

A. Publications

- 1) "Facile synthesis of trifluoromethyl-substituted enynes: Remarkable reactivity and stereoselectivity of tributyl(3,3,3-trifluoropropynyl)stannane in carbostannylation of alkynes"
S. Shimizu,* G. Jiang, M. Murai, Y. Takeda, Y. Nakao, T. Hiyama, E. Shirakawa, *Chemistry Letters*, 34, 1700–1701 (2005).
- 2) "Copper-catalyzed transformation of carbonyl-ene-nitrile compounds: Vinylation, imino ene reaction, and alkylation of 2-aza-2,4-cyclopentadienone intermediates generated *via* Ritter-type hydration and dehydrative cyclization reactions"
M. Murai, S. Kawai, K. Miki, K. Ohe,* *Journal of Organometallic Chemistry*, 692, 579–584 (2007).
- 3) "Novel generation of 3,3,3-trifluoropropynyllithium and transformation of the carbonyl adducts to trifluoromethyl-substituted allenes"
M. Shimizu,* M. Higashi, Y. Takeda, G. Jiang, M. Murai, T. Hiyama, *Synlett*, 1163–1165 (2007).
- 4) "Transition metal-catalyzed ring-opening, substitution, and cyclopropanation reactions *via* vinylcarbene complexes generated from *O*-propargyl thiocarbamates"
Y. Ikeda, M. Murai, T. Abo, K. Miki, K. Ohe,* *Tetrahedron Letters*, 48, 6651–6654 (2007).
- 5) "Copper-catalyzed addition reactions of aromatics and ketones to 2-aza-2,4-cyclopentadienone: Facile and efficient transformation of carbonyl-ene-nitriles to 1*H*-pyrrolin-2(5*H*)-ones"
M. Murai, K. Miki, K. Ohe,* *The Journal of Organic Chemistry*, 73, 9174–9176 (2008).
- 6) "A new route to 3-acyl-2-aminobenzofurans: Palladium-catalyzed cycloisomerisation of 2-(cyanomethyl)-phenyl esters"
M. Murai, K. Miki, K. Ohe,* *Chemical Communications*, 45, 3466–3468, (2009).
- 7) "New preparation and synthetic reactions of 3,3,3-trifluoropropynyllithium, -borate and -stannane: Facile synthesis of trifluoromethylated allenes, arylacetylenes and enynes"
M. Shimizu,* M. Higashi, Y. Takeda, M. Murai, G. Jiang, Y. Asai, Y. Nakao, E. Shirakawa, T. Hiyama, *Future Medicinal Chemistry*, 1, 921–945 (2009).
- 8) "Atom-efficient synthesis of α -alkylidene-*N*-furylimines *via* catalytic vinylcarbene-transfer reactions to carbonyl-ene-nitrile compounds"
M. Murai, S. Yoshida, K. Miki, K. Ohe,* *Chemical Communications*, 46, 3366–3368 (2010).
- 9) "A stereoselective cyclization cascade mediated by SmI₂-H₂O: Synthetic studies towards Stolonidiol"
T. M. Baker, L. A. Sloan, L. H. Choudhury, M. Murai, D. J. Procter,* *Tetrahedron: Asymmetry*, 21, 1246–1261 (2010).
- 10) "Gallium(III)-catalyzed bromocyanation of alkynes: Regio- and stereoselective synthesis of β -bromo- α,β -unsaturated nitriles"
M. Murai, R. Hatano, S. Kitabata, K. Ohe,* *Chemical Communications*, 47, 2375–2377 (2011).
- 11) "Rhodium-catalyzed carbene transfer reactions *via* thienylcarbene complexes generated from thiocarbamoyl-ene-yne compounds"
A. Tsuneishi, K. Okamoto, Y. Ikeda, M. Murai, K. Miki, K. Ohe,* *Synlett*, 655–658 (2011).
- 12) "Practical synthesis of aromatic nitriles *via* gallium-catalyzed electrophilic cyanation of aromatic C–H bond"
K. Okamoto, M. Watanabe, M. Murai, R. Hatano, K. Ohe,* *Chemical Communications*, 48, 3127–3129 (2012).
- 13) "Pd- and Cu-catalyzed one-pot multicomponent synthesis of hetero α,α' -dimers of heterocycles"
T. Murata, M. Murai, Y. Ikeda, K. Miki, K. Ohe,* *Organic Letters*, 14, 2296–2299 (2012).
- 14) "Azulene-based conjugated polymers: Unique seven-membered ring connectivity leading to

