organic Synthesis in Taiwan) and CAOS-7 (the 7th Conference on Advanced Organic Synthesis), held on January 9–11, 2026, at the Hsinchu Campus of NYCU, Taiwan. On behalf of the Organizing Committee, I extend our warmest greetings to all participants joining this special event, which covers state-of-the-art topics in organic synthesis. We are confident that the three-day program will be highly fruitful through in-depth discussions and the strengthening of international collaborations among researchers, helping to shape the future of organic synthesis toward a sustainable society.

We would like to express our sincere gratitude to the Department of Applied Chemistry and the Center for Emergent Functional Matter Science at NYCU, as well as to MEXT, for their generous support. We are also deeply grateful to the secretaries of CEFMS, especially Ms. Yi-Ting Hsieh, for their invaluable assistance in the organization and smooth management of this symposium.

With best regards,

On behalf of the Organizing Committee

Takashi Oshima, Professor, Kyushu University,

Time Table

January 9 (Fri) (Day 1)

14:30 -	***Reception***
	Chairman: Yen-Ju Cheng (NYCU)
15:00-15:25	(S1) **Takashi Ohshima** (Kyushu University) *"Digitalization-driven Transformative Organic Synthesis (Digi-TOS)"*
15:25-15:50	(S2) **Yi-Lin Wu** (NYCU) *"Mechanism-Guided Design of a Bioorthogonal Reaction Platform: Controlling Reactivity and Selectivity in TAMM–Aminothiol Chemistry"*
15:50-16:15	(S3) **Seiji Suga** (Okayama University) *"Electro-organic Transformations on the Flow Systems"*
	--- Break---
	Chairman: Takashi Ohshima
16:30-16:55	(S4) **Cheng-Chung Wang** (Academia Sinica) *"Statistical Analysis: A New Perspective on Stereoselective Glycosylation"*
16:55-17:20	(S5) **Makoto Yasuda** (The University of Osaka) *"Machine Learning-Guided Design of Reactive Species and Catalysts for Selective Organic Transformations"*
17:20-17:45	(S6) **Wei-Yu Lin** (Kaohsiung Medical University) *"Sustainable Approaches to Selective Amide Bond Cleavage"*

Dinner --- 18:30 Ho Hotel

January 10 (Sat) (Day 2)

	Chairman: Makoto Yasuda
8:30-8:45	(S7) **Takashi Koike** (Nippon Institute of Technology) *“Generation and Reaction of Fluoroalkyl Radicals from Fluorinated Alkyl Benzoates by Photoredox Catalysis”*
8:45-9:00	(S8) **Tomoyuki Miyao** (Nara Institute of Science and Technology) *“In-silico Models for Reactivity Parameter Prediction”*
9:00-9:15	(S9) **Masaru Kondo** (University of Shizuoka) *“Bayesian Optimization-Assisted Multiparameter Screening of Flow Reaction Conditions”*
9:15-9:30	(S10) **Mikito Fujinami** (Waseda University) *“Integration of Computer Vision and Digital Technologies for Automated Recording of Chemical Experiments”*
9:30-9:45	(S11) **Yusuke Masuda** (Hokkaido University) *“Mechanistic Insights into Organophosphorus Radical Reactions Enabled by Combined Computational and Experimental Approaches”*
9:45-10:10	(S12) **Hsiao-Ching Yang** (National Tsing Hua University) “*Decoding MOF Proton-Driven Coordination and Nucleation Pathway via In Situ SWAXS and Molecular Dynamics Simulations”*

--- Break---

	Chairman: K. K. Tony Mong
10:20-10:35	(S13) **Kensuke Kiyokawa** (The University of Osaka) *“Synthesis of Aminobenziodoxolones and Their Application to Oxidative Amination of Arylboronic Acids”*
10:30-10:45	(S14) **Tomoya Miura** (Okayama University) *“Synthetic Transformations of 1,1-Di(boryl)propene Starting from Propyn”*
10:45-11:00	(S15) **Hidetoshi Noda** (Institute of Microbial Chemistry)

"A Catalyst Design for Selective Nitrene Transfers"

11:00-11:15 (S16) **Yuichiro Mutoh** (RIKEN)
"Transient η6-Coordination Enables Borylation of Arenes"

11:15-11:30 (S17) **Makoto Sako** (The University of Osaka)
"Development of Chiral Borinic Acid Catalysts and Their Applications to Enantioselective Reactions"

11:30-11:50 (S18) **Gary Jing Chuang** (Chung Yuan Christian University)
"Exploring the Reactivities of Bicyclo[2.2.2]octenones: From Solution to Solid"

--- Group Photo, Lunch & Poster Session ---

Chairman: Mahito Atobe

13:15-13:30 (S19) **Takafumi Yatabe** (The University of Tokyo)
"Product-Selective Dehydrogenative Aromatization Enabled by Supported Metal Nanoparticle Catalysts"

13:30-13:45 (S20) **Miho Hatanaka** (Keio University)
"Theoretical and Data-Driven Approaches to Lanthanide Photofunctional Materials"

13:45-14:00 (S21) **Hiroshi Ikeda** (Osaka Metropolitan University)
"Machine Learning-assisted Design and Characterization of Dithienobenzothiazole-Based Organic Semiconductors"

14:00-14:15 (S22) **Junichiro Yamaguchi** (Waseda University)
"Heteroaromatic Swapping and Stereoediting of Benzylic Alcohols"

14:15-14:30 (S23) **Shinya Shiomi** (Tokushima Bunri University)
"Formal Umpolung Synthesis of α-Branched Amides and Its Application to the Synthesis of MR16728"

14:30-14:45 (S24) **Yuki Nagashima** (The University of Tokyo)
"Computationally guided development of photoreactions using electropositive elements"

--- Break & Campus Walk ---

Chairman: Sung Hui-Ling

15:45-16:00 (S25) **Yuto Sumida** (Institute of Science Tokyo)

	“Photoinduced PCET-mediated C–C bond cleavage enaibling bond-reorganization”
16:00-16:15	(S26) **Tsuyoshi Mita** (Hokkaido University) *“Harnessing the CO2 Radical Anion for Molecular Scaffold Construction”*
16:15-16:30	(S27) **Takanori Iwasaki** (Kyushu University) *“Stable Yet Lewis-acidic Anions enabling Cooperative Catalysis with Cationic Transition Metal Complexes”*
16:30-16:45	(S28) **Yuki Saito** (The University of Tokyo) *“SiO2 Supported BArF as a Versatile Platform for Chiral Ir(I) Catalyzed Asymmetric Hydrogenations”*
16:45-17:00	(S29) **Naoki Noto** (Nagoya University) *“Transfer learning across different photoreactions”*
17:00-17:15	(S30) **Naoto Yamasaki** (Nagoya University) *“Efficient Synthesis of Cyclic (RGDfK) Using Microflow Reactor”*
17:15-17:30	(S31) **Yoichi Hoshimoto** (The University of Osaka) *“Triarylborane Catalysis with Crude H2”*
17:30-17:45	(S32) **Toshiyuki Itoh** (Kanazawa University) *“Design of Extremely Hygroscopic Ionic Liquids for The Liquid Desiccant-Type Air Conditioner”*

--- Dinner --- 19:00 菜園

January 11 (Sun) (Day 3)

Chairman: Kiyosei Takasu

08:30-08:45	(S33) **Jun Takaya** (Osaka University) *“Exploring Photochemistry of Boron-Based Frustrated Lewis Pairs”*
08:45-09:00	(S34) **Hiroyuki Miyamura** (National Institute of Advanced Industrial Science and Technology) *“Development of Highly Active Heterogeneous Bimetallic Nanoparticle Catalysts for Selective Hydrogenation and Its*

Application to Integrated Continuous-flow Organic Synthesis”

09:00-09:15 (S35) **Nobuyuki Mase** (Shizuoka University)
“Synthesis of novel plant hormones: Fine bubble and flow technology for fairy chemicals”

09:15-09:30 (S36) **Yoichi M. A. Yamada** (RIKEN)
“Nano-Structured Heterogeneous Catalysts in Batch and Flow”

09:30-09:45 (S37) **Takayuki Doi** (Tohoku University)
“Synthtetic Study for Neothioviridamide via the Formation of (Aminovinyl)- methylcysteine through Photocatalytic Oxidative Decarboxylation”

09:45-10:00 (S38) **Keisuke Fukaya** (Toyama Prefectural University)
“Computationally Guided Total Syntheses of Dimeric Pyrrole–Imidazole Alkaloids”

10:00-10:15 (S39) **Yuya Kakiuchi** (The University of Osaka)
“Discerning Reactivity of Metal-Nitrogen Multiple Bonds from15N Solid-state NMR Spectroscopy”

--- Break---

<u>Chairman: Takayuki Doi</u>

10:30-10:45 (S40) **Koji Oohora** (The University of Osaka)
“Artificial Enzymes Containing Non-natural Active sites”

10:45-11:00 (S41) **Tomoko Yajima** (Ochanomizu University)
“Visible light induced perfluoroalkylation of phenols”

11:00-11:15 (S42) **Ken-Ichiro Sotowa** (Kyoto University)
“Development and Application of Modular Automated Experimental System”

11:15-11:30 (S43) **Mahito Atobe** (Yokohama National University)
“Amido Bond Formation by Electrocatalytic Oxidation of Hemiaminals at Gold Electrodes”

11:30-11:45 (S44) **Ryosuke Kojima** (Kyoto University)
“Towards chemical reaction foundation model and synthetic route prediction tool”

11:45-12:00 (S45) **Kiyosei Takasu** (Kyoto University)

"Fused Cyclobutenes to trans-Cycloalkenes"

12:00-12:15 (S46) **Yusuke Sasano** (Tohoku University)
"Air-Stable Tetrazene Radical Cation Salts: Synthesis, Characterization, and Oxidation Catalysts"

--- Lunch ---

13:00- **Panel Discussion on**
Perspective in the Digitalization of Organic Synthesis
—Toward Data-Driven, Automated, and Predictive Molecular Construction—

Moderators: Tamio Hayashi (National Taiwan Normal University), Yoshito Tobe (National Yang Ming Chiao Tung University), Takashi Oshima (Kyushu University), Tomoko Yajima (Ochanomizu University), Naoto Chatani (Hiroshima University), Kazuyoshi Yamakawa (the University of Tokyo), Ilhyong Ryu (National Yang Ming Chiao Tung University)

--- Poster Presentation (Afternoon of 2nd Day) ---

P-1 **Airi Yamaguchi** (Ochanomizu University)
"Metal-Free Conversion of Amines to Perfluoroalkylated Amides via Visible-Light Photocatalyst"

P-2 **Ryotaro Shirai** (Waseda University)
"Pd-catalyzed carbon–carbon double bond cleaving difunctionalization of Vince lactam"

P-3 **Keisuke Kondo** (Hokkaido University)
"Arylation of Trialkyl Amines via C(sp3)–N Bond Cleavage Enabled by Organosodium Compounds"

P-4 **Miyuu Hattori** (Shizuoka University)
"Extrapolated Prediction of High Confidence Using Virtual Variables in Iodination of Polyfluoroperylene"

P-5 **Kanata Wada** (Osaka Metropolitan University)
"A SOMO–HOMO Inverted Radical Cation Derived from a Phenyl-substituted Highly Strained Cage Diketone"

P-6 **Dong-eun Yoo** (Hokkaido University)

“Selective Ring-Opening Monoaddition of Organopotassium Species to Lactones via Flash Microflow Technique”

P-7 **Shu-Fan Wu** (NYCU)
“ET-Induced Three-Component Coupling of Ketones, Alkenes, and BPSE. Reactivity Dependence on One-Electron Oxidizing Reagents

P-8 **Guganchandar Vedarethinam** (NYCU)
“Pd(II)-Catalyzed $C(sp^2)$*-H Alkenylation of 2-Amino Biaryls with Bulky Internal Alkynes: From Alkenylation to Orthogonal Policyclic Hydrocarbons”*

P-9 **Hung-Sheng Hsieh** (NYCU)
“Rh(III)-Catalyzed Regioselective [4+2] Annulation of 2-Benzyl-2H-indazole-6-carboxylic Acids with Ynamides to Access Indazole-Fused Pyrans”

P-10 **Cheng-Hsun Huang** (NYCU)
“Asymmetric Oxidative Dearomatization Using Chiral Hypervalent Iodine Catalysts: Enantioselective C-C Bond Formation Toward the Synthesis of Crinine-Type Alkaloids”

P-11 **Ke-Liang Chen** (NYCU)
“Catalytic Asymmetric Spirocyclizing Diels–Alder Reaction of α-Alkylidene Cyclic Vinylogous Esters Using a Chiral Oxazaborolidine Lewis Acid”

P-12 **Tzu-Hsuan Nancy Huang** (NYCU)
“Synthetic Strategy to Accomplish the Total Synthesis of Lipooligosaccharides of Mycobacterium gastri”

P-13 **Jing-Hui Zeng** (NYCU)
“Total Synthesis of Glycosyl Actinopyrone derivative and its Biosynthetic Precursor for Stereochemical Revision”

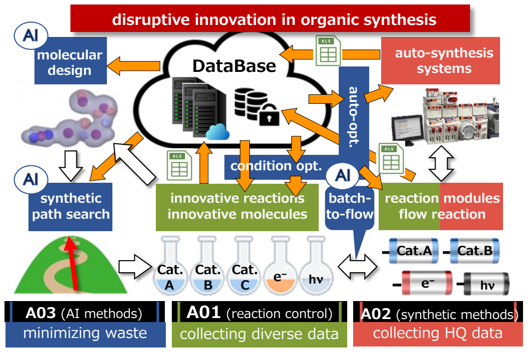
P-14 **Chia-Sheng Tsai** (NYCU)
“Synthesis of Multisubstituted Tellurophenes by S,O-Ligand Promoted Pd-Catalyzed C–H Olefination”

S1

Digitalization-driven Transformative Organic Synthesis (Digi-TOS)

Takashi Ohshima
Graduate School of Pharmaceutical Sciences, Kyushu University
E-mail: ohshima@phar.kyushu-u.ac.jp

Digitalization of organic reactions is essential for developing the next generation of organic synthesis with the aid of artificial intelligence (AI) and machine learning (ML). In this regard, we have recently launched the "Digitization-driven Transformative Organic Synthesis (Digi-TOS)", a unique digitization platform that promotes the integration of diverse fields of experimental chemistry and information science for transformative organic synthesis.[1] We are developing automated methods (molecular design, synthetic pathway search, reaction condition optimization, batch-to-flow conversion, and autonomous synthesis systems) that thoroughly leverage AI to accelerate the discovery of novel reactions and molecules. We are also building a highly reliable database (DB) that is optimized for ML in organic chemistry. In this presentation, I will outline three machine-learning–assisted approaches for data-driven organic synthesis.



Outline of “Digi-TOS” platform

First, we constructed a compact chemoselectivity data acquisition system using a functional group evaluation kit (FGE-kit).[2] The system rapidly generates functional-group compatibility information, and the resulting dataset provides a basis for ML-driven retrosynthetic model development.

Second, an activity-based ML model was applied to explore the drug-like chemical space efficiently. ML-proposed candidates were clustered, synthesized, and evaluated, enabling the discovery of compounds with activities exceeding those of the initial lead structures.

Third, an electrochemical method for converting bis-hydrazones into alkynes was optimized using ML. Parallel exploration of key electrolysis parameters yielded conditions that yielded 86% of diphenylacetylene in 20 experiments, and subsequent analysis identified factors governing the transformation.

[1] https://en.digi-tos.jp/

[2] Saito, N.; Nawachi, A.; Kondo, Y.; Choi, J.; Morimoto, H.; Ohshima, T. *Bull. Chem. Soc. Japan* **2023**, *96*, 465.

Takashi Ohshima was born in Ehime, Japan, in 1968. He received his Ph.D. from the University of Tokyo in 1996. He joined Otsuka Pharmaceutical Co. in 1996 and then The Scripps Research Institute as a Postdoctoral fellow in 1997. In 1999, he returned to the University of Tokyo as an Assistant Professor. He moved to Osaka University as an Associate Professor in 2005. He has been a Full Professor at Kyushu University since 2010.

S2

Mechanism-Guided Design of a Bioorthogonal Reaction Platform: Controlling Reactivity and Selectivity in TAMM–Aminothiol Chemistry

Yi-Lin Wu
Department of Applied Chemistry, National Yang Ming Chiao Tung University
E-mail: yilin.wu@nycu.edu.tw

Understanding and controlling reaction mechanism is central to the development of selective chemical transformations, particularly in complex molecular environments. I will present our recent studies on the condensation of 2-[(alkylthio)(aryl)methylene]malononitriles (TAMMs) with 1,2-aminothiols, focusing on reaction pathways, structure–reactivity relationships, and mechanistic control.

The TAMM–aminothiol reaction proceeds through thiolate exchange, cyclization, and competing elimination steps, with product distribution and kinetics dictated by substituent effects on the TAMM scaffold. Mechanistic analysis reveals how electronic and steric factors modulate these elementary steps, enabling a single reaction platform to be tuned for chemoselective and bioorthogonal protein labelling. Building on this foundation, sterically engineered *ortho*-substituted TAMMs were found to alter conformational dynamics and raise kinetic barriers for malononitrile elimination. Combined experimental, spectroscopic, and computational studies demonstrate unexpectedly that *ortho*-substituents stabilize enamine intermediates, leading to selective *N*-modification of terminal cysteine residues while preserving a free thiol functionality. This mechanistic control enables sequential and dual functionalization of peptides and proteins and introduces new molecular architectures for bioconjugation.

Together, these studies illustrate how detailed analysis of reaction pathways and energy landscapes can transform a single chemical transformation into a versatile and tunable platform for chemoselective synthesis in biologically relevant settings.

Yi-Lin Wu (吳宜霖),
MSc & PhD, ETH Zürich (2008 & 2012);
SNF Postdoctoral Researcher, Northwestern University (2012–2013);
Res. Asst. & Assoc. Professor, Northwestern University (2014–2018);
Lecturer & Senior Lecturer, Cardiff University (2019–2025);
Assoc. Professor, National Yang Ming Chiao Tung University (2025–).
Research Interests: Directing energy and charge flow pathways in dynamic supramolecular assemblies and reactive molecular ensembles.

S3

Electro-organic Transformations on the Flow Systems

Seiji Suga
Division of Applied Chemistry, Graduate School of Environmental, Life, Natural Science and Technology, Okayama University, Okayama, Japan
E-mail: suga@cc.okayama-u.ac.jp

Electro-organic transformations, which rely on electron-transfer processes occurring at electrode surfaces, provide a facile and environmentally benign means of accessing a wide range of valuable organic compounds. Our research group focuses on developing organic reactions mediated by electrochemically generated reactive species [1,2] (Figure 1a). In these systems, even a small amount of electron addition to, or removal from, the substrate can effectively promote the catalytic process [3,4] (Figure 1b). In particular, the latter reaction can be performed efficiently using an electrochemical flow reactor (Figure 2), and *machine-learning–based* optimization is highly effective in this process [5]. This approach also provides important insights into the reaction mechanism [6].

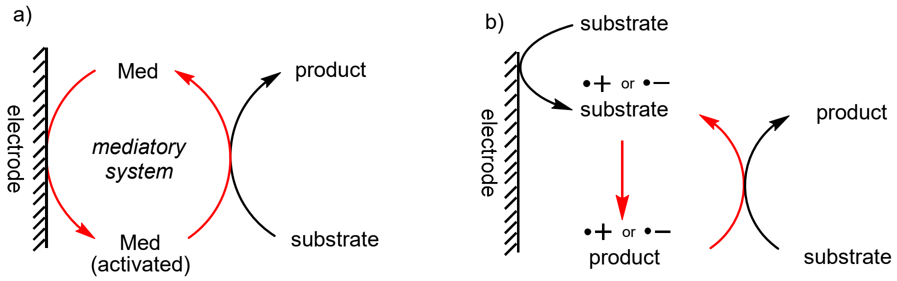


Figure 1. Electrochemical mediatory system and electron as a catalyst.

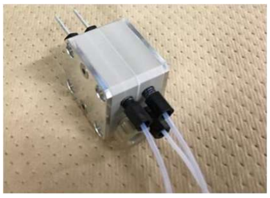


Figure 2. Flow Reactor

[1] Mitsudo, K.; Matsuo, R.; Yonezawa, T.; Inoue, H.; Mandai, H.; Suga, S. *Angew. Chem., Int. Ed.* **2020**, *59*, 7803–7807.

[2] Mitsudo, K.; Nagahara, T.; Kataura, N.; Okamura, Y.; Yonezawa, T.; Tachibana, Y.; Soltié, N.; Shigemori, K.; Sato, E.; Mandai, H.; Suga, S. *Commun. Chem.* **2025**, *8*, 366

[3] Sato, E.; Fujii, M.; Tanaka, H.; Mitsudo, K.; Kondo, M.; Takizawa, S.; Sasai, H.; Washio, T.; Ishikawa, K.; Suga, S. *J. Org. Chem.* **2021**, *86*, 16035–16044.

[4] Fujii, M.; Ueno, N.; Mitsudo, K.; Sato, E.; Suga, S. *Org. Lett.* **2025**, *27*, 6953-6958.

[5] Sato, E.; Tani, A.; Miyao, T.; Kunimoto, S.; Takizawa, S.; Mitsudo, K.; Suga, S. *Chem. Eur. J.* **2025**, *31*, e202501257.

[6] Okumura, Y.; Sato, E.; Mitsudo, K.; Suga, S. *JACS Au* **2025**, *5*, 3974-3981.

