

Curriculum Vitae

Hideaki Takano

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1. Education

- Apr. 2011 – Mar. 2015: **B.Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)
- Apr. 2015 – Mar. 2017: **M. Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)
- Apr. 2017 – Mar. 2020: **PhD.Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)

2. Career

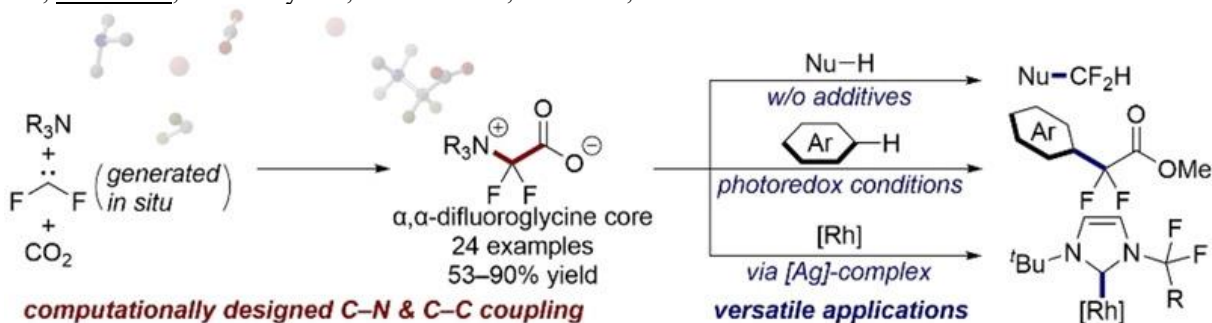
- Apr. 2020 – Sep. 2021: **Postdoctoral Researcher**, WPI-ICReDD, Hokkaido University (JST-ERATO Maeda Artificial intelligence for Chemical Reaction Design and Discovery Project)
- Oct. 2021 – **Specially Appointed Assistant Professor**, WPI-ICReDD, Hokkaido University (JST-ERATO Maeda Artificial intelligence for Chemical Reaction Design and Discovery Project)

3. Fellowship

- Apr. 2018 – Mar. 2020: **Research Fellowship for Young Scientists (DC2)**, Japan Society for the Promotion of Sciences (JSPS)
- Apr. 2018 – Mar. 2019: **Visiting Student**, Department of Chemistry, University of Cambridge (Prof. Robert J. Phipps), supported by Overseas Challenge Program for Young Researchers of JSPS

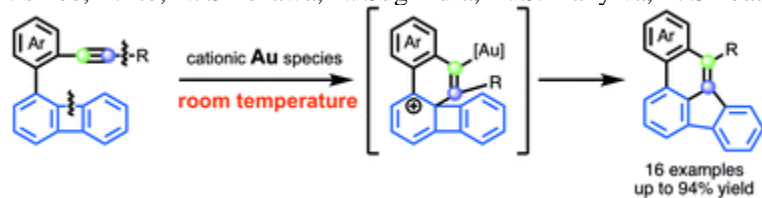
4. Publication

- Radical Difunctionalization of Gaseous Ethylene Guided by Quantum Chemical Calculations: Selective Incorporation of Two Molecules of Ethylene
ACS Omega, under revision
H. Takano, Y. You, H. Hayashi, Y. Harabuchi, S. Maeda, T. Mita
- Synthesis of Difluoroglycine Derivatives from Amines, Difluorocarbene, and CO₂: Computational Design, Scope, and Applications
Chem. Eur. J. **2021**, *27*, 10040-10047.
H. Hayashi, H. Takano, H. Katsuyama, Y. Harabuchi, S. Maeda, T. Mita



- 3). Gold-catalyzed dual C–C bond cleavage of biphenylenes bearing a pendant alkyne at ambient temperature
Org. Biomol. Chem. **2020**, *18*, 5826–5831.