- stimuli-responsiveness”
M. Murai, E. Amir, R. J. Amir, C. J. Hawker,* *Chemical Science*, 3, 2721–2725 (2012).
- 15) “Gold-catalyzed cycloisomerization reactions of 2-(2-propynyl)pyridine *N*-oxides leading to indolizinones”
M. Murai, S. Kitabata, K. Okamoto, K. Ohe,* *Chemical Communications*, 48, 7622–7624 (2012).
- 16) “Photoinitiated click reactions for the creation of spatially defined materials”
D. Miyajima, M. Murai, C. J. Hawker, *Koubunshi*, 61, 862–864 (2012).
- 17) “Zinc-porphyrins functionalized with redox-active peripherals: Enhancement of d π -p π interaction leading to unique assembly and redox-triggered remote switching of fluorescence”
M. Murai, M. Sugimoto, M. Akita,* *Dalton Transactions*, 42, 16108–16120 (2013).
- 18) “Copper-catalyzed C–H cyanation of terminal alkynes with cyanogen iodide”
K. Okamoto,* M. Watanabe, N. Sakata, M. Murai, K. Ohe,* *Organic Letters*, 15, 5810–5813 (2013).
- 19) “Bismuth(III)-catalyzed dehydrative etherification and thioetherification of phenolic hydroxy groups”
M. Murai,* K. Origuchi, K. Takai,* *Organic Letters*, 16, 3828–3831 (2014).
- 20) “Modulating structure and properties in organic chromophores: Influence of azulene as a building block”
M. Murai, S.-Y. Ku, N. D. Treat, M. J. Robb, M. L. Chabinyk, C. J. Hawker,* *Chemical Science*, 5, 3753–3760 (2014).
- 21) “Bismuth-catalyzed synthesis of PAHs with a phenanthrene backbone *via* cyclization and aromatization of 2-(2-arylphenyl)vinyl ethers”
M. Murai,* N. Hosokawa, D. Roy, K. Takai,* *Organic Letters*, 16, 4134–4137 (2014).
- 22) “Conjugated oligomers incorporating azulene building blocks –Seven- vs five-membered ring connectivity”
E. Amir, M. Murai, R. J. Amir, R. J. S. Cowart Jr, M. L. Chabinyk, C. J. Hawker,* *Chemical Science*, 5, 4483–4489 (2014).
- 23) “Modulating the properties of azulene-containing polymers through controlled incorporation of regioisomers”
K. Tsurui, M. Murai, S.-Y. Ku, C. J. Hawker,* M. J. Robb,* *Advanced Functional Materials*, 24, 7338–7347 (2014).
- 24) “Rhenium-catalyzed synthesis of 2*H*-1,2-oxaphosphorin 2-oxides *via* the regio- and stereoselective addition reaction of β -keto phosphonates with alkynes”
M. Murai,* M. Nakamura, K. Takai,* *Organic Letters*, 16, 5784–5787 (2014).
- 25) “Rhodium-catalyzed dehydrogenative germylation of C–H bonds: New entry to unsymmetrically functionalized 9-germafluorenes”
M. Murai,* K. Matsumoto, R. Okada, K. Takai,* *Organic Letters*, 16, 6492–6495 (2014).
- 26) “Iridium-catalyzed intermolecular dehydrogenative silylation of polycyclic aromatic compounds without directing group”
M. Murai,* K. Takami, K. Takai,* *Chemistry –A European Journal*, 21, 4566–4570 (2015).
- 27) “Isolation and structural characterization of *gem*-di(iodozincio)methane complexes stabilized with nitrogen ligands”
Y. Nishida, N. Hosokawa, M. Murai,* K. Takai,* *Journal of the American Chemical Society*, 137, 114–117 (2015).
- 28) “Rhenium-catalyzed *anti*-Markovnikov addition reaction of methanetricarboxylates to unactivated terminal acetylenes”
S. Hori, M. Murai,* K. Takai,* *Journal of the American Chemical Society*, 137, 1452–1457 (2015).