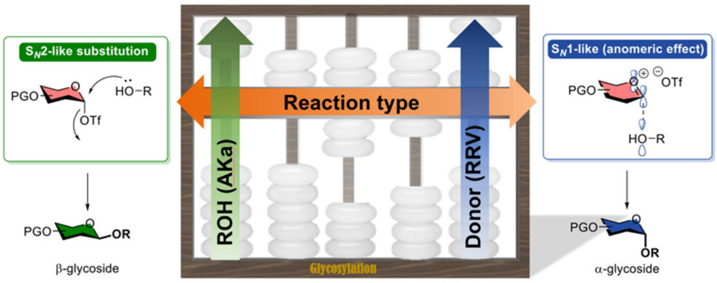
1995 Ph.D. Nagoya University (Prof. R. Noyori)
1995-1996 JSPS Postdoc, University of Oxford (Prof. J. E. Baldwin)
1996-1999 Assistant Professor, Kyoto University (Prof. J. Yoshida)
1999-2003 Lecturer, Kyoto University
2003-2008 Associate Professor, Kyoto University
2008-current Professor, Okayama University
2023-current Executive Director and Senior Vice President, Okayama University

S4

Statistical Analysis: A New Perspective on Stereoselective Glycosylation Reactions

Cheng-Chung Wang
Institute of Chemistry, Academia Sinica
E-mail: wangcc@chem.sinica.edu.tw

Carbohydrates are ubiquitous biomolecules that mediate numerous biological processes and exhibit important pathogenic effects. However, chemical synthesis of glycoconjugates has been hampered by challenges in glycosylation reaction, of which the stereoselectivity and yield are paramount but unpredictable. We develop a database composed of relative reactivity value (RRV) [1] and acceptor nucleophilic constant (Aka)[2] to quantify the reactivity of glycosyl donors and nucleophilicity of hydroxyl groups in glycosylation influenced by the steric, electronic and structural effects, providing a connection between experiments and computer algorithm. A diverse range of glycosylation donors and acceptors with well-defined reactivity and promotors were organized and processed by the designed program "GlycoComputer" for prediction of glycosylation reaction without involving sophisticated computational processing. The applicability of this system was further tested by the synthesis of a Lewis A skeleton to show that the stereoselectivity and yield can be accurately estimated.[6]



[1] Chang, C.-W.; Wu, C.-H.; Lin, M.-H.; Liao, P.-H.; Chang, C.-C.; Chuang, H.-H.; Lin, S.-C.; Lam. S.; Verma, V. P.; Hsu, C.-P.;* Wang, C.-C.* *Angew. Chem. Int. Ed.* **2019**, *58*, 16775-16779.

[2] Chang, C.-W.; Lin, M.-H.; Chan, C.-K.; Su, K.-Y.; Wu, C.-H.; Lo, W.-C.; Lam, S.; Cheng, Y.-T.; Liao, P.-H.; Wong, C-H.;* Wang, C.-C.* *Angew. Chem. Int. Ed.* **2021**, *60*, 12413-12423.

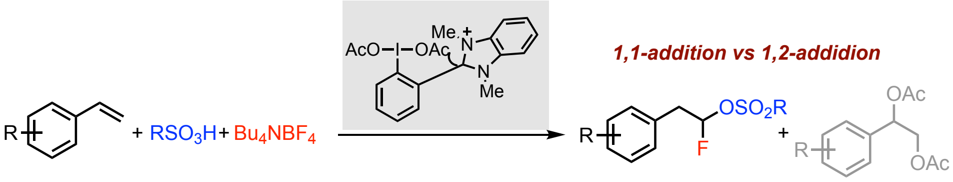
Dr. Cheng-Chung Wang received his Ph.D. from TIGP, Academia Sinica in 2007, followed by postdoctoral research at ETH and the Max-Planck-Institute. He joined the Institute of Chemistry, Academia Sinica in 2009, and was promoted to research fellow in 2022. His work centers on carbohydrate synthesis and AI-assisted glycosylation. His honors include the Carbosynth Oral Communication Prize (2018), Everlight Chemical Green Chemistry Thesis Award (2021), ACP Lectureship Award (2022), NSTC Outstanding Research Award, and Distinguished Alumnus of National Sun Yat-Sen University (2024).

S5

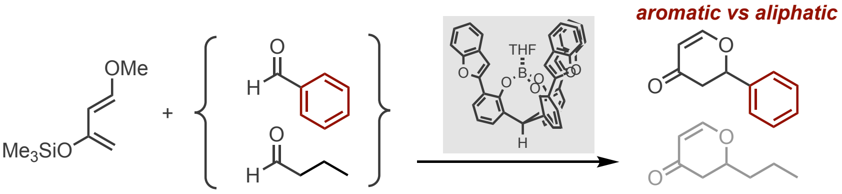
Machine Learning-Guided Design of Reactive Species and Catalysts for Selective Organic Transformations

Makoto Yasuda
Department of Applied Chemistry, Graduate School of Engineering, The University of Osaka
E-mail: yasuda@chem.eng.osaka-u.ac.jp

Two types of selective reactions were reported, employing novel reagents and catalysts designed with the aid of machine learning. The first example is a 1,1-regioselective addition to alkenes.[1] We explored the 1-fluoro-1-sulfonyloxylation of styrenes using Bu_4NBF_4 and sulfonic acids in the presence of a hypervalent iodine reagent, $ArI(OAc)_2$. Regression analysis of the substituent effects on $ArI(OAc)_2$ revealed that both electronic (electron-withdrawing ability) and steric factors significantly affect the 1,1-heterodifunctionalization. Guided by this analysis, we designed novel hypervalent iodine reagent, which provided high regioselectivity.



The second selective transformation involves differentiating aromatic and aliphatic compounds.[2] We developed a π-pocket Lewis acid catalyst that selectively recognizes aromatic aldehydes. Machine learning analysis showed that conventional steric and electrostatic descriptors could not fully explain the observed selectivity. An ensemble model predicted—and experiments confirmed—high aromatic selectivity for the catalyst bearing three 2-benzofuryl groups around a boron center. SHAP (Shapley Additive Explanations) analysis revealed that the selectivity originates from the three-dimensional size of the catalyst weighted by its polarizability, offering valuable insights for designing Lewis acid catalysts that exploit non-covalent interactions.



[1] M. Fujie, K. Mizufune, Y. Nishimoto, M. Yasuda *Org. Lett.* **2023**, *25*, 766.

[2] a) H. Nakajima, M. Yasuda, R. Takeda, A. Baba *Angew. Chem., Int. Ed.* **2012**, *51*, 3867. b) Y. Tsutsui, I. Yanaka, K. Takeda, M. Kondo, S. Takizawa, R. Kojima, A. Konishi, M. Yasuda *Org. Biomol. Chem.* **2024**, *22*, 4283.

Makoto Yasuda
Osaka University (BS, 1990, MS 1992, Ph.D. 1995). Assist. Prof. Osaka University (1995-2006). Postdoctoral fellow, University of Alberta (1998-1999, Prof. J. M. Stryker). Assoc. Prof. Osaka University (2006-2014). Prof. Osaka University (2014-present).
[Field of research] Organic chemistry, organometallic chemistry, coordination chemistry

S6

Sustainable Approaches to Selective Amide Bond Cleavage

Karthick Govindan, Nian-Qi Chen, and Wei-Yu Lin*
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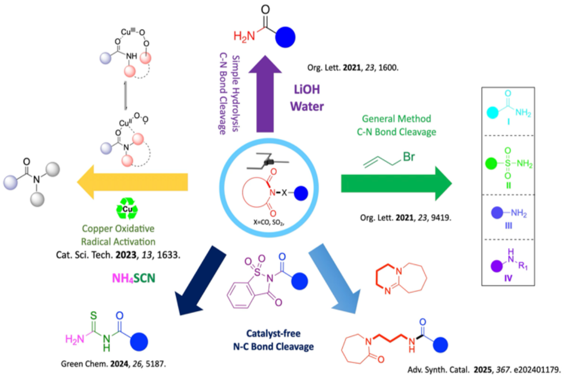
In recent years, the development of nonplanar amide precursors and exploration of their unique reactivity have significantly advanced the field of organic synthesis. Among these, twisted amides have emerged as a powerful platform for enabling amide bond functional group interconversions, greatly expanding the synthetic utility of amide derivatives. Herein, we report a novel methodology that harnesses selective ring opening followed by C–N bond cleavage to efficiently construct nitrogen-containing functional groups via a key reactive intermediate. The transformation is straightforward to perform, exhibits broad substrate tolerance, and provides access to a diverse array of valuable functionalized products. Notably, the versatility and practicality of this strategy are further demonstrated using a flow chemistry approach to afford the desired products in high efficiency. The potential of these new strategies is underscored through various synthetic applications, highlighting their value in modern organic synthesis.



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S7

Generation and Reaction of Fluoroalkyl Radicals from Fluorinated Alkyl Benzoates by Photoredox Catalysis

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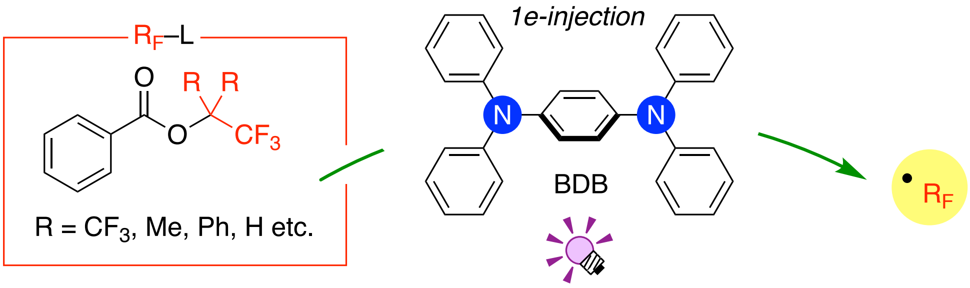
Photoredox catalysis with metal-based complexes and organic dyes has become a useful tool for synthetic radical chemistry.[1] Recently, we have found that small aromatics bearing two diarylamino termini such as 1,4-bis(diphenylamino)benzene (BDB) serve as efficient organic photoredox catalysts for reductive generation of fluorinated alkyl radical species from appropriate electron-accepting reagents (R_F–L).[2] In particular, BDB realizes generation of fluorinated alkyl radicals from the corresponding alkyl benzoates, which are readily accessible from commercially available fluorinated alcohols.[3] In this presentation, new synthetic strategies for radical fluoroalkylation will be discussed.



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S8

In-silico Models for Reactivity Parameter Prediction

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Methyl cation affinity (MCA) or methyl anion affinity (MAA) of a substrate is defined as the energy difference (negative of the energy) for the virtual reaction of a methyl cation or methyl anion with the substrate[1]. Molecules with higher MCA (MAA) are nucleophilic (electrophilic) because the corresponding product is stable. These thermodynamic energy differences showed strong correlations with Mayr's nucleophilicity and electrophilicity parameters after taking solvent effect into account [2,3]. A recently proposed efficient workflow for MCA and MAA calculation gradually increases calculation complexity from force field to DFT [4]. To further enhance calculation speed, which can be applied to millions of compounds for in-silico reaction prediction applications, atom-based machine learning modeling was proposed [5]. However, the proposed surrogate models lack sufficient prediction accuracy for applications. The root mean square error (RMSE) for MCA prediction was 17.45 [kJ/mol], and for MAA was 22.08 [kJ/mol].

Herein, we report highly accurate models for predicting MCA and MAA at atomic sites. The proposed modeling structure consists of the Uni-Mol [6] encoder block and a feed-forward network. All model parameters of the proposed models are fine-tuned during training. The prediction accuracy for both MCA and MAA improved compared with previously proposed methods. Furthermore, important conformation for the MCA and MAA prediction was identified. In my presentation, the discussion will include data-driven prediction models for reaction parameters and their potential applications.

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S9

Bayesian Optimization-Assisted Multiparameter Screening of Flow Reaction Conditions

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Flow chemistry has been widely adopted in fine-chemical synthesis as a sustainable approach that enhances reaction efficiency, safety, and reproducibility. Development of flow reactions requires systematic screening of both flow-specific parameters (e.g., flow rate, mixer type) and conventional reaction variables (e.g., temperature, concentration). To accelerate this inherently time-consuming process, machine-learning-assisted optimization methods are increasingly employed. In this study, we focused on multiparameter screening of flow-reaction conditions using Bayesian optimization (BO).

1. BO-driven screening of flow-reaction conditions including a mixer type

A mixer type is a critical determinant of performance in flow chemistry. However, digitalizing and optimizing mixer type—a categorical, engineering-based parameter—remains challenging for chemists. We applied categorical BO with one-hot encoding to screen micromixer types and organocatalytic conditions for a Brønsted acid-catalyzed biaryl synthesis in flow. BO-driven screening across six parameters, including mixer type, identified optimal conditions that afforded the product in 95% yield after performing 15 experiments.[1]

2. BO-assisted screening for flow reactions involving *in situ*-generated cyanogen chloride

Cyanogen chloride (Cl–CN) is a valuable electrophilic cyanating reagent. We previously reported a one-pot synthesis of sulfonyl cyanides from sodium sulfinates using Cl–CN generated *in situ* from KCN and $NaClO \cdot 5H_2O$. Given that Cl–CN is highly toxic, volatile, and unstable, we envisioned that a flow setup would improve safety and reaction performance. Application of constrained BO-assisted screening to the flow reaction between benzylamine and *in situ*-generated Cl–CN enabled rapid identification of suitable conditions, providing *N*-benzyl cyanamide in 74% yield after performing only eight experiments.

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Masaru Kondo received his Ph.D. degree in 2017 from the Nagoya Institute of Technology. He worked at Princeton University in 2017 as a postdoctoral researcher. He served as an assistant professor at SANKEN, Osaka University, from 2017 to 2021, and Ibaraki University from 2021 to 2023. He is currently an assistant professor at the University of Shizuoka, starting in 2023. His research interests include efficient synthesis of *N*-heteroaromatic compounds, data-driven efficient reaction screening, and organic synthesis based on fatty acid chemistry.

S10

Integration of Computer Vision and Digital Technologies for Automated Recording of Chemical Experiments

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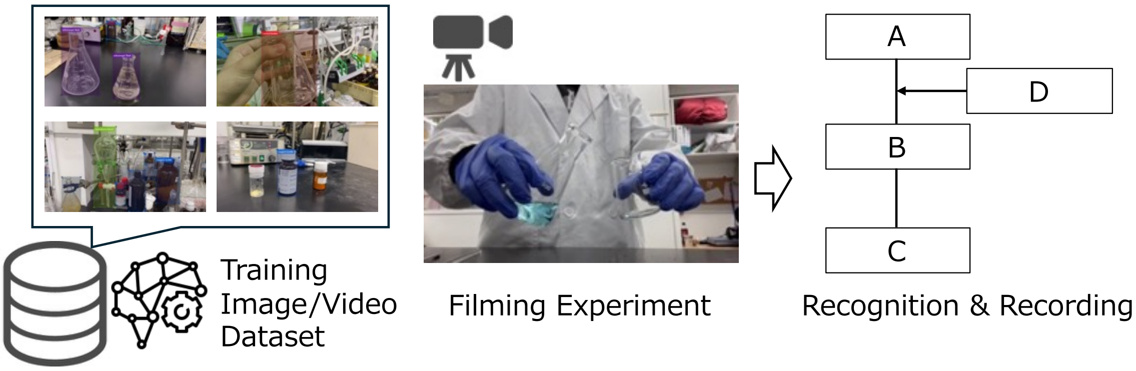
Ensuring seamless integration of recorded experimental results with downstream data analysis requires capturing experimental information electronically in a structured and standardized format. However, electronic laboratory notebooks (ELNs) have seen limited adoption, mainly due to the limited flexibility, relatively significant effort required for data entry, and dependence on individual recording practices. Recent advances in computer vision have increased interest in the automated recognition and recording of chemical experiments. Our group has built a large-scale image dataset[1], developed image- and action-recognition models specified to laboratory environments[2], and created methods for transforming experimental videos into flowchart-based representations.[3] Recent progress in multimodal experimental recording that combines sensor information, as well as approaches for quantitatively characterizing operator-dependent chemical manipulations beyond conventional experimental records, will be presented.



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S11

Mechanistic Insights into Organophosphorus Radical Reactions Enabled by Combined Computational and Experimental Approaches

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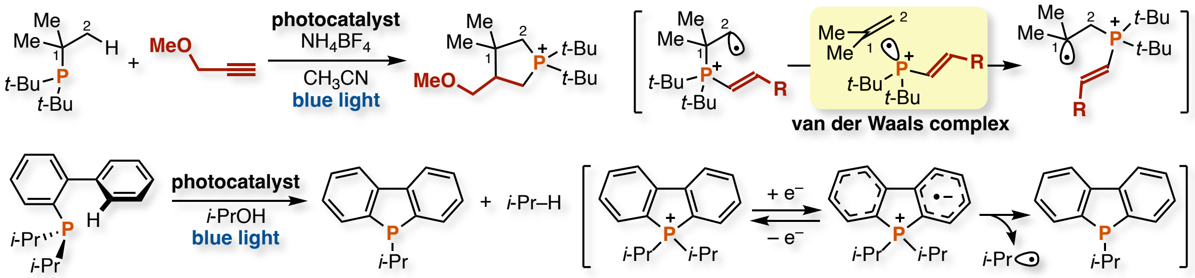
Quantum chemical calculations are becoming one of the most powerful tools for elucidating reaction mechanisms in organic chemistry. While they were once employed to rationalize experimental results, they now play a crucial role in mechanistic analysis and even provide valuable guidance for experimental design. In this presentation, I will discuss a series of mechanistic studies on photocatalytically induced radical reactions of organophosphorus compounds, in which computationally predicted reaction pathways were verified experimentally.

For example, we have developed a photocatalytic [3+2] cycloaddition of tri-*tert*-butylphosphine with terminal alkynes involving a 1,2-phosphorus migration of β-phosphonioalkyl radicals (Figure, top).[1] Combined theoretical and experimental studies suggest that the 1,2-phosphorus migration proceeds through a phosphine radical cation–alkene van der Waals complex as a key intermediate. Furthermore, we investigated the photocatalytic cyclization of 2-phosphinobiaryls to afford dibenzophospholes (Figure, bottom).[2] Theoretical calculations indicated two unexpected electron-transfer pathways operating outside the product-forming radical chain cycle. Experimental studies corroborated these pathways, showing the crucial role of the catalyst's redox properties in the reaction.



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S12

Decoding MOF Proton-Driven Coordination and Nucleation Pathway via In Situ SWAXS and Molecular Dynamics Simulations

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The aqueous synthesis of ZIF-8, where Zn^{2+} coordinates with 2-methylimidazole, begins with a proton-transfer controlled deprotonation step that directly governs ligand activation, coordination kinetics, and the ultimate framework topology. To provide molecular-level clarity relevant to synthetic chemists, we integrate metadynamics simulations and operando in situ small- and wide-angle X-ray scattering (in situ SWAXS) to continuously track the reaction microstructure from the moment Zn^{2+} and imidazole encounter each other in water. Our time-resolved data disentangles the sequence of early events: proton transfer–enabled ligand activation, formation of transient Zn–Im oligomers, growth into nanoscale coordination clusters, and their transformation into ZIF-8 nuclei. We further resolve the cooperative ordering steps that drive the transition from amorphous intermediates into crystalline sodalite-type domains. Coupled with kinetic modelling and simulation, these results provide a complete reaction-pathway map from initial acid–base/coordination chemistry to nucleation and final crystal maturation. This operando-scattering approach establishes a mechanistic foundation for rational control of MOF formation conditions, offering organic chemists a quantitative, real-time window into how proton transfer, ligand coordination, and structural self-assembly co-determine synthetic outcomes.

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Her research focuses on operando X-ray and neutron scattering combined with multiscale simulations to study reaction pathways and nucleation-to-crystallization processes in metal–organic frameworks and aqueous systems. Her work aims to provide molecular-level insights into coordination chemistry and chemical self-assembly. She has published in journals including Nature Communications, ACS Nano, and Angewandte Chemie, and has received the Ta-You Wu Memorial Award.

S13

Synthesis of Aminobenziodoxolones and Their Application to Oxidative Amination of Arylboronic Acids

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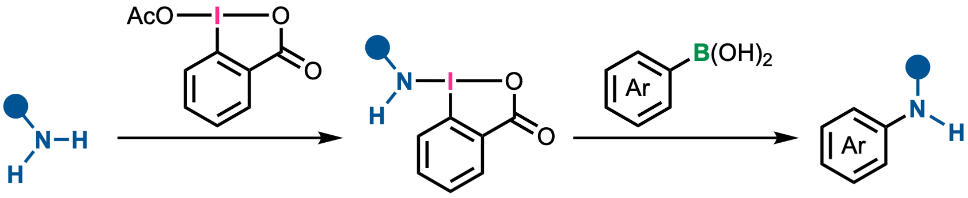
Hypervalent iodine(III) compounds bearing transferable nitrogen functional groups—commonly known as amino-λ³-iodanes—have long been recognized as useful reagents for oxidative amination, a valuable strategy for constructing nitrogen-containing organic molecules. However, their broader synthetic utility has been hampered by the limited availability of suitable reagents, particularly those derived from simple aliphatic and aromatic amines. We herein report a versatile and practical method for synthesizing amino-λ³-iodanes and demonstrate their application in the transition-metal-free oxidative amination of arylboronic acids.[1] A straightforward protocol was established for the preparation of aminobenziodoxolones from readily available amines, including ammonia, primary amines, and secondary amines. The resulting aminobenziodoxolones serve as efficient electrophilic aminating reagents, enabling the synthesis of a wide range of arylamines from readily available arylboronic acids.



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Kensuke Kiyokawa received his Ph.D. in 2012 from Osaka University under the direction of Prof. Akio Baba. In 2012, he was appointed to the position of Assistant Professor in the Department of Applied Chemistry in Prof. Minakata's group at Osaka University. His current research interest is the development of new synthetic methodologies using iodine compounds.

