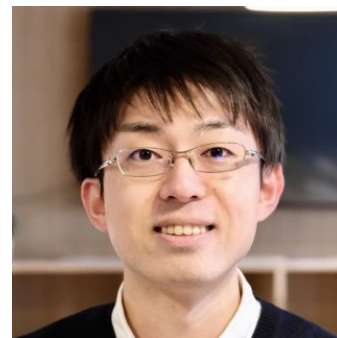


Hiroki Hayashi

Specially Appointed Assistant Professor
Institute for Chemical Reaction Design and Discovery
(WPI-ICReDD), Hokkaido University
Kita 21, Nishi 10, Kita-ku, Sapporo, Hokkaido, 001-0021, JAPAN
Phone: +81-11-706-9654
Fax: +81-11-706-9655
E-mail: hhayashi@icredd.hokudai.ac.jp



Personal Data

| | |
|----------------|----------------------------------|
| Date of Birth | November 11 th , 1988 |
| Place of Birth | Aichi, Japan |
| Gender | Male |
| Nationality | Japan |

Education

| | |
|-----------|---|
| 2011.3 | B. Eng. , School of Engineering, Nagoya University, Japan (Prof. Kazuaki Ishihara) |
| 2013.3 | M. Eng. , Graduate School of Engineering, Nagoya University, Japan (Prof. Kazuaki Ishihara) |
| 2016.3 | PhD. Eng. , Graduate School of Engineering, Nagoya University, Japan (Prof. Kazuaki Ishihara) |
| 2014.9–12 | Visiting Scholar , Department of Chemistry, University of Berkeley, California, United States (Prof. John F. Hartwig) |

Academic Career

| | |
|----------------|---|
| 2016.4–2017.3 | Postdoctoral Researcher , Department of Chemistry, University of Berkeley, California, United States (Prof. John F. Hartwig) |
| 2017.4–2020.1 | Assistant Professor , Faculty of Arts and Science, Kyushu University (Assoc. Prof. Tatsuya Uchida) |
| 2020.2–present | Specially Appointed Assistant Professor , WPI-ICReDD, Hokkaido University (JST-ERATO Maeda Artificial Intelligence for Chemical Reaction Design and Discovery Project) |

Fellowships & Grants

| | |
|---------------|--|
| 2015.4–2016.3 | Research Fellow of the Japan Society for the Promotion of Sciences (DC2) |
| 2016.4–2017.3 | 2016 The Naito Foundation Postdoctoral Fellow for Research Abroad |
| 2020.4–2022.3 | JSPS Grant-in-Aid for Young Scientists (20K15284) |
| 2021.8–2022.2 | 2021 The NOASTEC Foundation Subsidy for Young Scientists |
| 2023.4–2026.3 | JSPS Grant-in-Aid for Young Scientists (23K13737) |

Awards

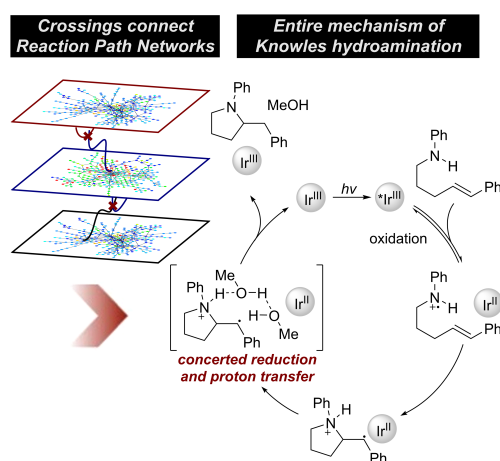
| | |
|------|---|
| 2012 | Very Important Presentation Award at the 43rd Annual Meeting of Union of Chemistry-Related Societies in Chubu Area, Japan |
| 2013 | Poster Award at the 1st IGER Annual Meeting, Japan |
| 2014 | Poster Award at the 31st Seminar of Organic Synthetic Chemistry, Japan |
| 2015 | Reaxys PhD Prize Finalist, UK |
| 2015 | Otsu Conference Award Fellow, Japan |
| 2016 | Presentation Award at the 96th CSJ Annual Meeting, Japan |
| 2020 | The Central Glass Award in Synthetic Organic Chemistry, Japan |
| 2021 | The Best Poster Presentation Award at the 7th Hokkaido University Cross-Departmental Symposium, Japan |
| 2023 | The Chemical Society of Japan Lecture Award for Young Chemists |