- 29) "Transition metal-catalyzed facile access to 3,11-dialkylfulminenes for transistor application"
M. Murai,* H. Maekawa, S. Hamano, Y. Kubozono, D. Roy, K. Takai,* *Organic Letters*, 17, 708–711 (2015).
- 30) "Rhenium-catalysed dehydrogenative borylation of primary and secondary C(sp³)-H bonds adjacent to a nitrogen atom"
M. Murai,* T. Omura, Y. Kubozono, K. Takai,* *Chemical Communications*, 51, 4583–4586 (2015).
- 31) "Palladium-catalyzed three-component coupling reactions of 2-(cyanomethyl)phenol, aryl halides, and carbon monoxide"
M. Murai, K. Okamoto, K. Miki, K. Ohe,* *Tetrahedron*, 71, 4432–4437 (2015).
- 32) "Iridium-catalyzed dehydrogenative silylation of azulenes based on the regioselective C-H bonds activation"
M. Murai,* K. Takami, H. Takeshima, K. Takai,* *Organic Letters*, 17, 1798–1801 (2015).
- 33) "Acceleration effects of phosphine ligands on the rhodium-catalyzed dehydrogenative silylation and germylation of unactivated C(sp³)-H bonds"
M. Murai,* H. Takeshima, H. Morita, Y. Kuninobu, K. Takai,* *The Journal of Organic Chemistry*, 80, 5407–5414 (2015). Selected as a *Featured Article* and *ACS Editor's Choice*.
- 34) "Rhodium-catalyzed synthesis of benzosilolometallocenes via the dehydrogenative silylation of C(sp²)-H bonds"
M. Murai,* K. Matsumoto, K. Takeuchi, K. Takai,* *Organic Letters*, 17, 3102–3105 (2015).
- 35) "Stereospecific deoxygenation of aliphatic epoxides to alkenes under rhenium catalysis"
T. Nakagiri, M. Murai,* K. Takai,* *Organic Letters*, 17, 3346–3349 (2015).
Highlight in "*Organic Chemistry Highlights*".
- 36) "Short synthesis of [5]- and [7]phenacenes with silyl groups at the axis positions"
D. Roy, H. Maekawa, M. Murai,* K. Takai,* *Chemistry –An Asian Journal*, 10, 2518–2524 (2015).
- 37) "Rhodium-catalyzed synthesis of chiral spiro-9-silabifluorenes via dehydrogenative silylation: Mechanistic insights into the construction of tetraorganosilicon stereocenters"
M. Murai,* Y. Takeuchi, K. Yamauchi, Y. Kuninobu, K. Takai,* *Chemistry –A European Journal*, 22, 6048–6058 (2016). Selected as a *Hot Paper*.
- 38) "Palladium-catalyzed direct arylation of azulene based on the regioselective C-H bond activation"
M. Murai,* M. Yanagawa, M. Nakamura, K. Takai,* *Asian Journal of Organic Chemistry*, 629–635 (2016).
- 39) "Synthesis of sila[n]helicenes via dehydrogenative silylation of C-H bonds under rhodium catalysis"
M. Murai,* R. Okada, A. Nishiyama, K. Takai,* *Organic Letters*, 18, 4380–4383 (2016).
- 40) "Molybdenum-catalyzed stereospecific deoxygenation of epoxides to alkenes"
S. Asako,* T. Sakae, M. Murai, K. Takai,* *Advanced Synthesis and Catalysis*, 358, 3966–3970 (2016).
Selected as a *Very Important Paper*.
- 41) "Rhenium-catalyzed 1,1-difunctionalization of 1,*n*-diynes with carbon nucleophiles followed by sequential cyclization leading to tetrahydroindenone derivatives"
M. Murai,* E. Uemura, S. Hori, K. Takai,* *Angewandte Chemie International Edition*, 56, 5862–5866 (2017).
- 42) "Iridium-catalyzed dehydrogenative dimerization of benzylmethylsilanes via silylation of C(sp³)-H bonds adjacent to a silicon atom"
M. Murai,* Y. Takeuchi, K. Takai,* *Chemistry Letters*, 46, 1044–1047 (2017).