S14

Synthetic Transformations of 1,1-Di(boryl)propene Starting from Propyne

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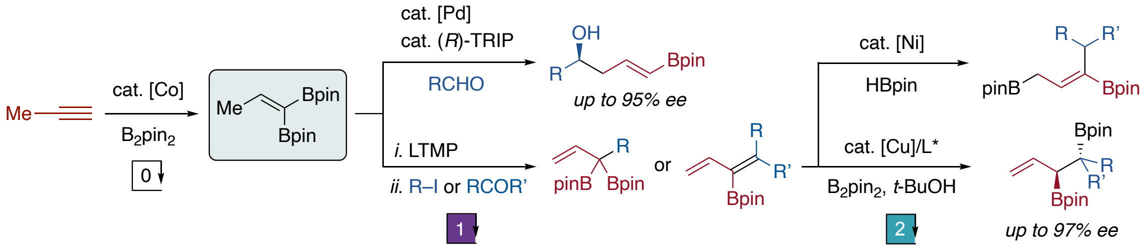
Propyne is produced from the cracking process of large hydrocarbon molecules in the petrochemical industry, most of which is an undesirable byproduct. This C3 source is an attractive raw material to fine synthetic chemistry, yet is rarely employed. We present here synthetic transformations starting from propyne.

First, propyne was converted into 1,1-di(boryl)propene on a gram scale under slightly modified conditions to those that were originally reported by the Chirik and Hu groups.[1,2] Then, we have developed synthetic transformations of 1,1-di(boryl)propene into 1) (*E*)-δ-boryl-substituted *anti*-homoallylic alcohols,[3] 2) α-boryl-α-substituted allylboronates,[4] and 3) boryl-1,3-dienes. Furthermore, the resulting boryl-1,3-dienes were found to be useful synthetic intermediates not only in oxidation reaction[5] but also in transition metal-catalyzed reactions.



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S15

A Catalyst Design for Selective Nitrene Transfers

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Selective functionalization of C(sp^3)–H bonds without directing groups remains a key challenge in organic synthesis. Metal-bound nitrenes and carbenes enable such transformations, and paddlewheel dirhodium complexes offer a suitable platform for tuning reactivity through ligand design. Although desymmetrized paddlewheel complexes developed by Hashimoto, Fürstner, and Davies created confined catalytic pockets effective for carbene transfer, these monocarboxylate-derived catalysts often lack sufficient reactivity for nitrene transfer.

The dicarboxylate-based $Rh_2(esp)_2$ introduced by Du Bois transformed nitrene chemistry[1] and represents one of the most effective catalysts for C–H amination. However, most derivatives maintained the symmetry of the parent scaffold, leaving unexplored the possibility of differentiating the two rhodium centers.

To address this issue, we pursued ligand designs that reshape the $Rh_2(esp)_2$ core. We first suppressed its conformational dynamics by introducing a substituent, allowing for the isolation of *anti* and *syn* conformers. These conformationally constrained catalysts improved nitrene-transfer selectivity.[2] Nevertheless, given the distinct metal sites in *syn* complexes, a suitable catalyst modification should lead to further selectivity enhancement. We, then, developed a ligand-linking strategy that imparts functional asymmetry to the paddlewheel core. Tethering carboxylates biases substrate approach toward a single rhodium center, creating catalysts with one active site and one partner that mainly provides electronic and structural support.

This lecture will outline the progression from conformational control to metal-site differentiation and illustrate how rational design within a bimetallic scaffold can enable selective nitrene-transfer reactivity.

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Hidetoshi Noda was born and raised in Tokyo, Japan. He received his B.S. and M.S. from the University of Tokyo (Japan) in the group of Prof. Dr. Masakatsu Shibasaki and his Dr. sc. from ETH Zürich (Switzerland) under the supervision of Prof. Dr. Jeffrey W. Bode. In 2015, he joined the Institute of Microbial Chemistry (BIKAKEN), Tokyo, as a JSPS Postdoctoral Fellow. He was tenured at the same institute in 2017, and he currently works there as a Chief Researcher. His research interests are at the interface between chemistry and biology.

S16

Transient η^6-Coordination Enables Borylation of Arenes

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Functionalization of the C–H bond in an arene enables the rapid construction of molecular complexity. To achieve efficient transformations, specialized substrates, such as arenes bearing a directing group and/or complex catalysts are often required. η^6-Coordination of an arene to a metal fragment such as [$Cr(CO)_3$] is known to reduce the electron density of the arene and has been widely utilized in organic synthesis. Yet its application to the C–H functionalization of arenes remains scarce, and the reported reactions require the isolation of the arene complex as a starting material [1,2]. To the best of our knowledge, only one example has been reported in which an arene complex was generated via arene exchange in situ, followed by a one-pot Pd/Ag-catalyzed C–H arylation [3]. Herein, we report that simple arenes can be borylated with $B_2(pin)_2$ in the presence of KF via in situ arene exchange with [$Cr(CO)_3(\eta^6$-np)] (Figure 1) [4]. Mechanistic studies suggest that the reaction proceeds via nucleophilic attack of a borate species on the arene activated by η^6-coordination, followed by hydride migration.

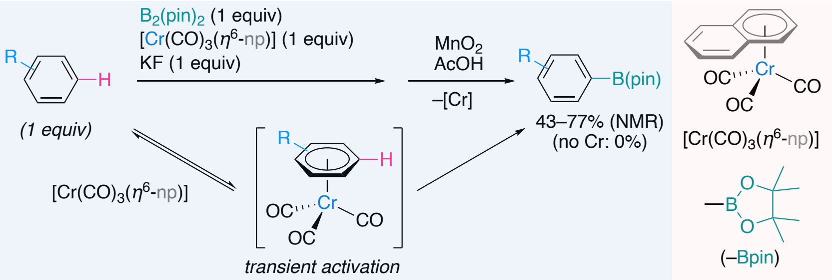

Figure 1. Borylation of simple arenes through transient η^6-coordination to [$Cr(CO)_3$].

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Yuichiro Mutoh, born in Gifu, Japan, earned his PhD in 2005 from Gifu University (Prof. Toshiaki Murai). After postdoctoral work at Kyoto University, he became an Assistant Professor at Chuo University in 2007. He joined the Tokyo University of Science in 2012, where he was promoted to a Junior Associate Professor in 2017. Since 2020, he has been a Senior Research Scientist at the RIKEN, collaborating with Dr. Laurean Ilies. His research focuses on molecular catalysts in organometallic chemistry and heavier main-group chemistry.

S17

Development of Chiral Borinic Acid Catalysts and Their Applications to Enantioselective Reactions

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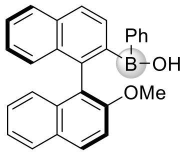
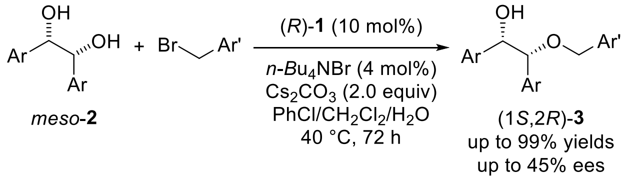
Boron-containing catalysts have emerged as powerful tools in modern organic synthesis due to their unique reactivity and broad applicability. Although many asymmetric organoboron catalysts based on boranes, boronic acids, and borates have been reported,[1] asymmetric catalysis using borinic acids remains poorly developed.[2] Given the growing interest in borinic acid chemistry, the creation of new chiral borinic acid catalysts represents an important challenge with significant potential. In this presentation, I would like to introduce our recent efforts to develop axially chiral borinic acid catalysts and to explore their synthetic applications.

A binaphthyl-type chiral borinic acid catalyst (*R*)-**1** was synthesized from (*S*)-BINOL, together with a library of related derivatives. These catalysts exhibit high stability toward moisture and oxygen, allowing practical handling. Their catalytic potential was first demonstrated in the enantioselective alkylative desymmetrization of *meso*-diols **2**, affording the corresponding products **3** with moderate enantioselectivity.[3a] We then applied the catalyst to a three-component Passerini-type reaction using isocyanides, aldehydes, and water. This method provides α-hydroxyamides in good yields with notable enantioselectivity, including for aliphatic aldehydes.[3b] Overall, these results establish chiral borinic acids as robust and versatile organocatalysts and expand their utility to water-tolerant enantioselective processes.

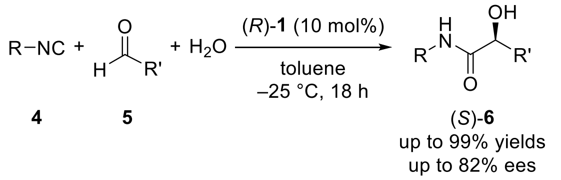


(*R*)-**1**

(A) Alkylative desymmetrization of *meso*-1,2-diols



(B) Three-component reaction; Passerini-type reaction



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Makoto Sako received his bachelor's degree under Prof. Toyoshi Shimada from the National Institute of Technology, Nara College, and later earned his master's and Ph.D. degrees from Osaka University under Prof. Hiroaki Sasai. During his doctorate, he conducted internships with Prof. Giang Vo-Thanh at Université Paris-Sud (2013) and Prof. Magnus Rueping at RWTH Aachen University (2015). He became an assistant professor at SANKEN in 2017 and has served in his current position in the laboratory of Prof. Mitsuhiro Arisawa since 2020. His research focuses on synthetic organic chemistry and novel asymmetric catalysis.

S18

Exploring the Reactivities of Bicyclo[2.2.2]octenones: From Solution to Solid

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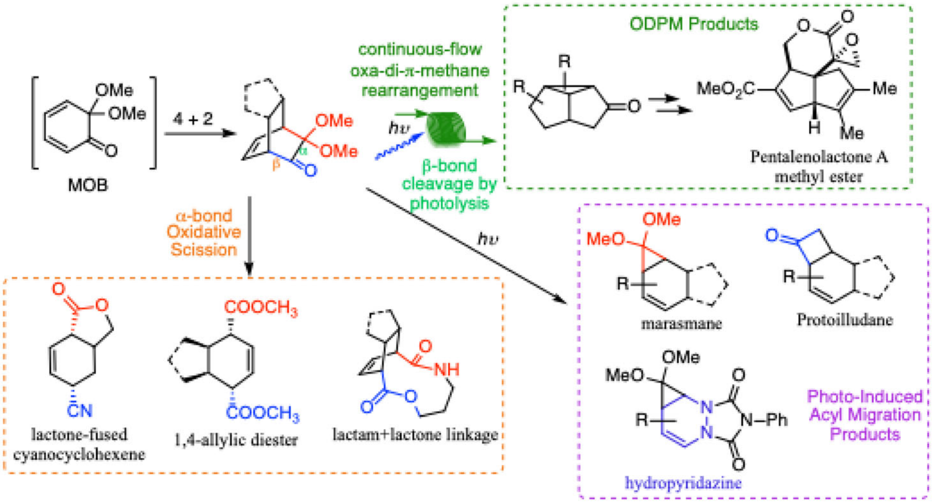
Bicyclo[2.2.2]octenones constitute a highly adaptable class of intermediates in organic synthesis, serving as useful starting points for assembling structurally complex molecules. These frameworks are conveniently generated via Diels–Alder cycloadditions of masked o-benzoquinones (MOBs), which provide a dependable strategy for accessing a broad array of architectures. Over the past few years, our group has focused on investigating the reactivity of bicyclo[2.2.2]octenones, paying attention to the unique properties of their α-dimethoxy ketone units in photochemical transformations and rearrangement reactions. This report outlines our recent discoveries, discuss the mechanistic features we have uncovered, and point to new synthetic opportunities enabled by these intriguing scaffolds.



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2019~ Prof., Dept of Chemistry, CYCU
Research Interest: Photo-induced rearrangements, Bimetallic catalysis.

S19

Product-Selective Dehydrogenative Aromatization Enabled by Supported Metal Nanoparticle Catalysts

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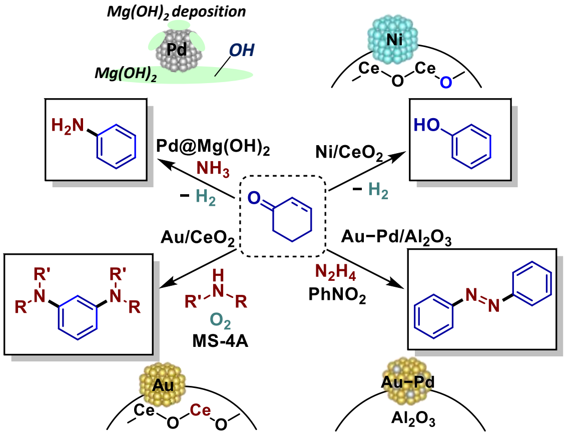
Dehydrogenative aromatization from cyclohexanones has attracted much attention for the synthesis of various aromatic compounds[1] because substituents on cyclohexanones can be regioselectively installed by well-established reactions without the limitation derived from aromatic compound substrates such as the *ortho*/*meta*/*para*-orientation.[2] Furthermore, if aerobic or acceptorless dehydrogenation systems are constructed, such dehydrogenative aromatization reactions are environmentally-friendly. However, there are still unachieved dehydrogenative aromatization reactions mainly because of the difficulty in controlling product selectivity. Recently, we have focused on multiple adsorption/activation of organic compounds on heterogeneous supported nanoparticle catalysts for developing unprecedented organic transformations. Based on the unique catalysis, which can be tuned and integrated by second metals and supports, we have successfully developed various product-selective dehydrogenative aromatization reactions.[3–6] In this presentation, we will focus on the unprecedented synthesis of azobenzenes from only non-aromatic compounds, cyclohexanones and $N_2H_4{\cdot}H_2O$, using an Al_2O_3-supported Au–Pd alloy nanoparticle catalyst in the presence of a suitable hydrogen acceptor: nitrobenzene.[6]



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Dr. Takafumi Yatabe is a lecturer at Department of Applied Chemistry in the University of Tokyo. In 2019, he obtained his PhD degree supervised by Prof. Kazuya Yamaguchi in the University of Tokyo on the development of environmentally-friendly organic reactions using heterogeneous catalysts. Then, he visited the group of Prof. Christophe Copéret in ETH Zürich until the end of 2019. In 2020, he was appointed as a research associate (assistant professor) in the group of Prof. Kazuya Yamaguchi. In 2025, he was promoted to the current position.

S20

Theoretical and Data-Driven Approaches to Lanthanide Photofunctional Materials

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Lanthanide (Ln) luminescence, originating from 4f-4f transitions, exhibits sharp emission spectra and has been applied in various optical materials. While the 4f-4f emission wavelengths of Ln complexes are almost independent of the surrounding environment, the emission intensities are heavily influenced by it, making appropriate ligand design crucial. To better understand and design optical materials, analyses of the potential energy surfaces (PES) of the ground and excited states are indispensable. However, ab initio calculations for Ln complexes are challenging due to the strong electronic correlation of the 4f electrons. To address this issue, we proposed the energy shift method, which describes the PES of $4f^N$ excited states and ligand-localized triplet states [1]. This method has contributed to the understanding and design of various Ln luminescent materials [2] and has also been applied to non-Ln systems [3]. However, it could not handle 4f-5d and charge transfer excited states, which are particularly important for cerium and europium complexes. To overcome this problem, we developed an updated method [4]. In addition, we built a cerium complex database containing 1.6k geometries and electronic properties calculated at the ωB97XD level. We plan to make this database public and evolve it into a platform for optical function prediction via machine learning. This presentation will describe our development of computational methods, applications to Ln materials, and our ongoing Ln open database project.

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Miho Hatanaka received her Ph.D. in 2011 from Keio University. After a four-year postdoctoral position at Kyoto University under Prof. Keiji Morokuma, she became an Assistant Professor at Kindai University in 2015. In 2017, she was promoted to Associate Professor at Nara Institute of Science and Technology. Since 2020, she has been an Associate Professor in the Department of Chemistry at Keio University, with a cross-appointment at IMS. In 2025, she was appointed as Professor at Keio University and IMS.

S21 Machine Learning-assisted Design and Characterization of Dithienobenzothiazole-Based Organic Semiconductors

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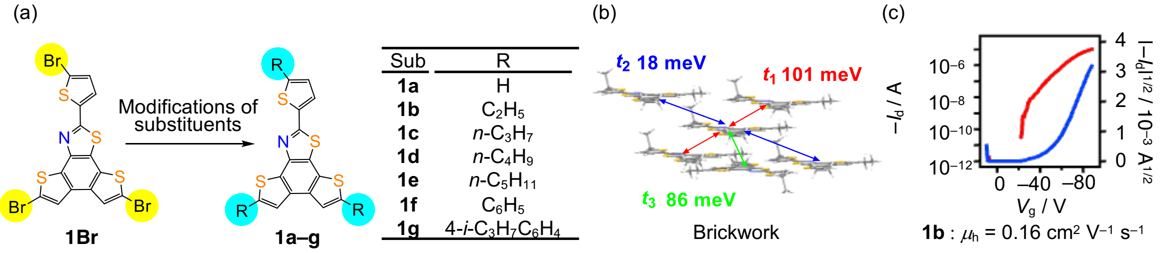
When designing the core skeleton of organic semiconductors, many factors should be considered, including the HOMO level, intermolecular interaction, and reorganization energy. Previously, we performed machine learning[1] and theoretical simulation[2] analyses to correlate the structural data of p-type organic semiconductors with hole mobility, and found that the number (N_{HBA}) of hydrogen bond acceptor (HBA) atoms such as N, O, and S is one of the most important descriptors. In this study, we synthesized dithienobenzothiazole (DBT) derivatives (**1a–g**, Fig. 1) with $N_{\mathrm{HBA}} = 5$ and evaluated their semiconducting performance. X-ray crystallographic analysis confirmed that the packing structure of **1b** (the diethyl and ethylthienyl derivative) in the crystal is classified into brickwork structures with multidirectional intermolecular charge-transfer integrals, as a result of incorporation of multiple HBA atoms. The solution-processed top-gate bottom-contact field-effect transistor of **1b** exhibits a hole mobility of 0.16 cm^2 V^{-1}s^{-1}. As a result, it was found that DBT derivatives exhibiting good performance have intermolecular interactions originating from the HBA atoms in the crystal, and that HBA contributes to the tight-packing structure.[3]



Sub	R
1a	H
1b	C_2H_5
1c	n-C_3H_7
1d	n-C_4H_9
1e	n-C_5H_{11}
1f	C_6H_5
1g	4-i-$C_3H_7C_6H_4$

Fig. 1 (a) Various molecular modification of **DBT** at the final step. (b) Crystal structure of **1b** and charge-transfer integral (t) between two neighboring molecules. (c) Characterization of OFET using thin-film of **1b** fabricated by solution-process

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2006-2010/2011-2021: Associate/Full Professor, Osaka Prefecture University
2022-current: Professor, Osaka Metropolitan University

- The Japan Photochemistry Association Award 2010
- The Society of Synthetic Organic Chemistry, Japan, The Kansai Branch Award 2010
- The Electrochemical Society of Japan, The Organic Electron Transfer Chemistry Academic Award 2020
- The Society of Organic π-Electron Systems, Japan, The Academic Award 2025

S22

Heteroaromatic Swapping and Stereoediting of Benzylic Alcohols

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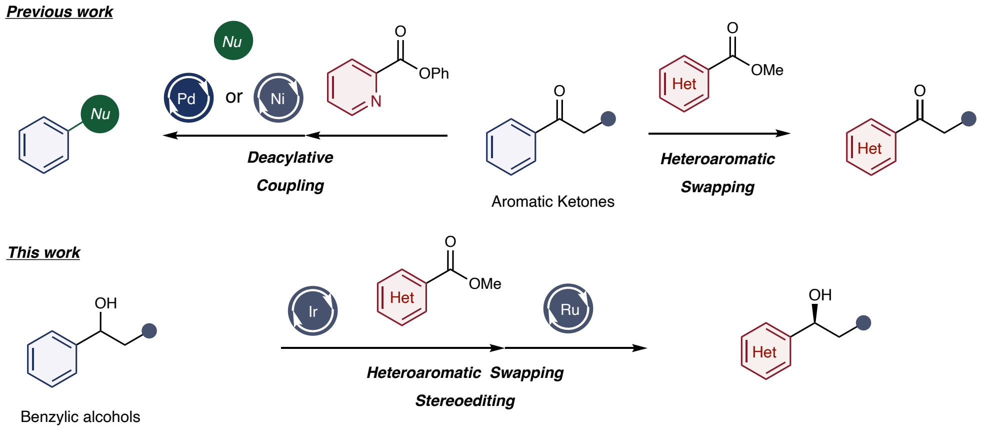
Benzylic alcohols contain a stereocenter and represent a privileged structural motif frequently found in pharmaceuticals. Because they are readily accessible through the reduction of aromatic ketones, a variety of asymmetric reductions have been extensively developed. We have recently reported deacylative coupling and heteroaromatic swapping reactions of aromatic ketones enabled by a Claisen–retro-Claisen sequence.[1,2] Building on these findings, we envisioned that benzylic alcohols themselves could serve as substrates for a heteroaromatic swapping reaction.

Here, we designed a catalytic hydrogen-transfer manifold in which oxidation of the alcohol, heteroaromatic swapping, and subsequent ketone reduction occur sequentially within a single reaction setup. This strategy enables the one-step conversion of benzylic alcohols into heteroaromatic alcohols. Using an iridium catalyst, we found that benzylic alcohols undergo efficient heteroaromatic swapping. Although enantioinduction was challenging under a single catalytic system, the addition of a chiral ruthenium catalyst after the swapping step allowed us to obtain enantioenriched heteroaromatic alcohols in a concise two-stage operation.



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S23

Formal Umpolung Synthesis of α-Branched Amides and Its Application to the Synthesis of MR16728

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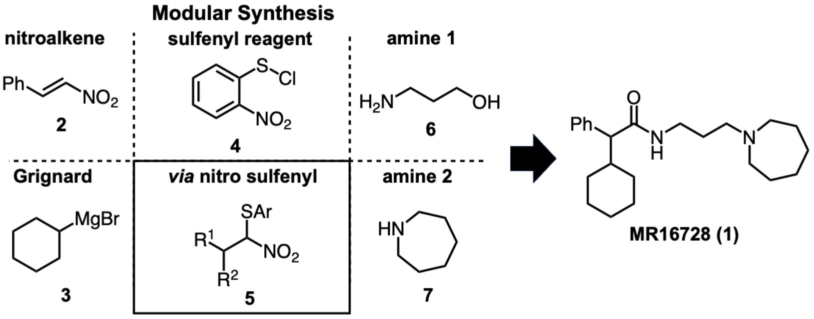
Amide scaffolds represent one of the most fundamental functional groups in organic and medicinal chemistry, widely present in natural products, bioactive compounds, peptides, and functional materials. In particular, α-branched amides have gained significant attention owing to their intriguing biological activities, making the development of efficient and concise synthetic methods an important challenge in both synthetic chemistry and drug discovery.