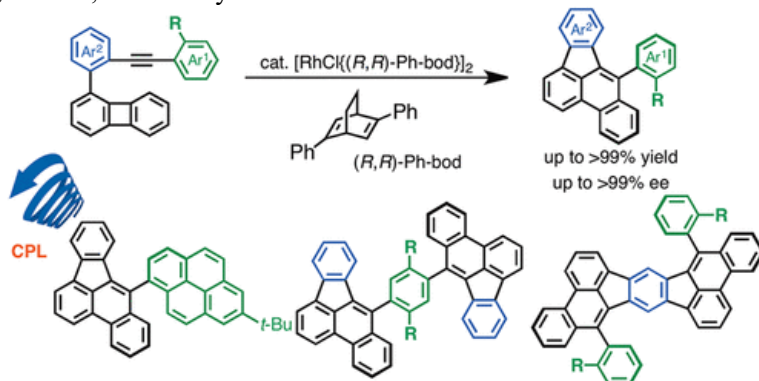
H. Takano, S. Okazaki, S. Nishibe, T. Ito, N. Shiozawa, N. Sugimura, K. S. Kanyiva, T. Shibata



- 4). Catalytic Enantioselective Synthesis of Axially Chiral Polycyclic Aromatic Hydrocarbons (PAHs) via Regioselective C-C Bond Activation of Biphenylenes

J. Am. Chem. Soc. **2020**, *142*, 4714-4722.

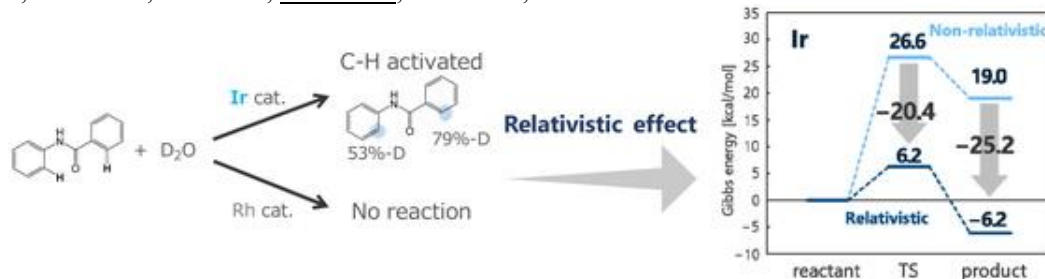
H. Takano, N. Shiozawa, Y. Imai, K. S. Kanyiva and T. Shibata



- 5). Relativistic Effect on Homogeneous Catalytic Reaction by Cationic Iridium Catalysts

J. Comput. Chem. Japan **2019**, *18*, 136–138.

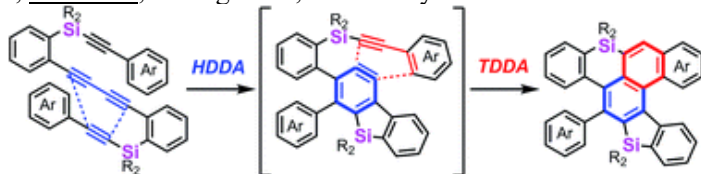
C. Takashima, Y. Ikabata, H. Kurita, H. Takano, T. Shibata, H. Nakai



- 6). Consecutive HDDA and TDDA reactions of silicon-tethered tetraynes for the synthesis of dibenzosilole-fused polycyclic compounds and their unique reactivity

Chem. Sci., **2019**, *10*, 6715–6720.