Publications

1. “Oxidation and Reduction Pathways in the Knowles Hydroamination via a Photoredox-Catalyzed Radical Reaction”

Yu Harabuchi, **Hiroki Hayashi**, Hideaki Takano, Satoshi Maeda, Tsuyoshi Mita

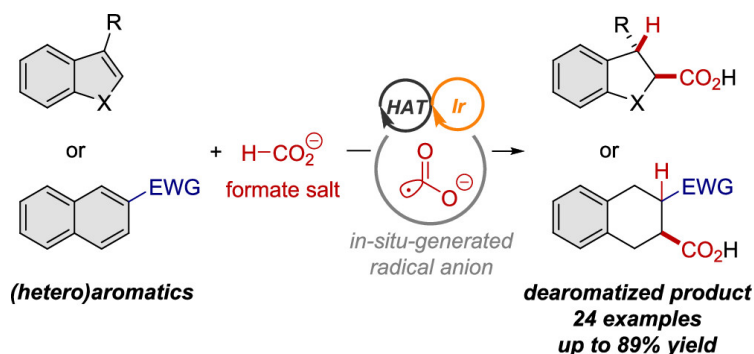
Angew. Chem. Int. Ed. **2023**, 62, e202211936.



2. “Photoredox/HAT-Catalyzed Dearomative Nucleophilic Addition of the CO₂ Radical Anion to (Hetero)Aromatics”

Saesh R. Mangaonkar, **Hiroki Hayashi**, Hideaki Takano, Wataru Kanna, Satoshi Maeda, and Tsuyoshi Mita

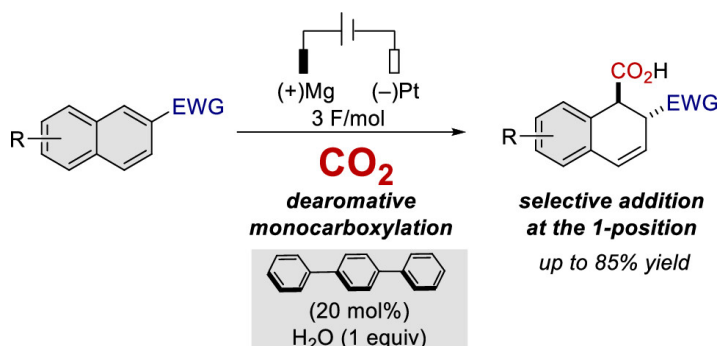
ACS Catal. **2023**, *13*, 2482–2488.



3. “Revisiting the Electrochemical Carboxylation of Naphthalene with CO₂: Selective Monocarboxylation of 2-Substituted Naphthalenes”

Vishal Kumar Rawat, **Hiroki Hayashi**, Hitomi Katsuyama, Saesh R. Mangaonkar, and Tsuyoshi Mita

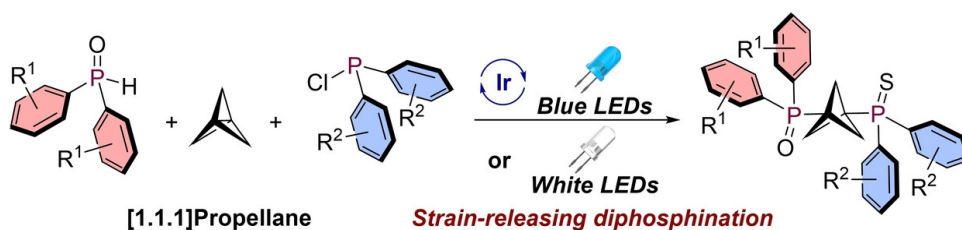
Org. Lett. **2023**, *25*, 4231–4235.