We recently developed a unique transformation that enables access to α-branched amides from nitroalkenes[1]. Our method features a one-pot synthesis of a multi-substituted nitro-sulfenyl intermediate followed by oxidative amidation, delivering the desired α-branched amide in a practical manner. This strategy allowed the modular synthesis of the acetylcholine-related drug-like molecule MR16728 (**1**). In the key sequence, the nitroalkene **2** was treated with cyclohexylmagnesium bromide (**3**), followed by nitrophenylsulfenyl chloride **4** to give the nitro-sulfenyl intermediate **5**. Subsequent oxidative amidation with amine **6** afforded the α-branched amide bearing a cyclohexyl moiety, which was then transformed into **1** through standard oxidation and reductive amination with azepane **7**. To date, more than ten analogues have been synthesized using this modular approach. In this presentation, we will also disclose previously unreported biological activities of these compounds.



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S24

Computationally guided development of photoreactions using electropositive elements

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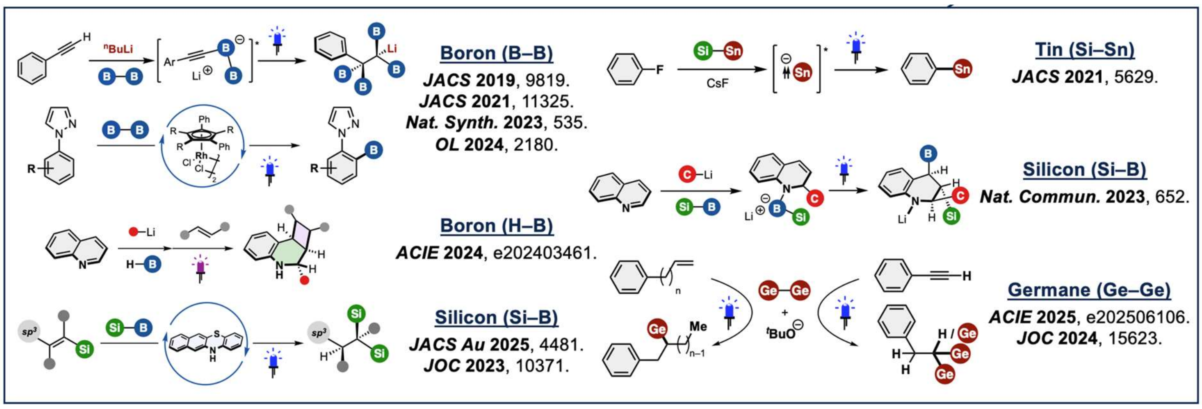
Photoinduced reactions have received much attention as a powerful tool to access kinetically or thermodynamically prohibited reactions on the ground state. In general, these reactions have been developed mainly by using electro-negative elements such as C, O, N, halogens as well as transition-metals. On the other hand, we have been interested in the excited states of electro-positive elements such as B, Si, Ge, and Sn, developing the highly reactive and selective photoinduced (catalytic) reactions. Especially, computational guidance could help us to efficiently develop photoinduced reactions depicted in the following figure. We would like to introduce and discuss a part of these results, including development of defluorostannylation of fluoroarenes (Sn),[1] dearomative silaboration of quinolines (Si),[2] dearomative cycloaddition of quinolines with alkenes (B),[3] and multiple germylation of terminal alkynes (Ge).[4]



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[3] Nagashima, Y.; Uchiyama, M, *et al. Angew. Chem. Int. Ed.* **2025**, *64*, e202506106.

Yuki Nagashima received his BSc (2012), MSc (2014), and PhD (2019) from the University of Tokyo. After working at the Mitsubishi Tanabe Pharma Corporation as a medicinal chemist (2014 to 2020), he moved to the Tokyo Institute of Technology (2020 to 2024). Since 2024, he has been working as an Assistant Professor at the University of Tokyo. His research interests include the development of organic photoreactions using the characteristics of diverse elements combined with computational chemistry.

S25

Photoinduced PCET-mediated C–C bond cleavage enaibling bond-reorganization

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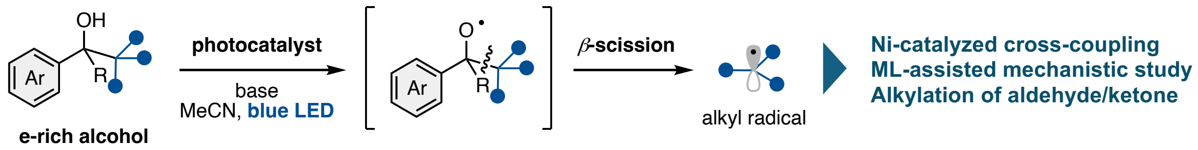
Carbon–carbon (C–C) bond formation is a central reaction in organic synthesis, whereas selective C–C bond cleavage remains challenging due to the high stability of these bonds. Mild cleavage of Csp^3–Csp^3 bonds under near-neutral, room-temperature conditions would be highly valuable, but only a few examples exist. We recently demonstrated that photodriven proton-coupled electron transfer (PCET) enables catalytic C–C bond cleavage of benzylic alcohols through β-scission of an alkoxy radical generated via single-electron oxidation and deprotonation.[1] Although visible-light PCET protocols have emerged, many rely on expensive Ir complexes and added base.[2] To overcome these limitations, we developed a *unimolecular* PCET system using an inexpensive benzophenone-type organic photocatalyst, eliminating the need for both precious metals and external base. This platform allows efficient generation of alkyl radicals, which we utilize as reactive intermediates for new C–C bond-forming "bond-reorganization" reactions. Because the byproducts are simple organic molecules, recovery and reuse are straightforward, offering potential for sustainable molecular-circulation chemistry. In this presentation, we describe visible-light-driven Csp^3–Csp^3 cleavage of secondary and tertiary alcohols followed by diverse transformations, including Ni-catalyzed cross-coupling, alkylation of electron-deficient ketones, and aldehyde alkylation. We also employed machine learning to analyze the Ni-catalyzed coupling: reaction yields were used to train predictive models based on quantum-chemistry-derived descriptors, allowing quantitative evaluation of key reaction-controlling factors.



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Yuto Sumida received his PhD from Kyoto University in 2010 under the supervision of Prof. K. Oshima. He spent nine months as a JSPS postdoctoral fellow in the group of Prof. D. Khane at Harvard University. In 2011, he became an Assistant Prof. at TMDU working with Prof. T. Hosoya. He moved to RIKEN Kobe as a Research Scientist in 2014. He has been an Assistant Prof. at Kanazawa University working with Prof. H. Ohmiya in 2019. He became an Associate Prof. at Science Tokyo working with Professor Takamitsu Hosoya since 2023.

S26

Harnessing the CO_2 Radical Anion for Molecular Scaffold Construction

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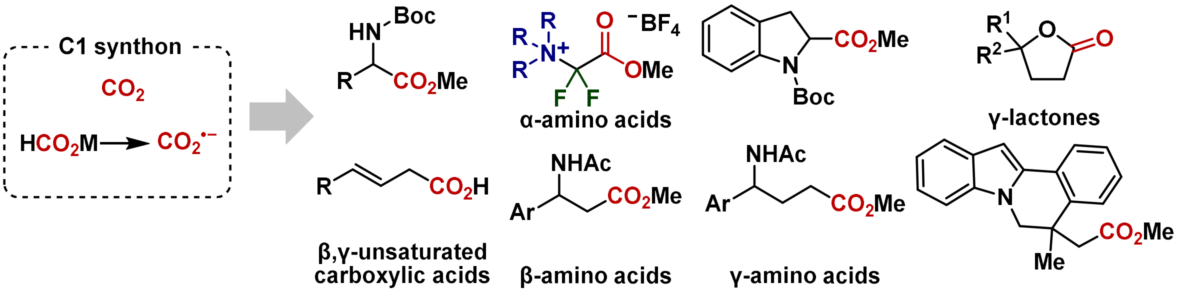
The CO_2 radical anion has emerged as a uniquely powerful C1 synthon for constructing synthetically valuable molecular scaffolds. Our research group has developed a series of radical transformations that directly utilize the CO_2 radical anion—generated from CO_2 or formate salts—enabling efficient access to α-, β-, and γ-amino acids, γ-lactones, and other value-added compounds. Guided by quantum chemical calculations, we elucidated the underlying reaction pathways and designed new ones that selectively promote C–C bond formation through the addition of the CO_2 radical anion. The products obtained from these CO_2 radical anion–based transformations serve as key intermediates for pharmaceuticals and functional materials. Collectively, these studies demonstrate how computationally assisted reaction design can fully exploit the unique reactivity of the CO_2 radical anion for building diverse and functionally rich molecular architectures.



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HP: https://mitagrouphp.icredd.hokudai.ac.jp/en.html

S27

Stable Yet Lewis-acidic Anions enabling Cooperative Catalysis with Cationic Transition Metal Complexes

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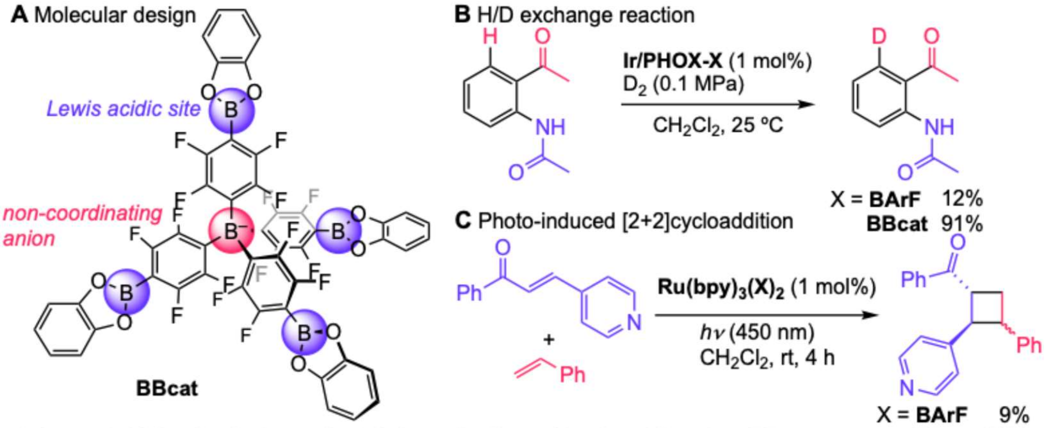
Although supporting ligands of transition metal catalysts have extensively been studied, counter anions of transition metal catalysts are often neglected their roles in catalytic cycle. Primarily counter anions are nucleophilic and their application in catalysis is based on their Brønsted basic nature. We developed a stable yet Lewis-acidic anion, **BBcat**, based on tetrakis(pentafluorophenyl)borate and featuring Lewis-acidic catechol borane (Scheme 1A).[1] Lewis acidic nature of **BBcat** was assessed by NMR analysis to have enough Lewis acidity. The combination of **BBcat** and cationic Ir complex catalyzed the C–H bond cleavage of acetophenone derivatives possessing Lewis basic functional groups, whereas commonly used non-coordinating anion, such as **BArF**, was ineffective counter anion, and the Lewis basic functional groups were also essential for acceleration (Scheme 1B).[1] A similar acceleration effect was achieved for photo-induced [2+2]cycloaddition of Lewis basic chalcone derivatives catalyzed by the combination of cationic Ru complex and **BBcat** (Scheme 1C).[2]



Scheme 1. Molecular design and catalytic applications of Lewis acidic anion, **BBcat**

[1] R. Mandai, T. Iwasaki, K. Nozaki, *Angew. Chem. Int. Ed.*, **2025**, *64*, e202503322.

[2] R. Mandai, T. Iwasaki, K. Nozaki, *manuscript submitted.*

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S28 SiO_2 Supported BArF as a Versatile Platform for Chiral Ir(I) Catalyzed Asymmetric Hydrogenations

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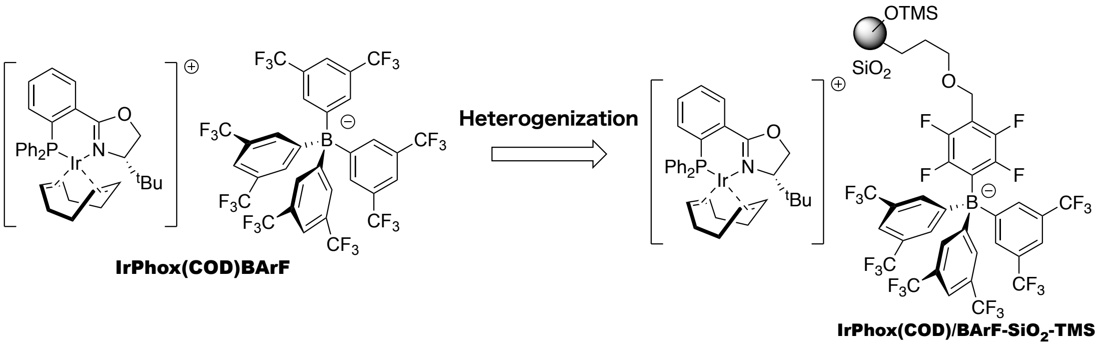
Cationic Ir(I) complexes are widely studies catalysts that exhibit high activity and high selectivity for the stereoselective hydrogenation of various olefins. On the other hand, since iridium is a rare and expensive metal, there is strong demand for the recovery and reuse of catalysts. We focused on the structure of tetraarylborate (BArF), which is used as a common counter anion for cationic Ir(I) complexes, and immobilized the borate salt on SiO_2 through appropriate linker design and to immobilize the cationic Ir(I) via electrostatic interactions.

The designed silica-supported borate was synthesized in 11 steps from a commercially available carboxylic acid. The cationic iridium complex IrPhox(COD)BArF was selected for immobilization. When the asymmetric hydrogenation of α,β-unsaturated ketones[1] was examined using the obtained immobilized catalyst, we found that fluorine substitution on the aromatic ring of the linker moiety was essential for achieving high activity. Furthermore, by applying TMS capping to the support to deactivate the silanols on the silica surface, the catalytic activity wa improved. By using the optimized support, the desired hydrogenation reaction proceeded with a yield of over 90% and an enantioselectivity of 98% ee,.



[1]S-.M. Lu, C. Bolm, *Angew. Chem. Int. Ed.* **2008**, *47*, 8920-8923.

Yuki Saito is a project associate professor at the University of Tokyo in Japan. In 2018, he received his Ph.D. degree under the supervision of Prof. Shū Kobayashi at the University of Tokyo, Japan. After a year as a JSPS research fellowship for young scientists (PD), he became a project assistant professor in the same group at the University of Tokyo. In 2024, he was appointed as a project associate professor in the continuous-flow fine synthesis social cooperation laboratory at the University of Tokyo.

S29

Transfer learning across different photoreactions

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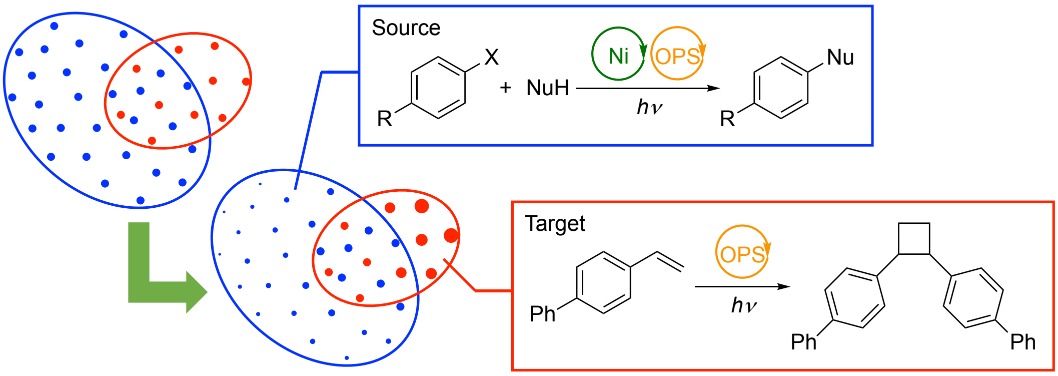
Although machine learning (ML) provides a powerful tool for catalyst optimization in organic reactions, including photocatalysis,[1] the limited availability of experimental training data often constrains its practical utility. Given that experienced organic chemists can draw on knowledge from previous experiments, it is an intriguing challenge to replicate this ability of human researchers to enhance ML predictions.[2]

Here, we demonstrate that domain adaptation (DA), an underexplored transfer learning (TL) strategy in catalysis research, substantially improves the prediction of catalytic activities of organic photosensitizers (OPSs).[3] By sharing information from nickel/photocatalytic C–O, C–S, and C–N cross-coupling reactions with that from a [2+2] cycloaddition, our TL protocol significantly enhances the predictive performance for photocatalytic activity. Notably, this approach also enables the efficient identification of promising OPSs for alkene photoisomerization, another distinct photoreaction, even when only ten training data points are available. These findings highlight DA as a practical and broadly applicable strategy for transferring knowledge on catalytic activity across different types of reactions.



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[2] a) T. Cernak, P. M. Zimmerman, et al., *Chem. Sci.* **2022**, *13*, 6655–6668. b) X. Hong, L. Ackermann, et al., *Nat. Commun.* **2023**, *14*, 3149. c) E. King-Smith, *Chem. Sci.* **2024**, *15*, 5143–5151.

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Brief CV
– March 2020 Doctoral Program, Tokyo Institute of Technology
April 2020 – March 2021 Otsuka Pharmaceutical Co., Ltd.
April 2021 – Present Assistant Professor, Nagoya University

S30

Efficient Synthesis of Cyclic (RGDfK) Using Microflow Reactor

○Naoto Yamasaki,[1] Mina Kim,[1] Kana Miyamoto,[1] Yuma Otake,[2] Kyohei Adachi,[2] Daisuke Kubo,[2] Shinichiro Fuse[1]*
[1] *Department of Basic Medicinal Sciences, Graduate School of Pharmaceutical Sciences, Nagoya University*
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Small cyclic peptides exhibit valuable biological activities and, because they also show high membrane permeability and excellent metabolic stability, have emerged as important targets in modern drug discovery research. However, a significant limitation is that current synthetic methods rely almost exclusively on solid-phase peptide synthesis, resulting in high production costs. Recently, we established a method that enables peptide chain extension by two residues in a single step through the in situ generation of *α*-amino acid *N*-carboxy anhydride (*α*-NCA),[1] as well as a rapid cyclization for small cyclic peptides that avoids dimerization.[2] To further validate these methods for practical applications and to deepen our understanding of microflow-based peptide synthesis, we attempted the efficient synthesis of Cyclic (RGDfK) (**1**), a known inhibitor of *αvβ*3 integrin, using our microflow chemistry.

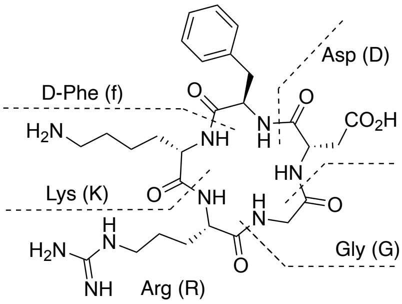

Figure 1 Cyclic (RGDfK) (**1**)

We first aimed to prepare the tripeptide Lys–Arg–Gly and to optimize a three-component coupling reaction using Boc-Arg(Pbf)-OH for in situ α-NCA formation. During this process, we found that slight variations in the residual water content within the reaction system caused fluctuations in the yield of the desired product. By adjusting the water content of Boc-Arg(Pbf)-OH solution to 3000–4000 ppm, the tripeptide was obtained in yields above 75%. Subsequently, coupling of the deprotected tripeptide with Asp and D-Phe successfully afforded the pentapeptide precursor required for cyclization. After the removal of the protecting group, our peptide cyclization method is applied, and the desired protected cyclic peptide was obtained in a high-yield. In this presentation, we will report the detailed experimental results and an analysis using in situ FT-IR for the tripeptide synthesis.

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Naoto Yamasaki, Ph.D.

Naoto Yamasaki received his Ph. D. in Pharmacy from Tokushima Bunri University. He was a postdoctoral researcher at Tokushima Bunri University from 2018 to 2021, and a postdoctoral fellow at Scripps Research from 2021 to 2023. In 2023, he joined the faculty at Nagoya University as an assistant professor in the Fuse Laboratory. His research interests include total synthesis of bioactive compounds such as terpenoids, carotenoids, peptides, and microflow synthesis.

S31

Triarylborane Catalysis with Crude H_2

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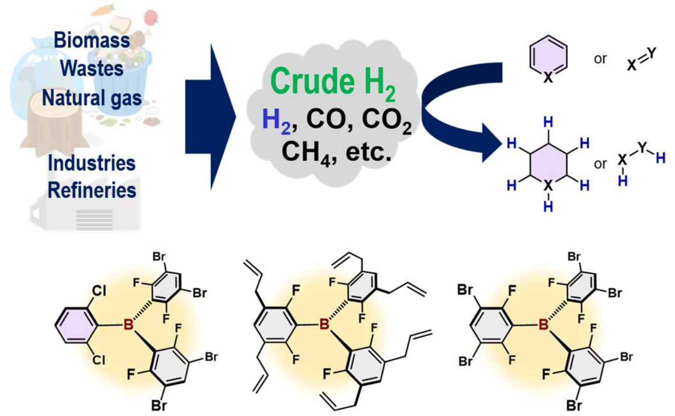
Molecular hydrogen (H_2) is one of the most promising energy carriers for the near future owing to its high gravimetric energy density and the relatively low environmental impact of its combustion products. In the mid-term, a large amount of H_2 is expected to be produced from a wide range of hydrocarbon and renewable resources, including biomass and waste, via purification of crude H_2, a gaseous mixture of H_2, CO, CO_2, and other components. We recently reported a strategy to separate H_2 from a gaseous mixture of H_2/CO/CO_2/CH_4 and simultaneously store it in *N*-heterocyclic compounds acting as liquid organic hydrogen carriers (LOHCs) through the triarylborane-catalyzed hydrogenation, which can be applied to produce H_2 via subsequent dehydrogenation.[1] We also extended this concept for alcohol synthesis via the hydrogenation of carbonyl compounds directly using crude H_2 and triarylborane catalysts.[2] In our system, even in the co-presence of CO and CO_2, carbonyl groups were selectively hydrogenated without side reactions such as carbonylation, dehalogenation, hydroformylation, and isomerization of olefins.