- 43) “Rhodium-catalyzed silylative and germylative cyclization with dehydrogenation leading to 9-sila- and 9-germafluorenes: A combined experimental and computational mechanistic study”
M. Murai,* R. Okada, S. Asako, K. Takai,* *Chemistry –A European Journal*, 23, 10861–10870 (2017).
Selected as a *Hot Paper*.
- 44) “Iridium-catalyzed hydrosilylation of cyclopropanes *via* regioselective carbon–carbon bond cleavage”
M. Murai,* A. Nishiyama, N. Nishinaka, H. Morita, K. Takai,* *Chemical Communications*, 53, 9281–9284 (2017).
- 45) “Structural characterization and unique catalytic performance of reactive silyl-substituted geminal dichromiomethane complexes stabilized with diamine ligand”
M. Murai,* R. Taniguchi, N. Hosokawa, Y. Nishida, H. Mimachi, T. Oshiki, K. Takai,* *Journal of the American Chemical Society*, 139, 13184–13192 (2017).
Selected as *JACS Spotlights (J. Am. Chem. Soc., 139, 12863–12864 (2017))*.
- 46) “Azulene-fused linear-shaped polycyclic aromatic hydrocarbons with low bandgap and unique stimuli-responsiveness”
M. Murai,* S. Iba, H. Ota, K. Takai,* *Organic Letters*, 19, 5585–5588 (2017).
- 47) “Rhenium-catalyzed *ortho*-alkylation of phenols”
Y. Kuninobu,* M. Yamamoto, M. Nishi, T. Yamamoto, T. Matsuki, M. Murai,* K. Takai,* *Organic Syntheses*, 94, 280–291 (2017).
- 48) “Straightforward approach to borylcyclopropanes by chromium-promoted cyclopropanation of unactivated alkenes”
M. Murai,* C. Mizuta, R. Taniguchi, K. Takai,* *Organic Letters*, 19, 6104–6107 (2017).
- 49) “Iridium-catalyzed sequential silylation and borylation of heteroarenes based on the regioselective C–H bond activation”
M. Murai,* N. Nishinaka, K. Takai,* *Angewandte Chemie International Edition*, 57, 5843–5847 (2018).
- 50) “Amine-promoted *anti*-Markovnikov addition reaction of 1,3-dicarbonyl compounds with terminal alkynes under rhenium catalysis”
M. Murai,* E. Uemura, K. Takai,* *ACS Catalysis*, 8, 5454–5459 (2018).
- 51) “Catalytic cleavage and reformation of ethereal σ -bonds”
M. Murai,* K. Origuchi, K. Takai,* *Chemistry Letters*, 47, 927–930 (2018).
- 52) “Unsymmetrical difunctionalization of two different C–H bonds in one-pot under transition metal catalysis”
M. Murai,* K. Takai,* *Synthesis* (Mini review), 51, 40–54 (2019).
Invited contribution to the “*Golden Synthesis Anniversary Special Issue*” (P. Knochel, Ed.).
- 53) “Regioselective arene homologation through rhenium-catalyzed deoxygenative aromatization of 7-oxabicyclo[2.2.1]hepta-2,5-diene”
M. Murai,* T. Ogita, K. Takai,* *Chemical Communications*, 55, 2332–2335 (2019).
- 54) “Palladium-catalyzed double-bond migration of unsaturated hydrocarbons controllable by second metal catalysts”
M. Murai,* K. Nishimura, K. Takai,* *Chemical Communications*, 55, 2769–2772 (2019).
- 55) “Chromium-mediated stannylcyclopropanation of alkenes with (diiodomethyl)stannanes”
M. Murai,* R. Taniguchi, C. Mizuta, K. Takai,* *Chemical Communications*, 21, 2668–2672 (2019).
- 56) “Regioselective functionalization of 9,9-dimethyl-9-silafluorenes by borylation, bromination, and nitration”
M. Murai,* N. Nishinaka, M. Kimura, K. Takai,* *The Journal of Organic Chemistry*, 84, 5667–5676 (2019).