4. “Synthesis of Bicyclo[1.1.1]pentane (BCP)-Based Straight-Shaped Diphosphine Ligands”

Hideaki Takano, Hitomi Katsuyama, **Hiroki Hayashi**, Miyu Harukawa, Makoto Tsurui, Sunao Shoji, Yasuchika Hasegawa, Satoshi Maeda, Tsuyoshi Mita

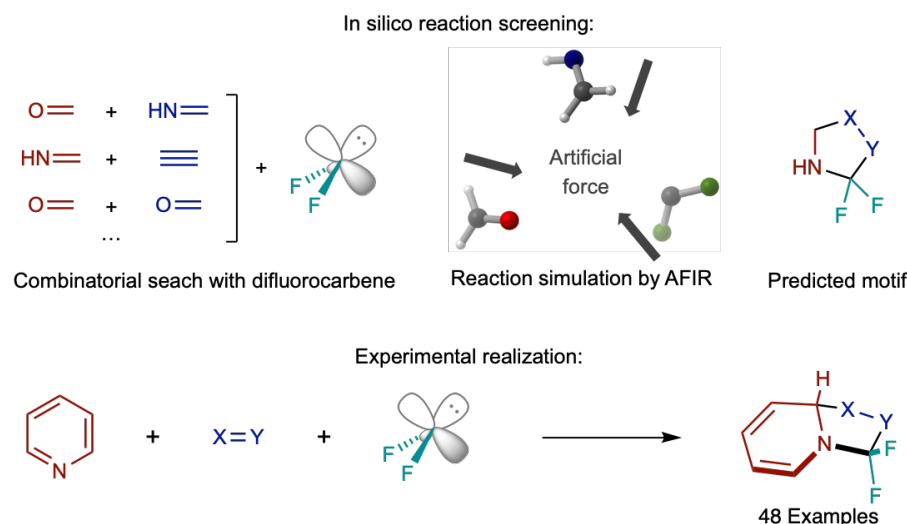
Angew. Chem. Int. Ed. **2023**, *62*, e202303435.



5. "In Silico Reaction Screening with Difluorocarbene for *N*-difluoroalkylative Dearomatization of Pyridines"

Hiroki Hayashi, Hitomi Katsuyama, Hideaki Takano, Yu Harabuchi, Satoshi Maeda, Tsuyoshi Mita

Nat. Synth. **2022**, *1*, 804–812.



6. "Prediction of High-Yielding Single-Step or Cascade Pericyclic Reactions for the Synthesis of Complex Synthetic Targets"

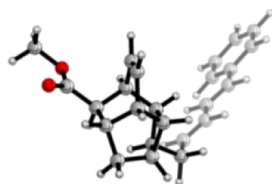
Tsuyoshi Mita, Hideaki Takano, **Hiroki Hayashi**, Wataru Kanna, Yu Harabuchi, Kendall, Houk. Satoshi Maeda

J. Am. Chem. Soc. **2022**, *144*, 22985–23000.

Automatic exploration for pericyclic reaction pathways:

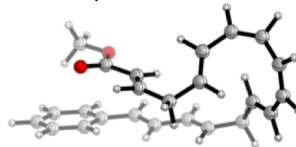
cycloadditions, ene reactions, group transfer reactions, cheletropic reactions, electrocyclic reactions, sigmatropic rearrangements