[1] Hashimoto, T.; Asada, T.; Ogoshi, S.; Hoshimoto, Y. *Sci. Adv.* **2022**, *8*, eade0189.
[2] Sakuraba, M.; Ogoshi, S.; Hoshimoto, Y. *Tetrahedron Chem* **2024**, *9*, 100059.

Yoichi Hoshimoto received his Ph.D. from Osaka University under the supervision of Professor S. Ogoshi in 2013. He is currently an Associate Professor and has been recognized as a “TechnoArena Professor” since 2025 at the Center for Future Innovation (CFi), the Graduate School of Engineering, The University of Osaka. His recent research interests include homogeneous catalysis with transition-metal and main-group-element complexes and the development of original *N*-heterocyclic carbenes.

S32

Design of Extremely Hygroscopic Ionic Liquids for The Liquid Desiccant-Type Air Conditioners

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Due to their many attractive physicochemical properties, ionic liquids (ILs) have received extensive attention with numerous applications proposed in various fields of science and technology.[1] We have been interested in their moisture absorption capability because this makes ILs possible candidates for desiccants for the liquid desiccant-type air conditioners (LDAC).[2] LDACs are expected to contribute to the reinforcement of basic infrastructure because the electric energy consumption of LDACs is more than 20% lower than that of conventional compressor-type air conditioners.[2] However, origin of the moisture absorption capability of ILs is still not well understood. For insight into this, we systematically synthesized various types of ILs by the combination of the dimethyl phosphate anion with alkyl group-substituted cyclic cations—imidazolium, pyrazolium, 1,2,3-triazolium, and 1,2,4-triazolium cations—and performed a detailed analysis of the dehumidification properties of these ILs and their aqueous solutions. Among the monocationic ILs, the best performance was obtained with 1-cyclohexylmethyl-4-methyl-1,2,4-triazolium dimethyl phosphate, whose DC (per mol) value is 14 times higher than that of popular solid desiccants like $CaCl_2$ and silica gel.[3] Dicationic ILs, such as 1,1'-(propane-1,3-diyl)bis(4-methyl-1,2,4-triazolium) bis(dimethyl phosphate), showed an even better moisture absorption, with a DC (per mol) value about 20 times higher than that of $CaCl_2$.[3] We further found that three types of nanostructures exist in these ILs aqueous solutions and these forms depend on the alkyl substituents of cationic part of ILs and water contents. Water molecules from air are absorbed mainly into polar regions of nanostructured ILs, defined primarily by phosphonium anions (in the space between the phosphonium anions in the nanostructure of aggregation form of the IL); the results suggest that the introduction of an appropriate alkyl side chain in the cationic moiety can be the key to the design of efficient desiccant ILs for LDAC.[3]

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Toshiyuki Itoh, B 1954 in Mie, Japan. Tokyo University of Education (BS 1976), The University of Tokyo (Ph.D. 1986), Colorado State University (Postdoc, 1990-1991), Okayama University (1987-2002), Tottori University (2002-2019). Emeritus Professor of Tottori University (2019), Toyota Physical and Chemical Research Institute (2020-2024), Kanazawa University (2024-present). Awards: The Society of Synthetic Organic Chemistry Award, Japan (2010), The 8th Green and Sustainable Chemistry Award, Japan (2009).

S33

Exploring Photochemistry of Boron-Based Frustrated Lewis Pairs

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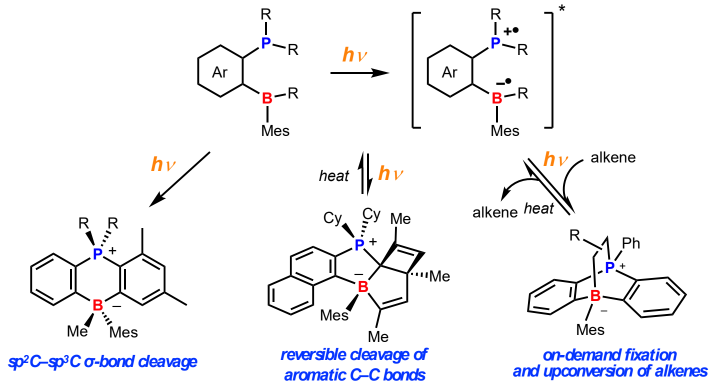
Intramolecular Frustrated Lewis Pairs (FLPs), which possess a Lewis acidic atom and a Lewis basic atom in neighboring but intact positions, are widely utilized as useful reagents and catalysts in organic synthesis. We have been exploring the photoreactivity of boron-based intramolecular FLPs and reported an $sp^2C–sp^3C$ σ-bond cleavage reaction of *o*-phosphinophenylboranes to give phosphonium-borate compounds via Frustrated Radical Pairs (FRPs), which was generated by photo-induced charge transfer from the boron atom to the phosphorus atom.[1] The FRP also enabled reversible insertion of the boron atom into aromatic C–C bonds.[2] Recently, we developed a light/heat-responsive FLP system for on-demand fixation of ethylene via FRPs, realizing reversible capture and release of ethylene and other alkenes orthogonally triggered by visible light and heat.[3] The details of generality, reaction mechanism, and synthetic application to alkene upconversion will be discussed in the presentation.

Exploration of photochemistry of boron-based FLPs



[1] Ito, T.; Iwasawa, N.; Takaya, J. *Angew. Chem. Int. Ed.* **2020**, *59*, 11913.

[2] Kuroki, K.; Ito, T.; Takaya, J. *Angew. Chem. Int. Ed.* **2023**, *62*, e202312980.

[3] Yanagi, T.; Takaya, J. *J. Am. Chem. Soc.* **2025**, *147*, 15740.

Dr. Jun Takaya received his PhD from Tokyo Institute of Technology under the direction of Prof. Nobuharu Iwasawa (2004). After a JSPS postdoctoral period (2004-05, Prof. John F. Hartwig at Yale University), he was appointed to an Assistant Professor at Tokyo Institute of Technology in 2005 and promoted to Associate Professor in 2014. He moved to Osaka university as a Full Professor in 2024. He was working as a researcher of PRESTO, JST from 2017 to 2020.

S34

Development of Highly Active Heterogeneous Bimetallic Nanoparticle Catalysts for Selective Hydrogenation and Its Application to Integrated Continuous-flow Organic Synthesis

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Continuous-flow synthesis has been gathering much attention in synthetic organic chemistry. Especially, connecting several reactors to integrate different reactions for multi-step organic synthesis is a powerful method of synthesizing high-value compounds like pharmaceuticals continuously. However, there are some difficulties in such integrations of flow reactors: a lower concentration solution is required for substrates with poor solubility; the volume of solvent increases by connecting multiple flow reactors, resulting in lower concentrations of reactants; and the integration of reactions whose kinetics and reaction speeds are varied is difficult.

Anthraquinone derivatives are classes of compounds employed in the production of valuable materials. Leuco-quinizarin, the 2-electron reduced form of quinizarin (1,4-dihydroxy-anthraquinone), is a highly active and useful reactant for the synthesis of variety of anthraquinone derivatives. We developed Pt/DMPSi-Al_2O_3 and Pt-Ni/DMPSi-Al_2O_3 as highly active and selective heterogeneous catalysts for the hydrogenation of quinizarins to leuco-quinizarins under neutral and continuous-flow conditions. Remarkably, bimetallic effects of Ni and Pt nanoparticle systems were highlighted in the selective hydrogenation of substituted quinizarin. 1) In addition, the continuous-flow synthesis of leuco-quinizarin and its derivatization reaction were integrated to be a fully continuous process using Flow-Batch-Separator unified reactors for synthesis of valuable compounds.

[1] Miyamura, H.*; Sharma, A.; Takata, M.; Kajiyama, R.; Kobayashi, S.; Kon, Y. Selective Hydrogenation of Quinizarins to Leuco-quinizarins and Their Direct Derivatization Using Flow-Batch-Separator Unified Reactors under Continuous-Flow Conditions. *ACS Catal.* **2024**, *14*, 10317-10323.

Hiroyuki Miyamura received BS degree (2004), MSc (2006), and PhD degrees (2009) in Pharmaceutical Sciences from The University of Tokyo, Japan, under the supervision of Professor S. Kobayashi. In 2009, just after receiving his PhD degree, he was appointed to Assistant Professor in the Department of Chemistry, The University of Tokyo. He had developed heterogeneous supramolecular catalysts in University of California, Berkely with Prof. F. D. Toste, Prof. K. N. Raymond and Prof. R. G. Bergman (2018-2019). In 2022, he moved to National Institute of Advanced Industrial Science and Technology (AIST) as Senior Researcher.

S35

Synthesis of novel plant hormones: Fine bubble and flow technology for fairy chemicals

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Fairy chemicals (FCs), such as 2-azahypoxanthine (AHX), represent a potential new class of plant hormones, naturally occurring in plants and produced *via* a novel purine metabolic pathway. FCs contribute to plant resilience against various stresses and regulate plant growth. Despite their biological significance, efficient and sustainable synthetic routes remain limited. In this study, we developed a four-step method for synthesizing AHX from 2-cyanoacetamide, employing fine bubble and flow chemistry to enhance efficiency. Initially, oxime was synthesized from 2-cyanoacetamide *via* an oximation reaction. A cascade-type, one-pot selective Pt/C-catalysed reduction of oxime, followed by a coupling reaction with formamidine acetate, afforded the intermediate 5-amino-1*H*-imidazole-4-carboxamide (AICA). Fine-bubble technology markedly enhanced the conversion of oxime to AICA, yielding 69%. Subsequently, 4-diazo-4*H*-imidazole-5-carboxamide (DICA) was synthesized from AICA via diazotization. Notably, we successfully obtained stable solid-state DICA, overcoming previous reports of instability. Finally, intramolecular cyclization of DICA, catalysed by $PhI(OAc)_2$ (0.5 mol%) in water, yielded AHX with an overall yield of 47%. This study uses modern fine bubble and flow technologies to establish an efficient, scalable synthetic route for FCs. The process improves yield and selectivity and enhances environmental sustainability. These findings provide a foundation for further research on FCs and their agricultural applications, paving the way for future studies on their physiological roles and potential benefits in plant science.

[1] "Fine bubble technology for the green synthesis of fairy chemicals" Manna, A. K.; Doi, M.; Matsuo, K.; Sakurai, H.; Subrahmanyam, C.; Sato, K.; Narumi, T.; Mase, N., *Org. Biomol. Chem.* **2024**, *22* (17), 3396-3404.

Nobuyuki Mase was born in Tokoname, Japan, in 1971. He received his Ph.D. from Nagoya Institute of Technology under the supervision of Professor Takeshi Toru in 1999 and began his academic career at Shizuoka University (SU) the same year. From 2003 to 2004, he worked as a Visiting Professor in the group of Professor Carlos F. Barbas III at The Scripps Research Institute. He became an Associate Professor in Materials Science and Chemical Engineering at SU in 2007 and has been a Professor of Applied Chemistry and Biochemical Engineering there since 2014. Since 2022, he has also served as Director of the Research Institute of Green Science and Technology at SU.

S36

Nano-Structured Heterogeneous Catalysts in Batch and Flow

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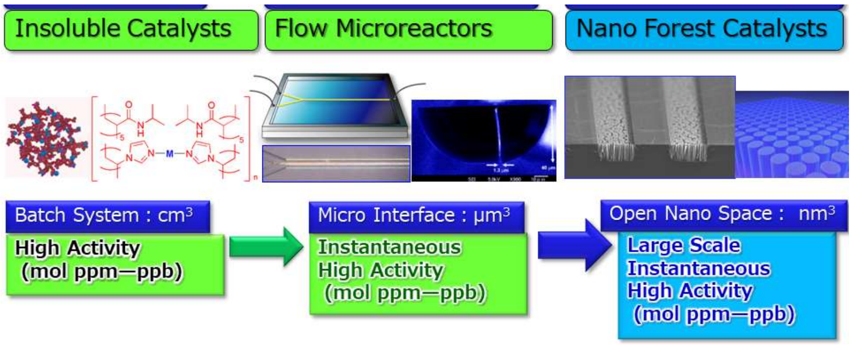
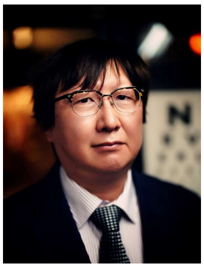
Our research focuses on developing highly efficient and recyclable nano-structured catalysts for organic transformations in batch and flow. We aim to unlock the full potential of catalysts to enable previously unexplored reactions. Additionally, we analyze the effects of light and microwave irradiation on catalytic performance and explore reactions that benefit from these conditions. A key aspect of our work is designing catalysts tailored for environmentally friendly processes, promoting sustainable chemistry.

To achieve these goals, we employ various strategies. First, we synthesize self-organized catalysts by integrating polymer ligands and metal species, ensuring precise structural control. Second, we develop spatial catalysts by incorporating micro/nanomaterials into catalytic matrices, significantly enhancing efficiency and selectivity. Finally, we explore electromagnetic wave-activated catalysts, which utilize light or microwave irradiation to drive catalytic transformations.



In this lecture, I will present case studies from our recent work, demonstrating the effectiveness of these approaches in advancing catalytic science.

[1] (batch) *JACS Au* **1**, 2080 (2021), and references cited therein; (flow) *Chem. Eur. J.* **30**, e202304335 (2024)
[2] (personal account) *Synlett* **34**, 1739 (2023); (batch) *ACS Catal.* **10**, 2148 (2020); (flow) *Chem.-Methods* e202500050 (2025); *J. Org. Chem.* **90**, 1447 (2025).
[3] *ACS Catal.* **13**, 12665 (2023)



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Visiting Professor, Kyushu University
Visiting Professor, Institute of Science Tokyo
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1999 Assistant Professor, Teikyo University
2003 Research Associate, The Scripps Research Institute, USA
2003 Assistant Professor, Institute for Molecular Science (and The Graduate University for Advanced Studies)
2007 Deputy Team Leader, RIKEN
2018 Team Leader, RIKEN (Adjunct Professor, Saitama University)
2025 Team Director, RIKEN (~current)

S37

Synthtetic Study for Neothioviridamide via the Formation of (Aminovinyl)methylcysteine through Photocatalytic Oxidative Decarboxylation

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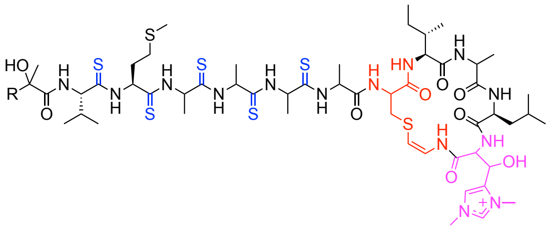
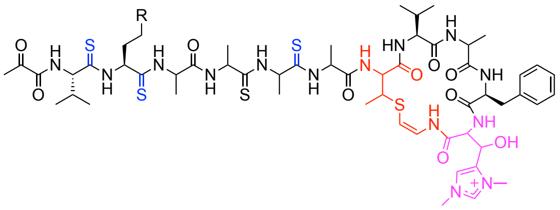
Thioviridamide isolated from an actinomycete identified as *Streptomyces olivoviridis* is a cyclic peptide natural product that possesses unique structures, such as an (aminovinyl)methylcysteine moiety, multiple thioamide bonds, and *N,N*-dimethyl-3-hydroxyhistidinium [1–2]. Since JBIR–140, a thioviridamide derivative, was isolated together with thioviridamide by heterologous expression using the entire gene cluster for thioviridamide biosynthesis [3], the heterologous expression using the gene clusters similar to those of thioviridamide have been investigated to discover further unique analogues like neothioviridamide [4], thiostreptamide S87, thioholgamides A and B, TVA-YJ-2, and thiosparsoamide. We have demonstrated photo-induced decarboxylative alkene formation of the (aminovinyl)methylcysteine moiety from lanthionine derivatives [5]. The scope of the reaction, its challenging application performed on a cyclic peptide, and the linkage of a side chain with multiple thioamide bonds toward the total synthesis of deoxyneothioviridamide will be presented.



thioviridamide (R = 2-oxopropyl)
JBIR-140 (R = H)



neothioviridamide, thiostreptamide S87, thioholgamide A, TVA-YJ-2, and thiosparsoamide (R = SMe); thioholgamide B (R = S(=O)Me)

[1] Hayakawa, Y.; Sasaki, K.; Adachi, H.; Furihata, K.; Nagai, K.; Shin-ya, K. *J. Antibiot.* **2006**, *59*, 1-5.

[2] Hayakawa, Y.; Sasaki, K.; Nagai, K.; Shin-ya, K.; Furihata, K. *J. Antibiot.* **2006**, *59*, 6-10.

[3] Izumikawa, M.; Kozone, I.; Hashimoto, J.; Kagaya, N.; Takagi, M.; Koiwai, H.; Komatsu, M.; Fujie, M.; Satoh, N.; Ikeda, H.; Shin-ya, K. *J. Antibiot.* **2015**, *68*, 533-536.

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[5] Kumashiro, M.; Ohsawa, K.; Doi, T. *Catalysts* **2022**, *12*, 1615.

1991.3	Ph. D. TokyoTech (Prof. Takashi Takahashi)
1991.4	Postdoc, Columbia University (Prof. G. Stork)
1993.10	Assistant Professor, TokyoTech
2001.2	Associate Professor, TokyoTech
2008.4	Professor, Tohoku University

S38

Computationally Guided Total Syntheses of Dimeric Pyrrole–Imidazole Alkaloids

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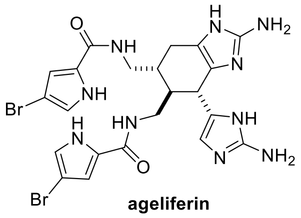
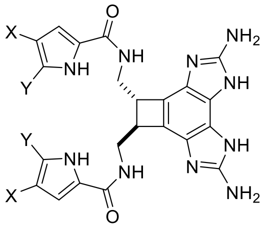
Predicting reactivity and designing reliable routes to complex natural products remain key challenges in total synthesis. In this presentation, I report the total syntheses of the dimeric pyrrole–imidazole alkaloids ageliferin and benzosceptrins, enabled by reactivity prediction with ConfoTS, a Python-based workflow for transition-state analysis.

For ageliferin, a virtual library of D-tartrate–based substrates for a dearomative Diels–Alder reaction of a hymenidin-derived unit was evaluated by analysis of transition-state energies. Analysis of this virtual library identified an optimal scaffold that underwent the cycloaddition with high stereoselectivity to construct a highly substituted six-membered core, leading to ageliferin in 15 steps from a known tetrahydropyridazine.[1] For the benzosceptrins, which feature a C_2-symmetric benzocyclobutane structure, ConfoTS was used to compute Gibbs energy profiles for a biosynthetically inspired 8π/6π electrocyclization pathway from nagelamide I–type substrates. These calculations guided substrate design and enabled the total syntheses of (±)-benzosceptrins A, B, and C.[2] Together, these studies demonstrate how prospective transition-state–based reactivity predictions can be integrated into synthetic planning for structurally complex dimeric pyrrole–imidazole alkaloids.



ageliferin



benzosceptrin A : X = Y = H
benzosceptrin B : X = Br, Y = H
benzosceptrin C : X = Y = Br

[1] Fujino, Y.; Fukaya, K.; Urabe, D. *J. Am. Chem. Soc.* **2025**, *147*, 34556–34563.

[2] Fujino, Y.; Matoba, T.; Amano, A.; Saito, K.; Fukuyama, K.; Fukaya, K.; Urabe, D. *manuscript submitted.*

Keisuke Fukaya received his B.S. (2012) and Ph.D. (2017) from Keio University, where he studied natural product synthesis under Professors Noritaka Chida and Takaaki Sato. He subsequently conducted postdoctoral research at the University of Texas at Austin with Professor Michael J. Krische. In 2018, he joined Toyama Prefectural University as an Assistant Professor and has been a Lecturer since 2024. His research centers on natural product synthesis and computational chemistry to enable efficient construction of complex molecules.

S39

Discerning Reactivity of Metal-Nitrogen Multiple Bonds from ^{15}N Solid-state NMR Spectroscopy

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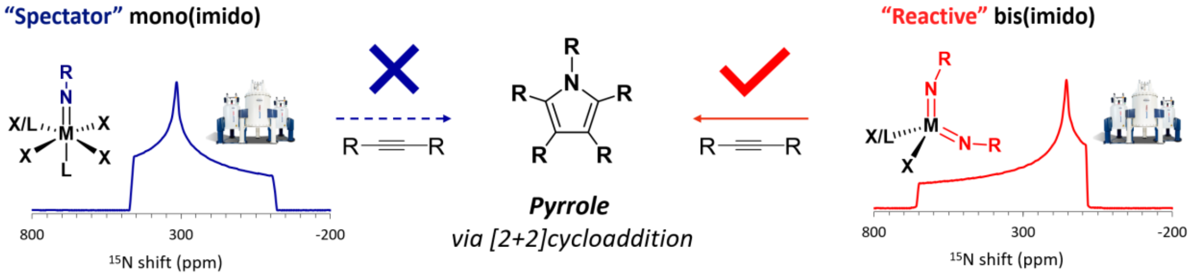
Metal-nitrogen multiple bonds – represented by terminal imido (M=NR) or hydrazide (M=NNR$_2$) complexes – serve as an ancillary ligand, or a key reactive intermediate for organic transformations, such as hydroamination, C-H bond functionalization and more recently, pyrrole formation reactions. Notably, the reactivity of M-N bond greatly varies depending on the metal center and other ligands. The most typical example can be found in different [2+2]-cycloaddition activities between d^0 mono(imido) species, which are often inert, and bis(imido)s which readily react with unsaturated bonds, calling for the rational catalyst design guidelines.