A. Mitake, R. Nagai, A. Sekine, H Takano, N. Sugimura, K. S. Kanyiva and T Shibata

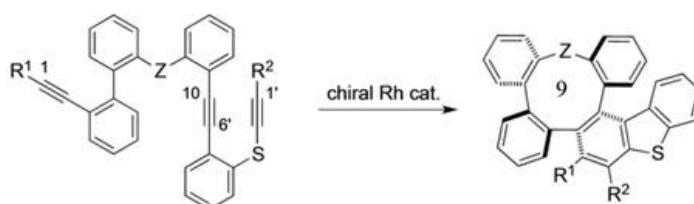


- 7). Enantioselective Synthesis of Nine- to Eleven-Membered Cyclic Polyphenylenes Containing Heteroatoms by Catalytic Intramolecular [2+2+2] Cycloaddition

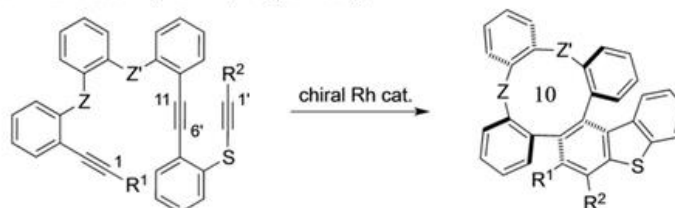
Asian. J. Org. Chem. **2019**, *8*, 970–977.

T. Shibata, T. Fusamae, H. Takano, N. Sugimura, K. S. Kanyiva

a) Chiral nine-membered ring from 1,10-diyne moiety



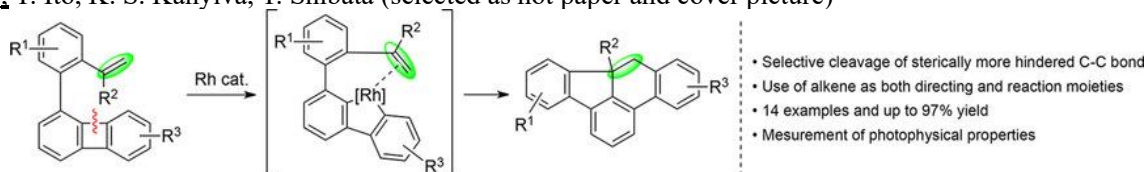
b) Chiral ten-membered ring from 1,11-diyne moiety



8). Regioselective Activation of a Sterically More Hindered C-C Bond of Biphenylenes Using an Alkene as Both a Directing Group and a Reaction Moiety

Chem. Eur. J. **2018**, *24*, 15173–15177.

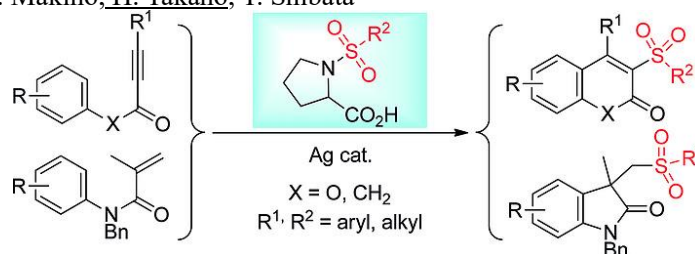
H. Takano, T. Ito, K. S. Kanyiva, T. Shibata (selected as hot paper and cover picture)



9). α -Amino Acid Sulfonamides as Versatile Sulfonylation Reagents: Silver-Catalyzed Synthesis of Coumarins and Oxindoles by Radical Cyclization

Eur. J. Org. Chem. **2018**, 5905–5909.

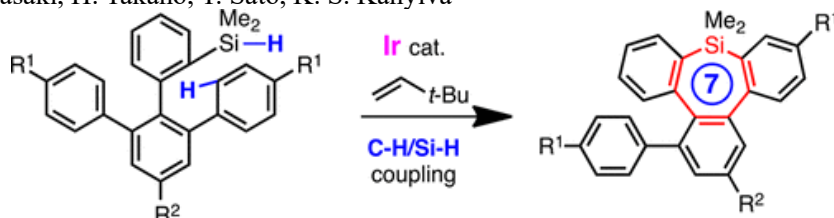
K. S. Kanyiva, D. Hamada, S. Makino, H. Takano, T. Shibata



10). A Ir-Catalyzed Synthesis of Substituted Tribenzosilolepins by Dehydrogenative C-H/Si-H Coupling