- 57) "Rhenium-catalyzed regioselective *ortho*-alkenylation and [3+2+1]cycloaddition of phenols with internal alkynes"
M. Murai,* M. Yamamoto, K. Takai,* *Organic Letters*, 21, 3441–3445 (2019).
- 58) "Rhenium-catalysed cyclization *via* 1,2-iodine and 1,5-hydrogen migration for the synthesis of 2-iodo-1*H*-indenes"
M. Murai,* K. Takai,* *Organic Letters*, 21, 6756–6760 (2019).
- 59) "Mechanistic insights into rhenium-catalyzed regioselective *C*-alkenylation of phenols with internal alkynes"
M. Murai,* M. Yamamoto, K. Takai,* *Chemistry – A European Journal*, 25, 15189–15197 (2019).
- 60) "Regioselective sequential silylation and borylation of aromatic aldimines as a strategy for programming synthesis of multifunctionalized benzene derivatives"
M. Murai,* N. Nishinaka, T. Enoki, K. Takai,* *Organic Letters*, 22, 316–321 (2020).
- 60) "Cyclization of 1,*n*-enynes initiated by the addition reaction of *gem*-dichromiomethane reagents to alkynes"
M. Murai,* R. Taniguchi, K. Takai,* *Organic Letters*, 22, 3985–3988 (2020).
- 61) "Cyclization of 5-alkynylketones with chromium alkylidene equivalents generated *in situ* from *gem*-dichromiomethanes"
M. Murai,* R. Taniguchi, T. Kurogi, S. Moritani, K. Takai,* *Chemical Communications*, 56, 9711–9714 (2020).
- 62) "Control of regioselectivity of carbene/alkyne metathesis in chromium-mediated coupling and cyclization with 1,6-enynes"
M. Murai,* R. Taniguchi, K. Takai,* *Bulletin of the Chemical Society of Japan*, 94, 2848–2852 (2021).
- 63) "Silylative cyclization with dehydrogenation leading to benzosilole-fused azulenes showing unique stimuli-responsive fluorescence"
M. Murai,* *Asian Journal of Organic Chemistry*, 11, 262–266 (2022).
- 64) "Diazulenylmethyl cations with a silicon bridge: A π -extended cationic motif to form *J*-aggregates with near-infrared absorption and emission"
M. Murai,* M. Abe, S. Ogi, S. Yamaguchi,* *Journal of the American Chemical Society*, 144, 20385–20393 (2022).
Press released by Nagoya Univ.
- 65) "Germanium- and tin-bridged diazulenylmethyl cations: Effects of the group 14 element on the structure and properties of the π -extended cation"
M. Murai,* M. Ito, S. Takahashi, S. Yamaguchi,* *Dalton Transactions*, 52, *in press* (2023).
- 66) "A kinetically stabilized nitrogen-doped triangulene cation: Stable and NIR fluorescent diradical cation with triplet ground state"
S. Arikawa, A. Shimizu,* D. Shiomi, K. Sato,* T. Takui, H. Sotome,* H. Miyasaka, M. Murai, S. Yamaguchi, S. Shintani,* *Angewandte Chemie International Edition*, 62, *in press* (2023).
- 67) "Azulene-fused linearly π -extended polycyclic aromatic hydrocarbons: Synthesis, photophysical properties, and OFETs applications"
M. Murai,* S. Iba, S. Hamao, Y. Kubozono, H. Ota, K. Takai,* *Bulletin of the Chemical Society of Japan*, 96, 1077 (2023).
Highlighted as a "Selected Paper".
- 68) "Dithienoazepine-based near-infrared dyes: Janus-faced effects of thiophene-fused structure on antiaromatic azepines"
M. Murai,* T. Enoki, S. Yamaguchi,* *Angewandte Chemie International Edition*, 62, e202311445 (2023).
Selected as a *Very Important Paper* and *Inside Cover*

Press released by Nagoya Univ.