In an effort to identify the reporter of the nature of M-N multiple bonds, we explored the use of ^{15}N solid-state (ssNMR) spectroscopy, primarily focusing on deciphering the reactivity of d^0 transition metal imido complexes. In fact, Chemical Shielding Tensors (CSTs) – readily available parameters from ssNMR spectra and computations – are diagnostic for the bonding and reactivity of imido ligand, where spectral line shapes reflect the M-N bond order. These results showcase the power of ssNMR as a catalyst-design guidelines, and further imply the potential of its parameters, accessible both from experiments and computations, as a convenient handle for data-science applications.



[1] Kakiuchi, Y.; Karmakar, P. S.; Roudin, J.; Tonks, I. A.; Copéret, C. *J. Am. Chem. Soc.* **2024**, *146*, 9860–9870.

[2] Karmakar, P. S.; Kakiuchi, Y.; Kim, J.; Harris, M. R.; Huh, D. N.; Sell, A. G.; Copéret, C.; Tonks, I. A. *J. Am. Chem. Soc.* **2025**, 147, 11019–11027.

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S40

Artificial Enzymes Containing Non-natural Active sites

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In nature, enzymes are responsible for the difficult chemical conversions with high efficiency and selectivity. However, most of these enzymes have strong limitation of the reactions only toward native substrates. Recently, creations of artificial enzymes have been reported by mutations and insertion of artificial metal complexes into protein matrices. Our group has especially focused on myoglobin (Mb), a small oxygen-binding hemoprotein, and prepared reconstituted Mb by replacement of heme with an artificial cofactor.[1−] We found that Mb reconstituted with metal complexes of porphycene, a constitutional isomer of porphyrin, catalyzes H_2O_2-dependent C–H bond hydroxylation and olefine cyclopropanation.[2,3]

Most recently, we employed lipocalin (Lip), a protein scaffold known to bind fluorescein (Flu), together with its variants.[3] The resulting Flu–Lip artificial enzymes were evaluated for catalytic activity in the photoinduced imine reduction of dihydroisoquinoline derivatives. To enhance activity, alanine scanning and site-directed mutagenesis were performed on residues near the dye-binding pocket. Among these, the H86D mutant showed markedly improved performance, with a turnover number (TON) approximately 3.5 times higher than that of the wild type. Further titration experiments analyzed by Stern–Volmer plots suggested that active variants displayed enhanced substrate-binding ability compared to the wild type, correlating with their higher TON values. These findings highlight the potential of protein scaffolds to provide not only asymmetric environments but also improved substrate affinity for photoredox catalysis.

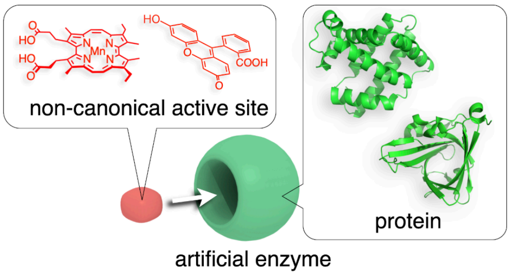

Fig. Schematic representation of artificial enzyme.

[1] K. Oohora, T. Hayashi, *Dalton Trans.*, **2021**, *50*, 1940.
[2] K. Oohora, T. Hayashi, et al., *J. Am. Chem. Soc.*, **2017**, *139*, 18460.
[3] Y. Kagawa. K. Oohora, T. Hayashi, et al., *Angew. Chem. Int. Ed.*, **2024**, *63*, e202403485.
[4] R. Kano, K. Oohora, T. Hayashi, *J. Inorg. Biochem.*, **2024**, *259*, 112657.

Koji Oohora received his Ph.D. degree from Osaka University under the supervision of Prof. Takashi Hayashi in 2011 and then promoted to be an Assistant Professor at Osaka University. He has been an Associate Professor at Osaka University since 2020. His research interests involve metalloprotein-based catalysts and materials.

S41

Visible light induced perfluoroalkylation of phenols

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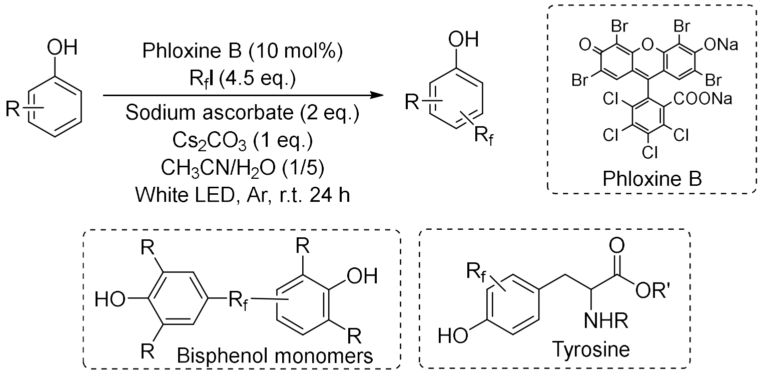
Fluoro-organic compounds are among the most abundant motifs in the pharmaceutical and agrochemical industries and in functional materials because of their unique fluorine-derived features. Also, fluorine-containing polymers are essential materials in our daily lives, such as heat resistance, water repellency, and low dielectric constant. We have conducted a series of studies on fluoroalkylation reactions using metal-free visible light reactions. During our studies, we have found that visible light fluoroalkylation is also effective for reactions with aromatic rings. Here, I will present the fluoroalkylation reactions of phenols using visible light reactions with organic catalysts.

In the reaction of phenol, phloxine B worked most effectively, in the presence of sodium ascorbate and cesium bicarbonate producing perfluoroalkylated product in good yields. This reaction did not use any transition metals and just photoirradiation using white LEDs. The reaction can produce fluorinated bisphenols or tyrosine. So we have also investigated polymer synthesis using our fluorinated bisphenols. And we also investigated the direct perfluorination of various amino acids and peptide.



I will also discuss the detailed reaction mechanism of this reaction and application for polymer synthesis and direct fluoroalkylation of peitides in the presentation.

[1] Sato, C.; Yamaguchi, A.; Shibata, H.; Katsuno, Y.; Kanbara, T. Yajima, T *J. Org. Chem.* **2025**, *90*, 24, 8434-8438.

1997 Ph.D, Tokyo Institute of Technology, Dept. of Chemical Engineering
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S42

Development and Application of Modular Automated Experimental System

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Recent advances in data science and computational technology have led to the development of automated experimental systems, thereby advancing research in chemical sciences[1]. Automated experimental technology minimizes the need for manual labor in experiments, enabling researchers to reduce the time spent on repetitive tasks and to prioritize conceptualizing, interpreting, and understanding the experiments and their results. However, existing automated experimental systems suffer from several issues that need to be addressed before they can be widely adopted. For instance, automated systems designed for specific reactions are difficult to apply to a more general class of reactions. Although systems capable of handling multiple synthesis experiments using different procedures exist, they often incur high implementation costs.

Our laboratory has developed an inexpensive and easily reconfigurable automated experimental system. The system consists of commercially available experimental devices which are converted into IoT modules using small PCs (Fig. 1). The system enables remote control of the experimental devices through these IoT modules. By converting experimental devices into IoT modules, we can design and implement automated experiments immediately even after changing the device components.

This system has been applied to a variety of chemical reaction experiments, including the Suzuki–Miyaura coupling, TEMPO oxidation of benzyl alcohol, and hydrogenation of aromatic ketones. Through these applications, we confirmed that this system is useful for both flow and batch systems. The labor savings afforded by automation are particularly significant in experiments that require extended durations.

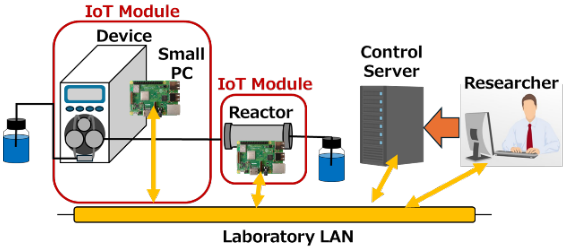

Fig. 1 Overview of Developed System

[1] Abolhasani, M., Kumacheva, E., The rise of self-driving labs in chemical and materials sciences, Nat. Synth, 2, 483-492 (2023).

Ken-Ichiro Sotowa specializes in continuous flow processes and laboratory automation. He earned his B.Eng. from Hiroshima University (1990) and PhD in chemical engineering from the University of Leeds (1997) under Prof. C. McGreavy. Following research on microreaction technologies at Kyushu and Tokushima Universities, he joined Kyoto University as professor in 2019, where he develops flexible automated experimental systems. He will serve as chair of the International Conference on Microreaction Technology (Kyoto, September 27-30, 2026).

S43

Amido Bond Formation by Electrocatalytic Oxidation of Hemiaminals at Gold Electrodes

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Amide is one of the most fundamental chemical bonds found in biological systems, and thus, a myriad of natural products and active pharmaceutical ingredients (API) contain amide bonds. With the rapid growth of peptide and oligonucleotide therapeutics, the importance of chemical tools in creating amide bonds by the coupling of carboxylic acids and amines is increasing. However, most synthetic methods for amide bond formation rely on the use of a (super)stoichiometric amount of the reagent, which generates an equimolar amount of chemical waste. Peptide and oligonucleotide processes typically generate 3000–15000 kg per kg of API. Thus, there is an increasing demand for the sustainable formation of amide bonds. In recent years, electrochemistry has attracted considerable attention as a sustainable method for organic synthesis.

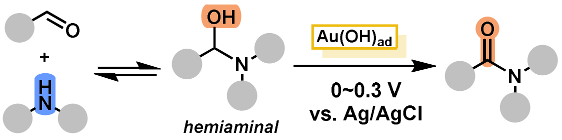

Figure 1. Concept of this work.

With these in mind, in the present work, we have demonstrated the electrocatalytic amide bond formation from aldehydes and amines in a continuous flow using gold (Au)-modified carbon felt for the first time (Figure 1).

The system demonstrated efficient amide synthesis from various aldehydes and amines (Figure 2). This approach achieves high selectivity and productivity through the chemoselective electrochemical oxidation of hemiaminals, offering a sustainable alternative for amide synthesis. In addition, mechanistic studies revealed that amine adsorption onto the Au surface is the key to chemoselectivity.

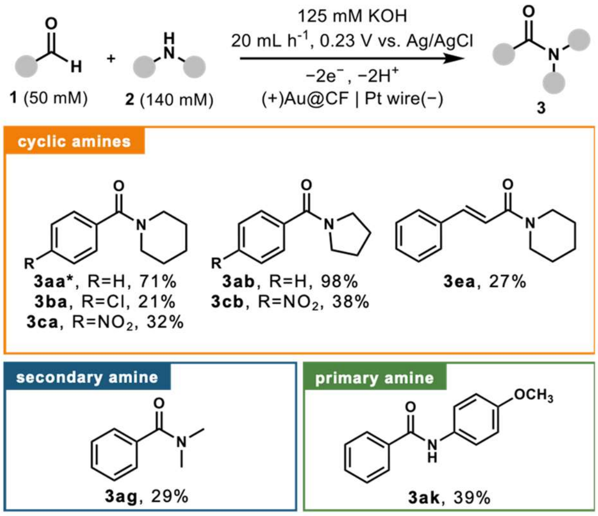

Figure 2. Substrate scope.

Reference

[1] J. Sato, M. Fujita, N. Shida, M. Atobe, *ACS Electrochemistry,* **2025**, *1*, 45–51.

Mahito Atobe
1993-1998: PhD Thesis with Prof. T. Nonaka, Department of Electronic Chemistry, Tokyo Institute of Technology
1996-2002: Research Associate of Tokyo Institute of Technology
2002-2007: Lecturer of Tokyo Institute of Technology
2007-2010: Associate Professor of Tokyo Institute of Technology
2010-present: Professor of Yokohama National University
Main Awards
2003: Young Research Award of the Electrochemical Society of Japan
2009: The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology: The Prize for Young Scientists

S44

Towards chemical reaction foundation model and synthetic route prediction tool

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Large-scale reaction databases are enabling advances in chemical research, including accurate reaction prediction and retrosynthetic analysis using AI. We developed ReactionT5 (https://github.com/sagawatatsuya/ReactionT5v2), a reaction prediction model trained on the Open Reaction Database (ORD), demonstrating strong performance in product, yield, and reverse reaction prediction with minimal fine-tuning [1]. To support widespread adoption, we maintain the models on platforms such as HuggingFace and provide documentation and tutorials for visualization and fine-tuning.

Beyond single-step prediction, we developed ReTReK, a multi-step retrosynthesis model [2] (https://github.com/clinfo/RetRekpy). Implemented as the Python package ReTReKpy, it allows researchers to easily use and extend the model with additional data for specialized reaction domains. We further enhanced benchmarking capabilities and are developing a user-friendly interface to support use by external researchers and industry. This presentation will introduce these software tools.

[1] T.Sagawa, R.Kojima: ReactionT5: a pre-trained transformer model for accurate chemical reaction prediction with limited data. In Journal of Cheminformatics, Springer, Vol. 17 No. pp. 126, 2025.

[2] S.Ishida, K.Terayama, R.Kojima, K.Takasu, Y.Okuno: AI-Driven Synthetic Route Design Incorporated with Retrosynthesis Knowledge. In Journal of Chemical Information and Modeling, 2022.

Received a B.E. in Computer Science in 2012, an M.E. in Information Science and Engineering in 2014, and a Ph.D. in Engineering in 2017 from the Tokyo Institute of Technology, Japan. Appointed as a program-specific associate professor (AMED) at the Graduate School of Medicine, Kyoto University, in 2017. Became a lecturer at the same graduate school in 2021. Serving as an associate professor at the Center for Digital Transformation of Healthcare, Graduate School of Medicine, Kyoto University, since 2024. Concurrent positions include associate professor in the Department of Biomedical Data Science, Graduate School of Medicine, Kyoto University, and team director at the Laboratory for Multimodal AI Framework, BDR, RIKEN, Japan.

S45

Fused Cyclobutenes to *trans*-Cycloalkenes

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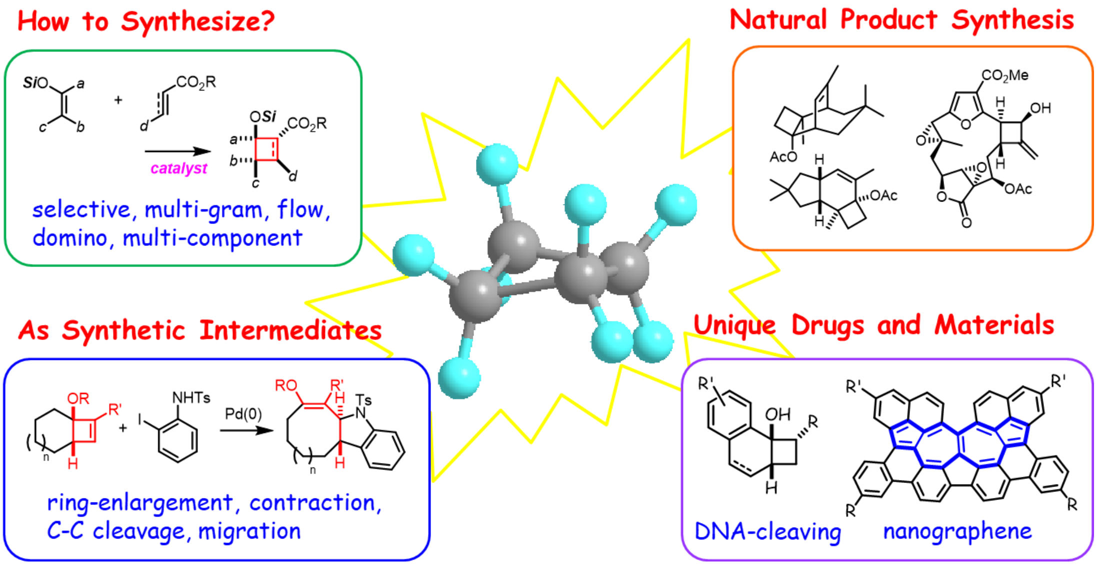
Four-membered carbocycles, such as cyclobutanes and cyclobutenes, are one of fundamental and important structural units. Due to the ring strain, the four-membered carbocycles have been utilized in synthetic chemistry. Despite their high utility, only a limited number of practical and efficient methods exist for their synthesis.

We have developed two classes of new synthetic methods to give multi-functionalized cyclobutanes and cyclobutenes. These findings led us to discover many interesting transformation reactions of the four-membered carbocycles driven by their ring-strain relief.^{2} In this symposium, I would like to talk about the synthesis of medium-sized trans-cycloalkenes from fused-cyclobutenes by electrocyclization.



[ref] *J. Am. Chem. Soc.* **2015**, *137,* 9579, *Angew. Chem. Int. Ed.* **2019**, *58*, 11836, *Synlett* **2023**, *34*, 1275, *Org. Lett.* ASAP.

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2005-2007	Lecturer, same as above.
2007-2011	Assoc. Prof., Kyoto Univ., Grad. Sc. of Pharm. Sci.
2012-current	Full Prof., same as above.

Awards: The Incentive Award in Synthetic Organic Chemistry, Japan, The PSJ Award for Young Scientists.

S46

Air-Stable Tetrazene Radical Cation Salts: Synthesis, Characterization, and Oxidation Catalysts

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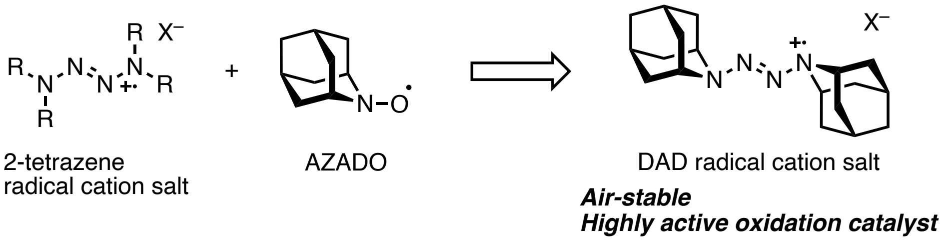
Stable organic radicals are widely studied for their unique properties, yet radical cation salts that persist under ambient conditions remain rare. Nitrogen-based radical cations typically require aromatic π-conjugation for stabilization, and isolable aliphatic examples are exceedingly uncommon. Tetrazene frameworks, composed of four linearly connected nitrogen atoms, offer a distinctive platform for such species; however, their radical cations have been rarely investigated, and no structurally authenticated examples have been reported to date.[1,2]

We designed a 2-tetrazene radical cation in which both nitrogen termini are embedded within rigid azaadamantane skeletons, identifying 1,2-di(2-azaadamantan-2-yl)diazene (DAD) as its neutral precursor. This design strategy was inspired by the highly robust and strongly active nitroxyl radical oxidation catalyst 2-azaadamantane *N*-oxyl (AZADO), whose rigid adamantane framework plays a crucial role in stabilizing its radical nature.[3]

In this study, we synthesized and isolated air-stable tetrazene radical cation salts generated by one-electron oxidation of DAD. The resulting radical cation shows exceptional persistence and serves as a highly active catalyst for alcohol oxidation.



2-tetrazene radical cation salt

AZADO

DAD radical cation salt

Air-stable
Highly active oxidation catalyst

[1] Tolles, W. M.; Moore, D. W.; Thun, W. E. *J. Am. Chem. Soc.* **1966**, *88*, 3476–3479.

[2] Nelsen, S. F.; Kessel, C. R.; Brien, D. J. *J. Am. Chem. Soc.* **1980**, *102*, 702–711.

[3] Shibuya, M.; Tomizawa, M.; Suzuki, I.; Iwabuchi, Y. *J. Am. Chem. Soc.* **2006**, *128*, 8412–8413.

2012-2014	Research Instructor at Tohoku University
2014	Ph.D. Tohoku University
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P-1

Metal-Free Conversion of Amines to Perfluoroalkylated Amides via Visible-Light Photocatalyst

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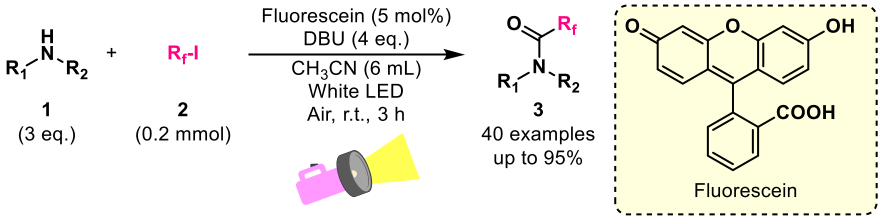
Fluorinated organic compounds show unique characteristics such as high metabolic stability, enhanced lipophilicity, and strong electron-withdrawing properties, making them indispensable in pharmaceuticals, agrochemicals, and functional materials. Among them, fluorinated amides are particularly valuable due to their broad applications across agrichemistry, medicine, and functional material science. Therefore, the development of efficient synthetic methods for accessing these perfluoroalkylated amides is highly important. Furthermore, from the viewpoint of green chemistry, sustainable, inexpensive, and operationally simple methods are highly demanded.

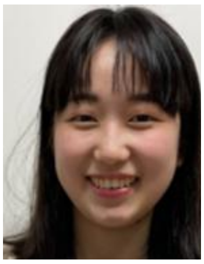
However, fluorinated amide compounds have traditionally been synthesized using explosive or highly unstable fluorine sources or transition-metal catalysts, which pose significant safety, handling, and environmental challenges.[1] In contrast, photochemical reactions are recognized as green and energy-efficient, operating under mild conditions. Our laboratory has reported a series of visible-light-driven reactions employing perfluoroalkyl iodides as fluorine sources and metal-free organic photocatalysts as a driving force of the reactions.

We herein report a metal-free, visible-light-induced perfluoroalkylation of amines, affording perfluoroalkylated amides under mild and environmentally friendly conditions (Scheme 1) . Notably, this method allows the use of inexpensive amines as starting materials and can be performed under ambient atmosphere. The reaction shows broad substrate scope, enabling efficient access to diverse fluorinated amides from various amines and perfluoroalkyl iodides.