J. Org. Chem. **2018**, *83*, 3426-3432.

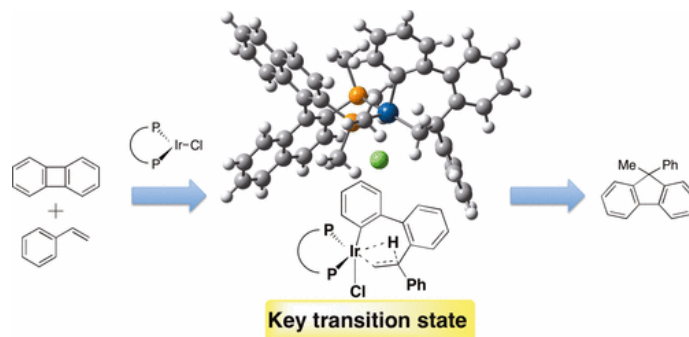
T. Shibata, N. Uno, T. Sasaki, H. Takano, T. Sato, K. S. Kanyiva



11). DFT Studies on the Mechanism of the Iridium-Catalyzed Formal [4 + 1] Cycloaddition of Biphenylene with Alkenes

ACS Omega **2017**, *2*, 5228–5234.

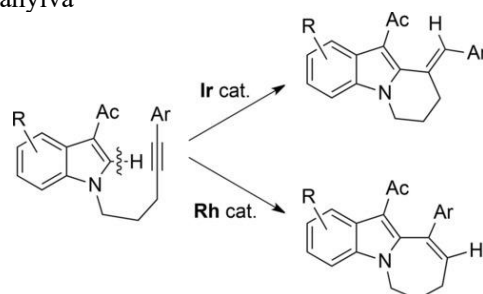
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata



- 12). Intramolecular C-H Alkenylation of *N*-Alkynylindoles: *Exo* and *Endo* Selective Cyclization by the Choice of Metal Catalysts

Adv. Synth. Catal. **2017**, *359*, 1849–1853.

T. Shibata, T. Baba, H. Takano, K. S. Kanyiva



- 13). Iridium-Catalyzed Formal [4+1] Cycloaddition of Biphenylenes with Alkenes Initiated by C-C Bond Cleavage for the Synthesis of 9,9-Disubstituted Fluorenes

Org. Lett. **2016**, *18*, 1860-1863.

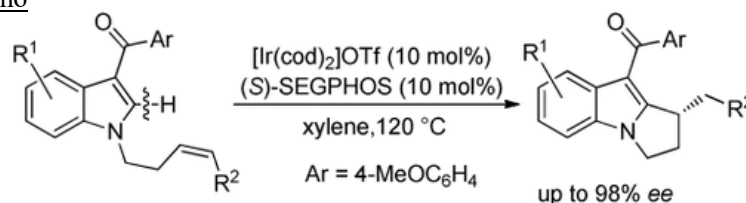
H. Takano, K. S. Kanyiva, T. Shibata



- 14). Iridium-Catalyzed Intramolecular Enantioselective C-H Alkylation at the C-2 Position of *N*-Alkynylindoles

Adv. Synth. Catal. **2015**, *357*, 1131-1135.

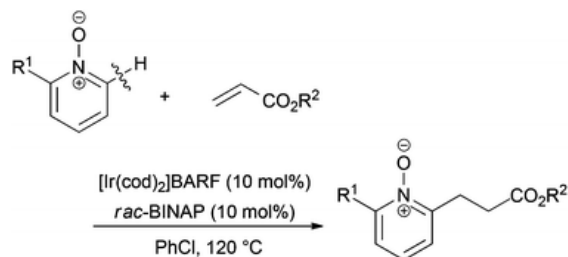
T. Shibata, N. Ryu, H. Takano



- 15). Cationic iridium-catalyzed C-H alkylation of 2-substituted pyridine *N*-oxides with acrylates

Org. Chem. Front. **2015**, *2*, 383-387.