- 69) "Dithieno[3,2-*b*;2',3'-*f*]phosphepinium-Based Near-Infrared Fluorophores: p_x - π^* Conjugation Inherent to Seven-Membered Phosphacycles"
K. Andoh, M. Murai,* P.-A. Bouit, M. Hissler, S. Yamaguchi,* *Angewandte Chemie International Edition*, 63, e202410204 (2024).
- 70) "Controlling Redox and Wire-Like Charge-Delocalization Properties of Dinuclear Mixed-Valence Complexes with $MCp^*(dppe)$ ($M = Fe, Ru$) Termini Bridged by Metalloporphyrin Linkers"
M. Murai, K. Ono, Y. Tanaka, M. Akita,* *ACS Organic & Inorganic Au*, 4, *accepted* (2024).
- 71) "Sulfur-Bridged Diazulenylmethyl Cations: Charge-Segregated Assembly of π -Conjugated Cations Toward Charge-Carrier Transport Application"
S. Takahashi, M. Murai,* T. Hattori, S. Seki,* T. Yanai, S. Yamaguchi,* *Under revision* (2024). *ChemRxiv* **2024**, preprint (DOI: 10.26434/chemrxiv-2024-k45wj).

B. Oral Presentation in the International Conference

- 1) "Development of azulene-based novel π -conjugated molecules: Enhancement of dipolar leading to unique stimuli-responsiveness"
M. Murai, C. J. Hawker, 12th International Kyoto Conference on New Aspects of Organic Chemistry (IKCOC 12)
Kyoto, November, 2012
- 2) "Rhenium-catalyzed *anti*-Markovnikov addition reaction of carbon nucleophiles to unactivated terminal acetylenes"
M. Murai, International Symposium on Pure & Applied Chemistry (ISPAC)
Ho Chi Minh, Vietnam, June, 2017 (Invited)
- 3) "Transition metal-catalyzed intermolecular dehydrogenative silylation of aromatic compounds without directing groups based on the regio- and chemoselective C-H bond activation"
M. Murai, 8th Annual Global Congress of Catalysis 2017
Shanghai, China, October, 2017 (Invited)
- 4) "Regioselective benzoannulation of PAHs *via* the rhenium-catalyzed deoxygenation of 7-oxabicyclo[2.2.1]-hepta-2,5-diene"
M. Murai, K. Takai, International Symposium on JST ACT-C Project ~Invention of π -Electronic Organic Molecules toward Electronic Energy Devices~
Okayama, July, 2017
- 5) "Rhenium-catalyzed *anti*-Markovnikov addition reaction of carbon nucleophiles to unactivated terminal acetylenes"
M. Murai, K. Takai, 14th International Kyoto Conference on New Aspects of Organic Chemistry (IKCOC 14)
Kyoto, November, 2018
- 6) "Rhenium-catalyzed intermolecular *anti*-Markovnikov addition reaction of 1,3-dicarbonyl compounds with terminal alkynes"
M. Murai, K. Takai, 28th International Conference on Organometallic Chemistry (ICOMC 2018)
Florence, Italy, July, 2018 (Invited)
- 7) "Regioselective benzannulation of PAHs *via* rhenium-catalyzed deoxygenation of 7-oxabicyclo[2.2.1]hepta-2,5-diene"
M. Murai, International Congress on Pure & Applied Chemistry (ICPAC)

Yangon, Myanmar, August, 2019 (Invited)

- 8) “Silicon-bridged diazulenylnmethyl cations as a π -extended cationic motif to form *J*-aggregates with near-infrared emission”
M. Murai, S. Yamaguchi, 15th International Symposium on Functional- π Electron Systems (F π -15)
Raleigh, USA, June, 2023
- 9) “Alignment of azulene-based cationic π -skeletons toward functional π -materials”
M. Murai, 15th International Kyoto Conference on New Aspects of Organic Chemistry (IKCOC 15)
Kyoto, November, 2023
- 10) “Design and synthesis of key nonbenzenoid core units realizing near-infrared emission”
M. Murai, 2023 International IRCCS–IRTG–ILR Symposium on “New Horizons of Molecular Functions”
Nagoya, December, 2023
- 11) “Si, Ge, and Sn-bridged π -conjugated carbocations: Azulene-fusing strategy for designing near-infrared dyes”
M. Murai, The 20th International Symposium on Silicon Chemistry (ISOS-2024)
Hiroshima, May 2024