Scheme 1.



[1] S. Liu, J. Zhou, L. Yu, Y. Liu, Y. Huang, Y. Ouyang, G-L. Liu, X-H. Xu, and N. Shibata, *Chem. Rev.* **2025**, *125*, *9*, 4603–4764



Airi Yamaguchi received her B.Sc. in Chemistry from Ochanomizu University in 2022 and her M.Sc. in 2024 under the supervision of Prof. Tomoko Yajima. She is currently pursuing her Ph.D. in the Department of Chemistry at Ochanomizu University, working with Prof. Yajima. Her research focuses on photoinduced organic reactions and the development of synthetic routes, particularly in the field of organofluorine chemistry.

P-2

Pd-catalyzed carbon–carbon double bond cleaving difunctionalization of Vince lactam

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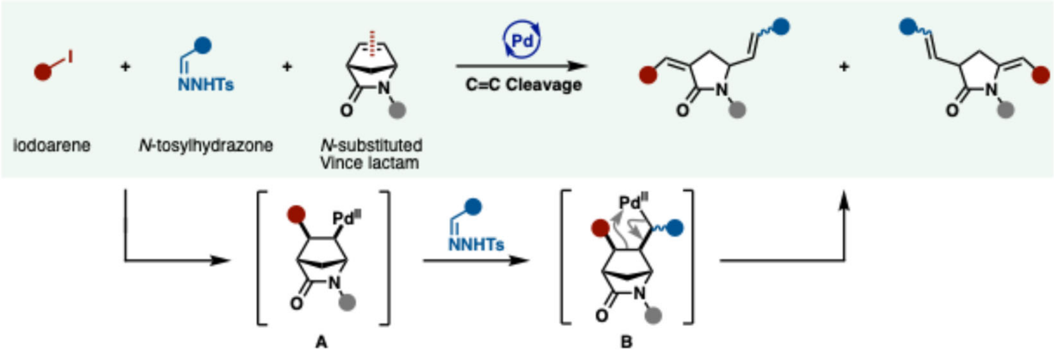
The cleavage of carbon–carbon double bonds, as seen in ozonolysis and olefin metathesis, is a powerful method for skeletal editing. Another notable example is the Pd-catalyzed difunctionalization of norbornene (NBE) with iodoarenes and *N*-tosylhydrazones to give disubstituted cyclopentanes, although this transformation was limited to unsubstituted NBE[1].

We focused on Vince lactam, a heterocycle with a [2.2.1] bicyclic framework, as an alternative NBE surrogate[2]. Vince lactam is a readily available pharmaceutical building block, but C=C bond cleavage has been reported only in limited cases such as ozonolysis. If a method could be developed to cleave this carbon–carbon bond while introducing difunctional groups, it would provide an excellent synthetic approach to disubstituted γ-lactams.

In this study, we report a palladium catalyzed difunctionalization of Vince lactam involving the cleavage of a carbon-carbon double bond, using iodoarenes and *N*-tosylhydrazones. The reaction proceeds via β-carbon elimination of the intermediate **B**, generated from alkylpalladium species **A** and *N*-tosylhydrazone. The method provides efficient access to substituted γ-lactams. Additionally, we found that the substituents on the nitrogen atom of the Vince lactam significantly influence regioselectivity.



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[2] Singh, R.; Vince, R. *Chem. Rev.* **2012**, *112*, 4642–4686.

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He received his B.Sc. from Waseda University in 2023 under the supervision of Prof. Junichiro Yamaguchi. He is currently pursuing his M.Sc. in the Department of Applied Chemistry, Waseda University, working with Prof. Yamaguchi. [Field of research] Organic Chemistry.

P-3

Arylation of Trialkyl Amines via C(sp^3)–N Bond Cleavage Enabled by Organosodium Compounds

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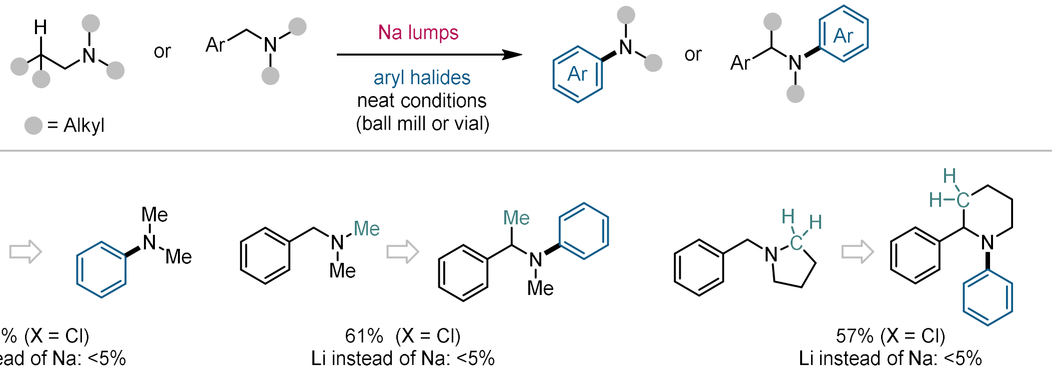
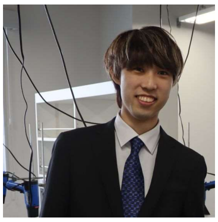
Organosodium compounds have recently attracted attention as sustainable alternatives to organolithium reagents. Beyond simple substitution, these compounds offer significant potential to access unique reactivities unattainable with organolithiums. However, exploration of these unique reactivities has remained limited due to poor solubility in organic solvents and difficulties in preparation. Recently, we developed a mechanochemical protocol for the generation and utilization of organosodium species[1], providing an operationally simple and rapid approach to probe their reactivities and develop new transformations.

Here, we report an unprecedented direct arylation of chemically inert trialkylamines via C(sp^3)–N bond cleavage, enabled by organosodium compounds under solvent-free conditions using either ball milling or simple magnetic stirring in a glass vial. A wide range of trialkylamines underwent site-selective C(sp^3)–N bond cleavage in the presence of aryl halides and metallic sodium to afford the corresponding arylated products in good yields. Moreover, when benzyl dialkylamines were used as substrates, the reaction proceeded with concomitant migration of one alkyl group on nitrogen. Notably, these new transformations barely proceeded with lithium metal, highlighting the distinct reactivity of organosodium species. Preliminary mechanistic studies suggest the involvement of aryne intermediates in these transformations.



[1] **<u>Kondo, K.</u>**; Lowe, M.; Davison, N.; Waddell, P. G.; Armstrong, R. J.; Lu, E.; Kubota, K.; Ito, H. *Nat. Synth.* **2025**, *accepted.*



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P-4

Extrapolated Prediction of High Confidence Using Virtual Variables in Iodination of Polyfluoroperylene

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Polyfluoroperylene (F8) and its derivatives are expected as new electronic materials. However, difficulty in large-scale F8 synthesis limits detailed condition studies (Fig.1.). Instead, we will explore the synthetic conditions for the target molecule F8 based on the results of examining the preliminary study molecules polyfluoronaphthalene. However, due to slight structural differences that result in differing electronic states, the target molecule cannot be obtained in high yield. To address this, we investigate the relationship between these molecules using iodinated F8 (PFIPR) as a case study, attempting to predict the yield of the target molecule.

To examine the first step of PFIPR synthesis in detail [1], yields were predicted using iodinated F7 naphthalene and F6 naphthalene as preliminary study molecules. The Generative Machine Learning Method with Virtual Variables (GMLV) [2] was used, which predicts yields by optimizing "virtual variables" representing molecular relationships. In this study, we examined the number of experimental data for the target molecule used in the input data and attempted GMLV model optimization.

The results shown in Fig.2. It was suggested that including at least one experimental data for the target molecule significantly improved prediction accuracy. Furthermore, errors tended to increase when data was biased toward specific temperature and time conditions.

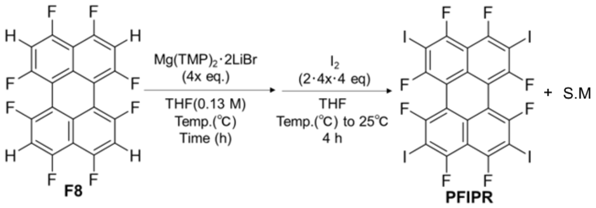


Fig.1. Synthesis of iodinated F8

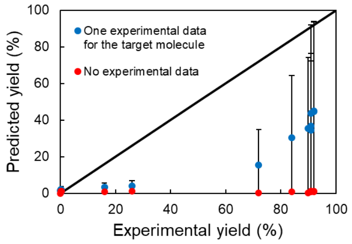
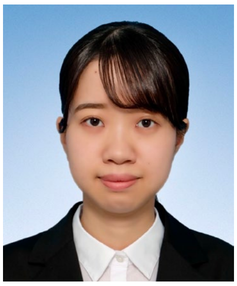


Fig.2. Comparison of yy Plots Based on the Presence or Absence of Experimental Data for Target Molecules

[1] K. Takeda, *et al. Artif. Intell. Chem.* Des. **2025**, 3, 1-10

[2] K. Takeda, *et al. Comput. Aided Geom.* Des. **2024**, 53, 2689-2694



Faculty of Engineering, Shizuoka University (April 2020 - March 2024)
Graduate School of Integrated Science and Technology, Shizuoka University (April 2024 -)

P-5

A SOMO–HOMO Inverted Radical Cation Derived from a Phenyl-substituted Highly Strained Cage Diketone

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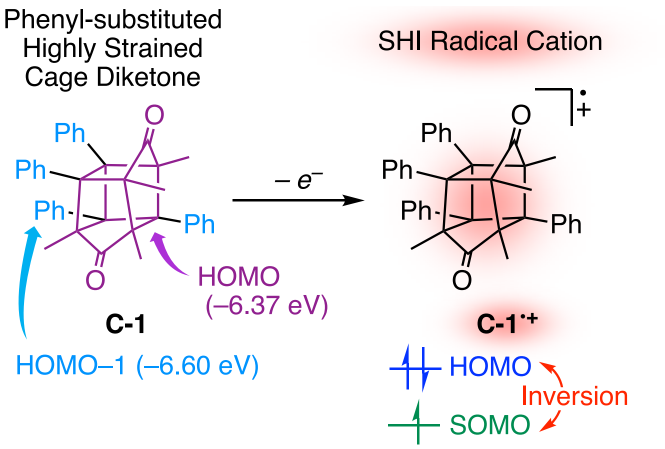
Recently, SOMO–HOMO inversion (SHI) open-shell species, in which the energy level of the SOMO is deeper than that of the HOMO have attracted much attention.[1] In this study, we conducted one-electron oxidation of **C-1** (Scheme 1) to generate a novel SHI radical cation **C-1**$^{\bullet+}$. This study was designed based on the finding that the HOMO and HOMO–1 of **C-1** are localized in a highly strained cage diketone and four phenyl groups, respectively, and possess energy levels close to each other.



Scheme 1. The generation of SHI radical cation **C-1**$^{\bullet+}$ by one-electron oxidation of the phenyl-substituted highly strained cage diketone **C-1**.

Density functional theory calculations and time-resolved ESR measurements of **C-1**$^{\bullet+}$ generated by the photoinduced electron-transfer reaction of **C-1** revealed that the g_{ZZ} value of the ZZ component of the g value is 2.0004, which is smaller than that of a free electron (2.0023) (Figure 1). This finding is direct evidence for the **C-1**$^{\bullet+}$ being an SHI radical cation based on the analysis using an equation shown in Figure 1.[2] In the presentation, we will also give details of the results of the transient-absorption spectroscopic analysis of **C-1**$^{\bullet+}$.

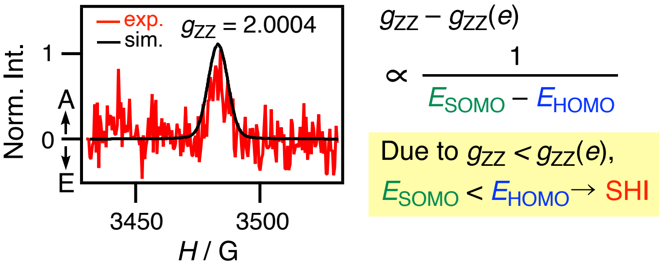
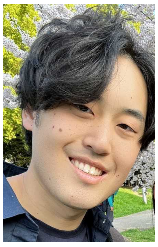


Figure 1. Time-resolved ESR spectrum of **C-1**$^{\bullet+}$ and the relationship between the g value and the energy level of the molecular orbital.

[1] Murata, R.; Wang, Z.; Abe, M. *Aust. J. Chem.* **2021**, *74*, 827–837.
[2] Ham, F. S. *J. Phys. Chem. Solids* **1963**, *24*, 1165–1174.



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Group of Prof. Hiroshi Ikeda

P-6

Selective Ring-Opening Monoaddition of Organopotassium Species to Lactones via Flash Microflow Technique

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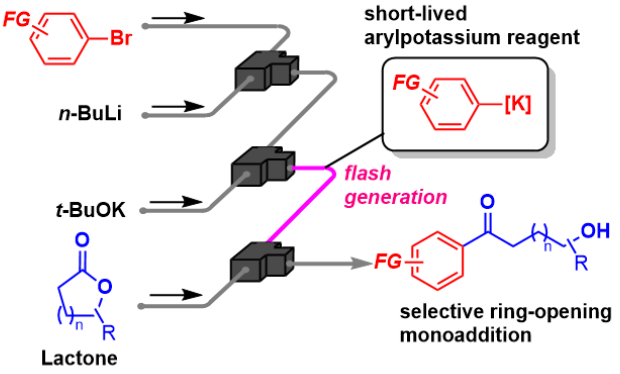
Polyesters derived from the ring-opening polymerization (ROP) of lactones are inherently biodegradable and have attracted considerable attention as sustainable alternatives to conventional plastics.[1] However, conventional ROP using organic bases or amphoteric metal alkoxides often suffers from side reactions such as backbiting and uncontrolled terminal functionalities, limiting the precise control of initiation and propagation.[2]

To address these issues, we aimed to achieve control over initiation and suppress side reactions by employing a rapid and irreversible anionic ROP. In this study, by utilizing the rapid mixing, instantaneous quenching, and precise temperature control of a flow microreactor, we successfully achieved anionic one-to-one ring-opening monoaddition via the selective nucleophilic addition of arylpotassium reagents to lactones. This reaction system enabled selective monoaddition even when using substituted organopotassium species or various lactones and lactams, and further revealed that polymerization is controllable under high-speed flow conditions by adjusting the equivalents of lactone in excess.



[1] Y. Ikada, H. Tsuji, Macromol. *Rapid Commun.* **2000**, *21*, 117–132.

[2] A. C. Albertsson, I. K. Varma, *Biomacromolecules* **2003**, *4*, 1466–1486.

Dong-eun Yoo

Ph.D. Candidate, Department of Chemistry, Hokkaido University (Nagaki Laboratory).

Research focuses on living anionic polymerization and monoaddition, and sequence-defined oligomerization

P-7

ET-Induced Three-Component Coupling of Ketones, Alkenes, and BPSE. Reactivity Dependence on One-Electron Oxidizing Reagents

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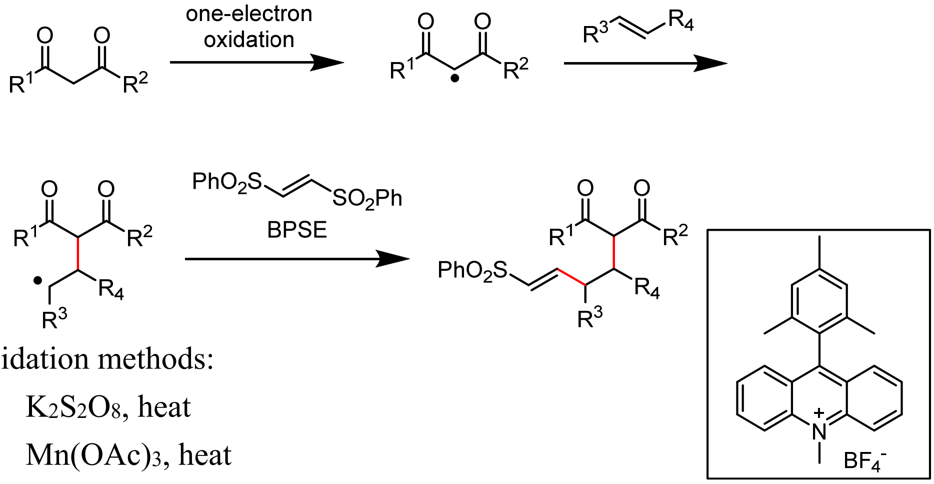
We report a protocol for δ,ε-unsaturated ketones by a three-component coupling of ketones, alkenes, and 1,2-bis(phenylsulfonyl)ethylene (BPSE) [1][2] using one-electron oxidizing reagents. In the presence of potassium persulfate, α-keto radicals are generated from β-diketones, which undergo polarity-matched addition to the ordinary alkenes and BPSE in order. In this study, we discuss the applicability of different oxidants and substrates for the transformation, which appears highly dependent on the oxidizing reagents. For example, while potassium persulfate and Fukuzumi's catalyst are limitedly effective for β-diketones, manganese(III) acetate works with malonates and even simple ketones. Behaviors of different alkenes and the role of BPSE in this system are also discussed.



Oxidation methods:

$K_2S_2O_8$, heat

$Mn(OAc)_3$, heat

Fukuzumi's catalyst, hν

Fukuzumi's catalyst

[1] For a review, see: Sumino, S.; Ryu, I.; Robert, F.; Landais, Y. *Synthesis*, **56**, 3233-3246 (2024).

[2] For our recent work using BPSE, see: (a) Tsai, C. -Y.; Jhang, Y. -J.; Wu, Y. -K.; Ryu, I. *Angew. Chem. Int. Ed.* **62**, e202311807 (2023). (b) Tsai, C. -Y.; Chen, C. -Y.; Wu, Y. -K.; Ryu, I. *Helv. Chim. Acta.* **107**, e202400017 (2024).

2020 ~ 2024: B.S. at National Taiwan Normal University, focused on asymmetric rhodium(I)-catalyzed addition reactions for undergraduate research.
2024 ~ present: M.S. student at National Yang Ming Chiao Tung University, currently studying radical-induced multi-component coupling and functionalization reactions.

P-8

Pd(II)-Catalyzed C(sp^2)-H Alkenylation of 2-Amino Biaryls with Bulky Internal Alkynes: From Alkenylation to Orthogonal Policyclic Hydrocarbons

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Palladium-catalyzed free-amine-directed C-H alkenylation of 2-amino biaryls with bulky internal alkynes is reported. These alkenylation products can be transformed to hetero policyclic orthogonal hydrocarbons via electrophilic aromatic substitution; for examples, 2,2′-binaphthyl-1,1′-bifunctional carboxylic acids, 6-phenanthridines, phenanthro-picenes, bulky aryl substituted phenanthrenes, and pyrene fused heptafluvene in moderate to good yields. These orthogonal hydrocarbons show attractive optoelectronic properties, evidenced by cyclic voltammetry, UV-vis and fluorescence data, act as candidates for organic electronic materials and chromophore reagents.

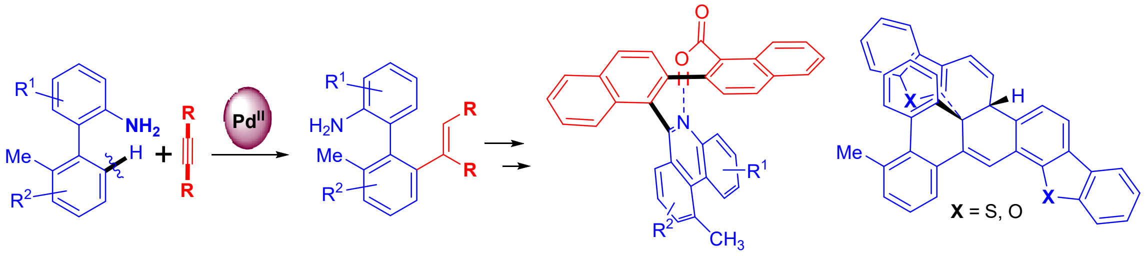
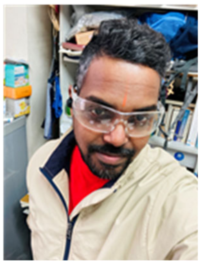


Figure 1. Unprecedented palladium-catalyzed C-H alkenylation of 2-amino biaryl with alkynes leading to orthogonal polycyclic hydrocarbon scaffolds.



I completed my M.Sc. in Chemistry in 2012 at St. Joseph's College, Tiruchirappalli, India. Since 2018, I have been pursuing my PhD under the supervision of Prof. Shih-Ching Chuang at National Yang-Ming Chiao Tung University, Taiwan. My research centres on the innovative synthesis of quaternary ammonium salts and Orthogonal polycyclic hydrocarbons, including polycyclic cinnolino[2,3-*f*]phenanthridin-9-ium and benzo[c]cinnolinium salts, supported by over seven years of hands-on expertise in their design and production

P-9

Rh(III)-Catalyzed Regioselective [4+2] Annulation of 2-Benzyl-2H-indazole-6-carboxylic Acids with Ynamides to Access Indazole-Fused Pyrans

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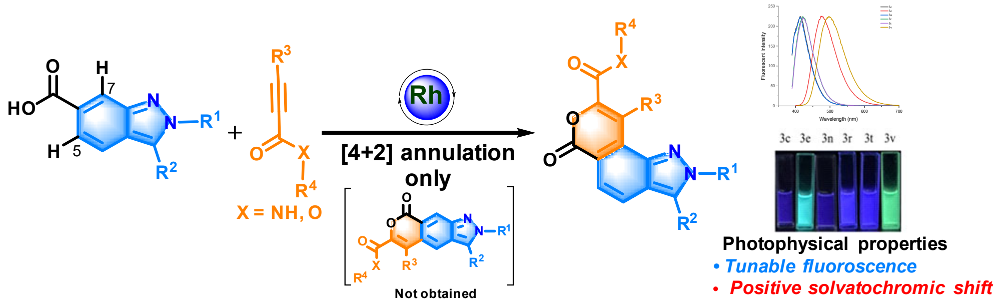
We report a Rh(III)-catalyzed C7–H activation/[4+2] annulation of 2-benzyl-2H-indazole-6-carboxylic acids with ynamides, enabling the regioselective synthesis of indazole-fused pyrans. Mechanistic studies highlight the pivotal role of the dual directing groups (indazole and carboxylic acid) in facilitating selective C7–H bond activation, even in the presence of the competing C5–H bond. This method provides a straightforward and efficient approach for accessing structurally diverse indazole-fused pyran derivatives under mild reaction conditions. In the photoluminescence study, the synthesized compounds exhibited tunable fluorescence (410–520 nm), covering most of the visible spectrum, along with a positive solvatochromic shift in solvents of varying polarity.