T. Shibata, H. Takano,

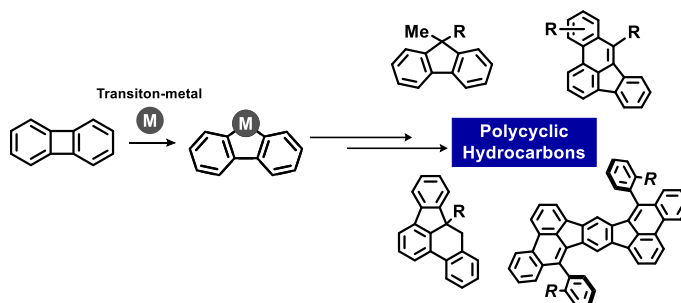


5. Review

- 1). Versatile Transformations of Biphenylenes by Transition-Metal Catalysts and Application for the Synthesis of Polycyclic Hydrocarbons

J. Synth. Org. Chem. Jpn. **2021**, *79*, 849-858.

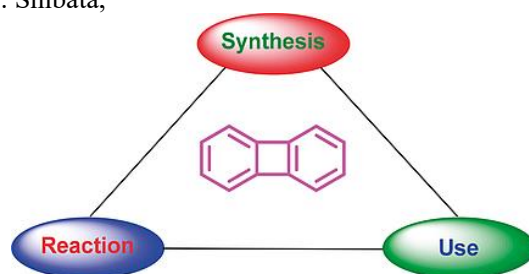
H. Takano, T. Shibata



- 2). Recent Advances of Biphenylene: Synthesis, Reactions and Uses

Eur. J. Org. Chem. **2019**, 2871–2883.

H. Takano, T. Ito, K. S. Kanyiva, T. Shibata,



6. Patent

- 1). エチレンを原料に用いた 1, 2-ビス (ジフェニルホスフィノ) エタン (DPPE) 誘導体の合成法

美多 剛, 前田 理, 高野 秀明

特願 2021-131481 出願 (2021 年 8 月 11 日)

7. Conference

- 1). エチレンガスのラジカルダブル官能基化反応を指向した AFIR 法に基づく新規反応開発
119th Symposium on Organic Synthesis, O-13, Online meeting, Nov 2021
高野秀明、美多剛、原渕祐、前田理
- 2). AFIR 法に基づくエチレンガスの光触媒を用いたラジカルダブル官能基化反応の開発
第 47 回反応と合成の進歩シンポジウム, 2O-16, Online meeting, Oct 2021
高野秀明、美多剛、原渕祐、前田理
- 3). Development of Radical Difunctionalization of Ethylene Gas Predicted by Quantum Chemical Calculations (Oral)
The 101st CSJ Annual Meeting, Online meeting, A21-3am-02, March 2021
H. Takano, T. Mita, Y. Harabuchi, S. Maeda
- 4). Development of Catalytic Transformation via Regioselective Cleavage of Sterically Hindered C-C Bond Promoted by Unsaturated Bonds as Both Directing Group and Reaction Site (Oral)
66th Symposium on Organometallic Chemistry, O1-01, Tokyo Metropolitan University (Japan), September 2019
H. Takano, T. Ito, N. Shiozawa, K. S. Kanyiva, T. Shibata
- 5). Rhodium-catalyzed regioselective activation of sterically hindered C-C bond of Biphenylene” (Poster)
ESOC2019 - 21st European Symposium on Organic Chemistry, PO-149, Vienna (Austria), July 2019
H. Takano, T. Ito, N. Shiozawa, K. S. Kanyiva, T. Shibata
- 6). ロジウム触媒を用いた立体的に混み合った C-C 結合開裂を伴う分子内環化反応の開発 (Poster)
52nd Summer School of Organometallic Chemistry, 1P-7, Okayama (Japan), June 2019
Hideaki Takano
- 7). Computational Study of Iridium Complexes as Transition States in Formal [4+1] Cycloaddition of Biphenylene with Alkenes: Rational Explanation of [4+1] Prior to [4+2] Cycloaddition (Poster)
The 24th International SPACC Symposium -Metal Complexes for Green and Sustainable Development-, P-13, University of Auckland (New Zealand), November 2017
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata