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[2] Dhole, S.; Liao, J.; Kumar, S.; Salunke, D.; Sun, C. *Adv. Synth. Catal.* **2018**, *360* (5), 942–950.

Mr. Hung-Sheng Hsieh holds a Bachelor of Science in Medicinal and Applied Chemistry from Kaohsiung Medical University (KMU) and a Master of Science in Medical Applied Chemistry from Chung Shan Medical University (CSMU). He is currently a Ph.D. candidate in the Laboratory of Combinatorial Drug Design, Department of Applied Chemistry at National Yang Ming Chiao Tung University (NYCU), where his research focuses on C-H activation of novel scaffolds in drug discovery applications. With five years of hands-on experience, he possesses extensive expertise in organic synthesis and catalysis.

P-10

Asymmetric Oxidative Dearomatization Using Chiral Hypervalent Iodine Catalysts: Enantioselective C-C Bond Formation Toward the Synthesis of Crinine-Type Alkaloids

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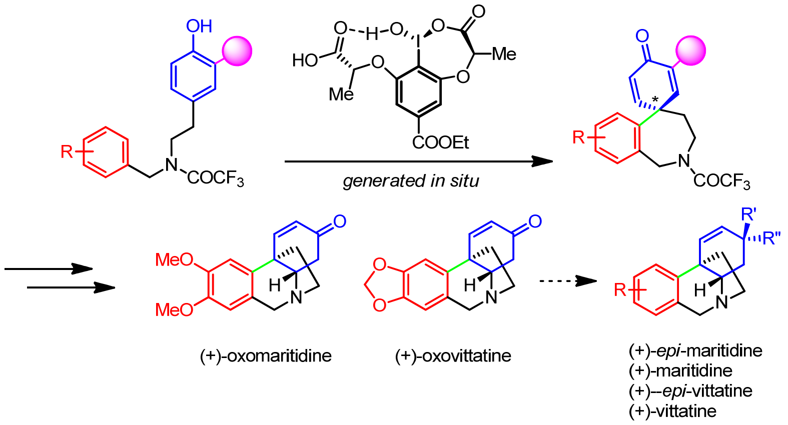
The oxidative dearomatization of simple phenols enables the formation of new C–C, C–N, C–O, and C–halogen bonds. Although numerous dearomatization protocols have been developed and applied in the synthesis of various natural products, hypervalent iodine–mediated oxidative dearomatization has emerged as a particularly versatile strategy due to its mild reaction conditions, low toxicity, and commercial availability.[1] In this study, we developed a novel and environmentally friendly chiral hypervalent iodine reagent capable of promoting asymmetric oxidative dearomatization under mild, metal-free conditions, addressing a previously underexplored area in chiral hypervalent iodine catalysis. This transformation allows the efficient construction of new carbon–carbon bonds with excellent stereocontrol. Furthermore, the developed methodology was successfully applied to the asymmetric synthesis of Crinine-type alkaloids, a family of natural products known for their significant biological activities.[2]



[1] Kumar, R.; Singh, F. V.; Takenaga, N.; Dohi, T. Asymmetric Direct/Stepwise Dearomatization Reactions Involving Hypervalent Iodine Reagents. *Chem. Asian J.* **2022**, *17*, e202101115.

[2] Berkov, S.; Atanasova, M.; Georgiev, B.; Bastida, J.; Doytchinova, I.; The Amaryllidaceae Alkaloids: an Untapped Source of Acetylcholinesterase Inhibitors. *Phytochem. Rev.* **2022**, *21*, 1415 - 1443.

Cheng-Hsun Huang received his B.S. degree from National Tsing Hua University in 2020 and has been pursuing his M.S. and Ph.D. in Applied Chemistry at National Yang Ming Chiao Tung University under the supervision of Prof. Yen-Ku Wu. He also served as a special research student in Prof. Kazuaki Ishihara's laboratory at Nagoya University from September to November 2025.

P-11

Catalytic Asymmetric Spirocyclizing Diels–Alder Reaction of *α*-Alkylidene Cyclic Vinylogous Esters Using a Chiral Oxazaborolidine Lewis Acid

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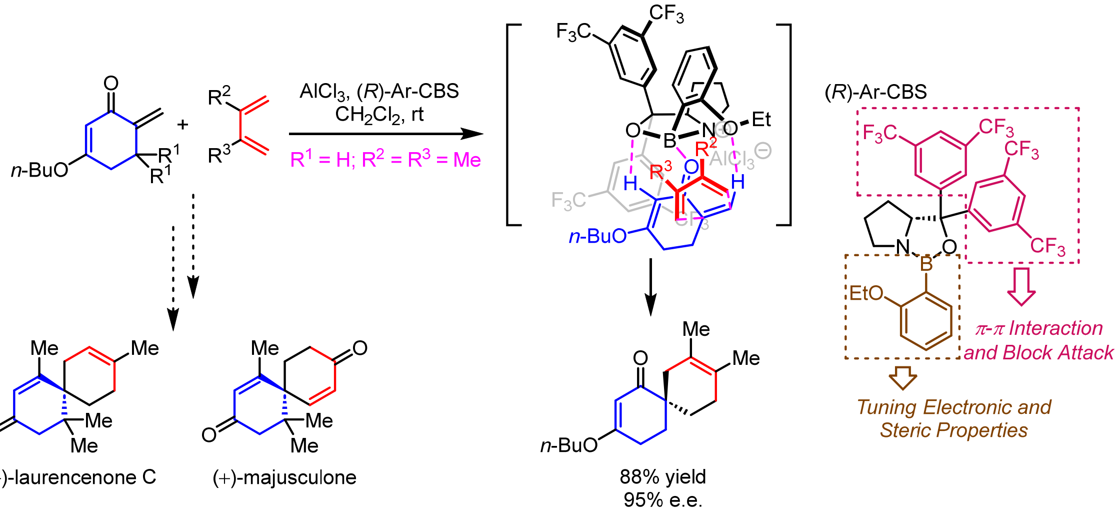
The transformation of *α*-alkylidene cyclic vinylogous esters into spirobicyclic products *via* a Diels–Alder reaction was developed using readily available catalytic systems. In our previous study, the AlMe₂Cl–catalyzed Diels–Alder reaction was successfully achieved and applied in the total synthesis of (±)-laurencenone C, along with 23 examples with yields up to 96%.[1] Recently, we further developed a chiral Lewis acid–mediated Diels–Alder reaction, in which an oxazaborolidine was found to deliver high yield and excellent enantioselectivity. The substituents of the oxazaborolidine core were systematically varied for the optimal performance.[2] This reaction scope is currently being investigated, and we will establish an updated approach to laurencenone C and other spiro-carbon-bearing natural products.



Scheme 1. Asymmetric Diels-Alder Reaction and Its Application in Total Synthesis.

[1] Cheng, Y.-T. M.S. Thesis, National Yang Ming Chiao Tung University, Hsinchu, 2023.

[2] (a) Corey, E. J.; Shibata, T.; Lee, T. W. *J. Am. Chem. Soc.* **2002**, *124*, 3808–3809. (b) Futatsugi, K.; Yamamoto, H. *Angew. Chem. Int. Ed Engl.* **2005**, *44*, 1484–1487. (c) Liu, D.; Canales, E.; Corey, E. J. *J. Am. Chem. Soc.* **2007**, *129*, 1498–1499.

Ke-Liang Chen (陳科諒). National Taitung University (BSc, 2019; MSc, 2021). Academia Sinica (Research Assistant, 2022-2023). PhD student, National Yang Ming Chiao Tung University (2023-present).
[Field of Research] Organic Chemistry.

P-12

Synthetic Strategy to Accomplish the Total Synthesis of Lipooligosaccharides of *Mycobacterium gastri*

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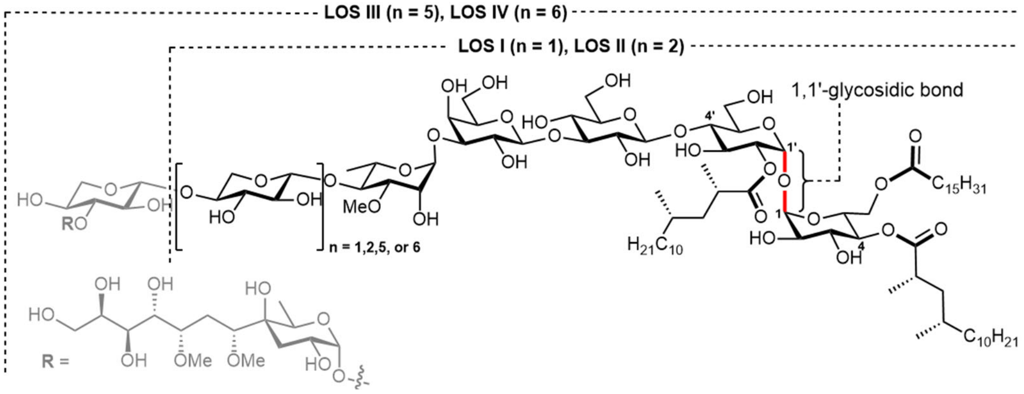
Mycobacterial lipooligosaccharides (LOS) are a class of complex glycolipids isolated from a variety of mycobacterial species.[1],[2] As distributed mainly at the periphery of the cell walls, the functional roles of these molecules remain largely unknown due to a lack of sample for biological studies.[3] This poster reports a practical strategy for the first total synthesis of two LOS structures namely LOS-I and LOS-II isolated from *Mycobacterium gastri*. The LOS-I and II comprise a trehalose substituted with three acyl chains at C4, C6, and C2′ positions. Extended from the C4′ position of the trehalose is a tetra- or pentasaccharide chain.[4] Our synthetic route features an asymmetrically protected trehalose core that enables regioselective acylation and glycosylation.[5] In present study, various carbonate participating groups were explored for construction of the β-glycosidic linkages.



[1] B. Bai, C.-J. Chu, T. L. Lowary. *Israel J. Chem*. **2015**, *55*, 360-372

[2] K. Shen, B. Bai, Y.-H. Liu, T. L. Lowary. *Angew. Chem. Int. Ed*. **2021**, *60*, 24859-24863

[3] M. Gilleron, J. Vercauterent, G. Piunz. *J. Biol. Chem*. **1993**, *268*, 3168-3179.

[4] M. Gilleron, G. Puzo. *Glycoconjugate J*. **1995**, *12*, 298-308.

[5] S. Mondal, C.-J. Tseng, J. J.-Y. Tan, D.-Y. Lin, H.-Y. Lin, J. H. Weng, C.-H. Lin, K.-K. T. Mong. *Angew. Chem., Int. Ed*., **2023**, *62*, e202212514

Tzu-Hsuan Nancy Huang received a B.Sc. and B.Ed. from the National Taiwan Normal University of Taiwan. She is currently pursuing the M.Phil. in the Department of Applied Chemistry in National Yang Ming Chiao Tung University. Her research mainly focuses on exploration of the electronic effects on neighboring participatory groups for deoxysugars and development of synthetic strategy for total synthesis of multi-acylated LOS.

P-13

Total Synthesis of Glycosyl Actinopyrone derivative and its Biosynthetic Precursor for Stereochemical Revision

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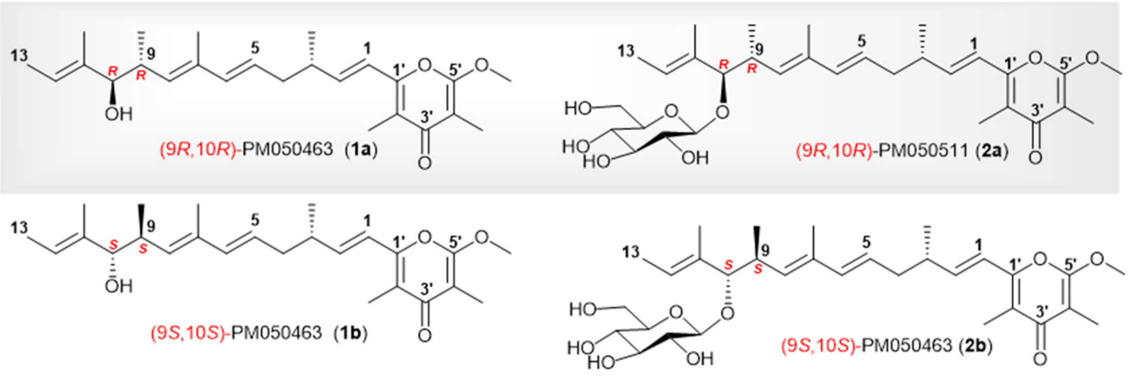
Actinopyrones and related derivatives are γ-pyrone metabolites that generated from a wide variety of *Streptomyces* species. [1] Based on the position and geometry of the double bond, presence or absence of a glucosyl residue, and substitution pattern of the γ-pyrone moiety, more than ten different actinopyrones and related derivatives have been characterized. [2,3] Despite the attractive biological properties such as anti-*Helicobacter pylori*, vasodilation, cytotoxicity, etc., the absolute configuration for some of the metabolites is still controversial. This poster describes the total synthesis of actinopyrones namely PM050463 (**1a**) and (**1b**), and PM050511 (**2a**) and (**2b**). Each are prepared on the base of the absolute configuration assigned in previous studies (**Figure 1**).[2,3] By comparing the NMR data of these diastereomers with the authentic samples, we confirmed the absolute stereochemistry of the natural products. The revised stereochemistry of the actinopyrones paves way for reassessment of the anti-*Helicobacter pylori* and cytotoxic properties.



(9*R*,10*R*)-PM050463 (**1a**)

(9*R*,10*R*)-PM050511 (**2a**)

(9*S*,10*S*)-PM050463 (**1b**)

(9*S*,10*S*)-PM050463 (**2b**)

[1] R. Th. Magar and J.-K. Sohng. *Appl. Microbiol. Biotechnol*. **2024**, *108*, article 471.

[2] C. Schleissner, M. Pérez, A. Losada, P. Rodríguez, C. Crespo, *et al*. *J. Nat. Prod.* **2011**, *74*, 1590–1596.

[3] H. Zhang, X. Zhang, Y. Huang, J. Yuan, X. Wei, J. Ju. *J. Nat. Prod*. **2022**, *85*, 625–633.

Jing-Hui, Zeng received a B.Sc. from the National Kaohsiung Normal University. She is currently pursuing the M.Phil. in the Department of Applied Chemistry in National Yang Ming Chiao Tung University. Her research mainly focuses on structural elucidation in the total synthesis of natural products.

P-14

Synthesis of Multisubstituted Tellurophenes by S,O-Ligand Promoted Pd-Catalyzed C–H Olefination

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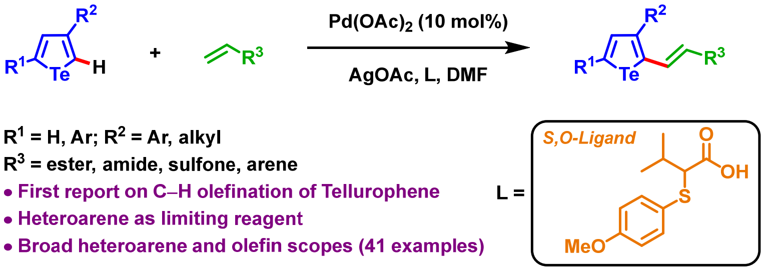
Tellurophene-based molecules and polymers have been found in applications across diverse fields, such as photodynamic therapy, pharmacology, light emitters, liquid crystals, organic photovoltaics, and organic field-effect transistors. [1] To the best of our knowledge, this study presents the first report on C–H olefination of tellurophenes, which has not been previously explored, unlike in other chalcogenophenes. [2] Traditional C–H olefination challenges include the need for excess starting materials and directing groups. To address these limitations, we developed a ligand-assisted Pd-catalyzed C–H olefination reaction for 2,4-disubstituted tellurophenes. This method can be applied to a variety of olefins, such as acrylate, acrylamide, vinyl sulfone, and styrene, demonstrating outstanding functional group tolerance across 41 examples. Mechanistically, the S,O-ligand is essential in enhancing the reactivity of the Pd catalyst by triggering the formation of more reactive Pd cationic species, [3] which accelerates the reaction and promotes Pd-catalyzed C–H functionalization. Our method provides an efficient route to functionalized tellurophenes, expanding their potential in advanced materials. Also, we discovered that these olefinated tellurophenes act as photosensitizers for singlet oxygen generation, making them promising for photodynamic therapy and other ROS-related applications.



R^1 = H, Ar; R^2 = Ar, alkyl
R^3 = ester, amide, sulfone, arene

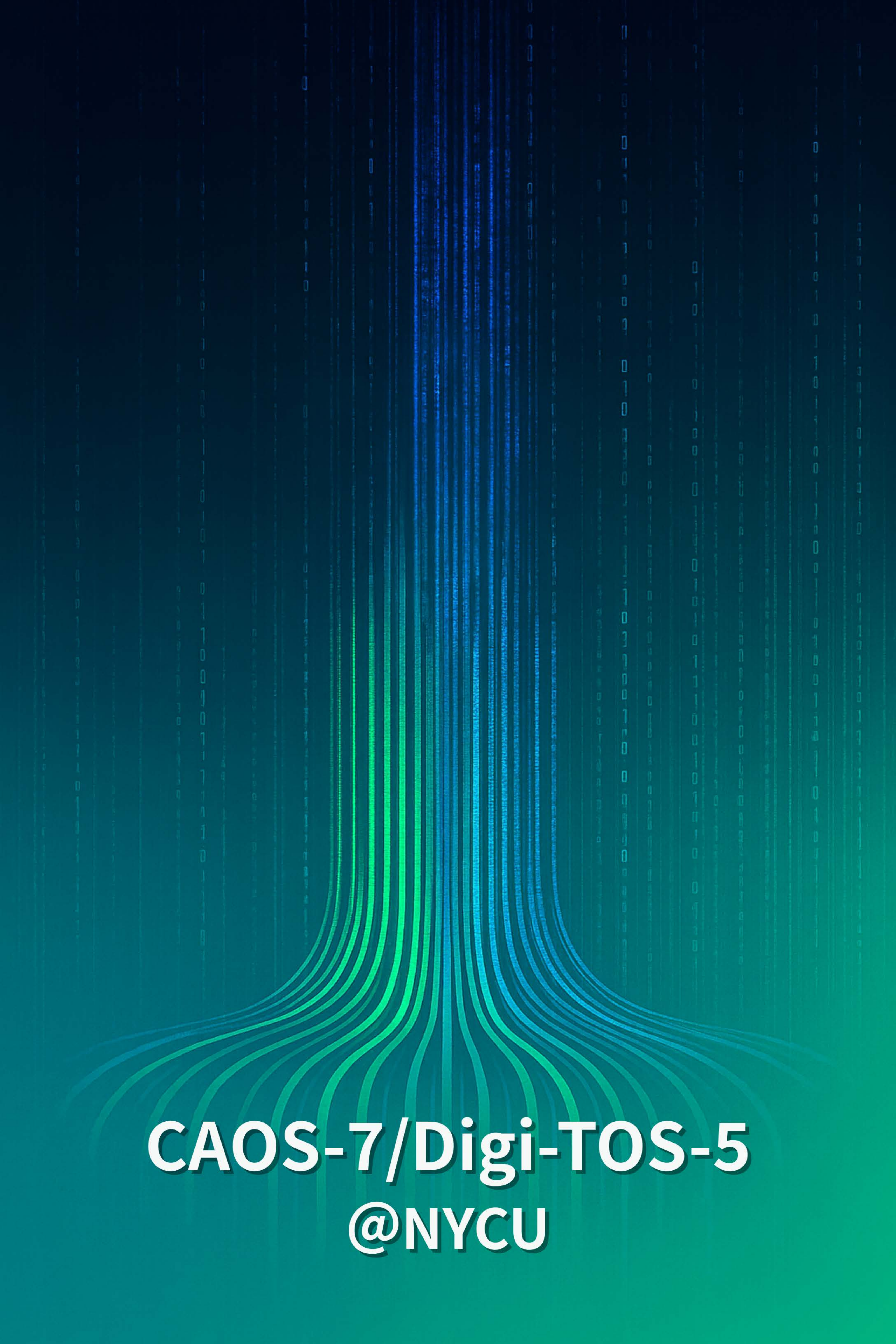
- First report on C–H olefination of Tellurophene
- Heteroarene as limiting reagent
- Broad heteroarene and olefin scopes (41 examples)

[1] Huang, K.-H.; Liu, H.-H.; Cheng, K.-Y.; Tsai, C.-L.; Cheng, Y.-J. *Chem. Sci.* **2023**, 14, 8552.

[2] Chen, S.-Y.; Sahoo, S. K.; Huang, C.-L.; Chan, T.-H.; Cheng, Y.-J. *Org. Lett.* **2020**, 22, 2318−2322.

[3] Naksomboon, K.; Gómez-Bengoa, E.; Mehara, J.; Roithová, J.; Otten, E.; Fernández-Ibáñez, M. A. *Chem. Sci.* **2023**, *14*, 2943−2953.

Chia-Shen Tsai (蔡佳燊), 2022; B.S. (National Chiayi University), 2023-; Ph.D. Student (Department of Applied Chemistry, National Yang Ming Chiao Tung University), Research interests: Synthesis and functionalization of tellurophene compounds and their application in material science development.



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