- 8). Computational Mechanistic Study for the Iridium-Catalyzed Formal [4+1] Cycloaddition of Biphenylene with Alkenes (Oral)
The 97th CSJ Annual Meeting, Keio University, Tokyo, 3E2-28, March 2017
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 9). Iridium-Catalyzed Formal [4+1] Cycloaddition for the Synthesis of 9,9-Disubstituted Fluorenes and DFT Studies of the Reaction Mechanism (Poster)
66th Symposium on Organometallic Chemistry, P2-37, Waseda (Japan), September 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 10). Synthesis of 9,9'-Disubstituted Fluorene Derivatives by Iridium Catalyst Initiated by C-C Bond Cleavage of Biphenylenes (Invited lecture)
ISPAC 2016, ORS12, Kuching (Malaysia), August 2016
H. Takano
- 11). Iridium-catalyzed reaction of biphenylenes with alkenes initiated by C-C bond cleavage (Poster)
International Conference on Organometallic Chemistry 2016, 186, Melbourne (Australia), July 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 12). イリジウム触媒を用いた C-C 結合開裂を経る[4+1]付加環化反応の開発 (Poster)
49th Summer School of Organometallic Chemistry, Gunma (Japan), July 2016
Hideaki Takano
- 13). Iridium-Catalyzed Formal [4+1] Cycloaddition Initiated by C-C Bond Cleavage of Biphenylenes (Poster)
109th Symposium on Organic Synthesis, P-22, Tokyo Institute of Technology (Japan), June 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 14). Synthesis of 9,9-Disubstituted Fluorene Derivatives by Iridium Catalyst via C-C Bond Activation of Biphenylenes (Oral)
The 96th CSJ Annual Meeting, 2H7-18, Doshisha University (Japan), March 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 15). C-H alkylation for 2-substituted pyridine N-oxide by a cationic iridium(I) catalyst" (Poster)
Pacifichem2015, ORGN2539, Hawaii (America), December 2015
H. Takano, T. Shibata
- 16). Chiral Cationic Iridium-Catalyzed Enantioselective Intramolecular C-H Alkylation at the C-2 Position of Indoles (Poster)
62nd Symposium on Organometallic Chemistry, P2-47, Kansai University (Japan), September 2015
H. Takano, N. Ryu, T. Shibata
- 17). Enantioselective intramolecular C-H alkylation at the C-2 position of indole by a chiral cationic iridium(I) catalyst (Poster)
OMCOS18, P-429, Barcelona (Spain), June 2015
H. Takano, N. Ryu, T. Shibata
- 18). Cationic Iridium-Catalyzed Enantioselective Intramolecular C-H alkylation at the C-2 Position of Indoles (Poster)
Symposium on Molecular Chirality 2015, PP-20D, Waseda University (Japan), June 2015
H. Takano, N. Ryu, T. Shibata
- 19). Ir(I)-Catalyzed C2-Selective C-H Alkylation of Pyridine N-Oxides (Oral)
The 95th CSJ Annual Meeting, 2E5-11, Nihon University (Japan), March 2015
H. Takano, T. Shibata

8. Award

- 2020 博士学位賞
- 2017 Yoshiro Sekine Award (Top grade award for M.S. in my major)
- 2016 27th International Conference on Organometallic Chemistry(ICOMC) Student Award and Travel Bursary (<http://icomc2016.com/student-award-travel-bursary/>)
- 2015 Top grade award for undergraduate school in my department

9. Membership

- The Chemical Society of Japan
- The Society of Synthetic Organic Chemistry, Japan