Input:
product in pericyclic reactions



AFIR

Output:
potential reaction pathways,
 ΔG^\ddagger , potential substrates

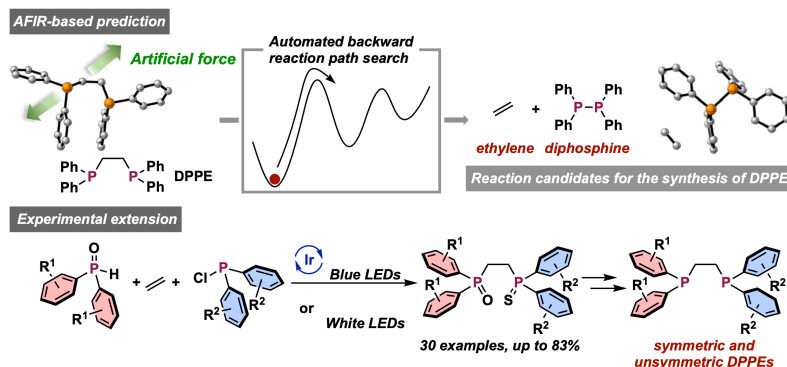


up to 52 atoms
precise stereochemistry
applicable to multi-step routes

7. “A Theory-driven Synthesis of Symmetric and Unsymmetric 1,2-Bis(diphenylphosphino) ethane Analogues via Radical Difunctionalization of Ethylene”

Hideaki Takano, Hitomi Katsuyama, **Hiroki Hayashi**, Wataru Kanna, Yu Harabuchi, Satoshi Maeda, Tsuyoshi Mita

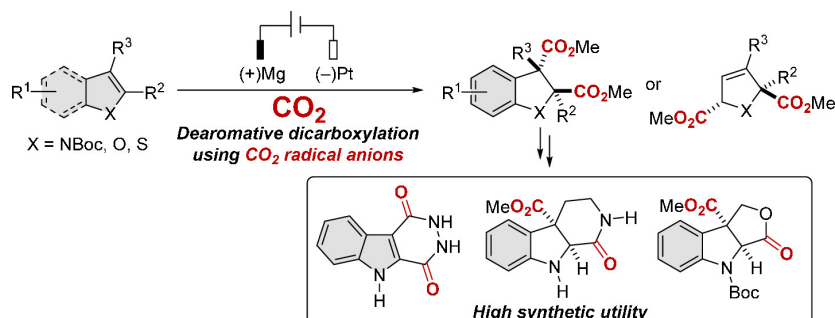
Nat. Commun. **2022**, *13*, 7034.



8. “Electrochemical Dearomative Dicarboxylation of Heterocycles with Highly Negative Reduction Potentials”

Yong You, Wataru Kanna, Hideaki Takano, **Hiroki Hayashi**, Satoshi Maeda, Tsuyoshi Mita

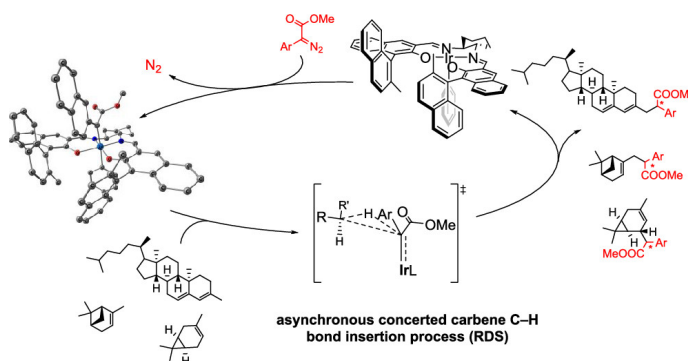
J. Am. Chem. Soc. **2022**, *144*, 3685–3695.



9. “Iridium(III)-Catalyzed Asymmetric Site-Selective Carbene C–H Insertion during Late-Stage Transformation”

Yuki Yamakawa, Takashi Ikuta, **Hiroki Hayashi**, Keigo Hashimoto, Ryoma Fujii, Kyohei Kawashima, Seiji Mori, Tatsuya Uchida, Tsutomu Katsuki

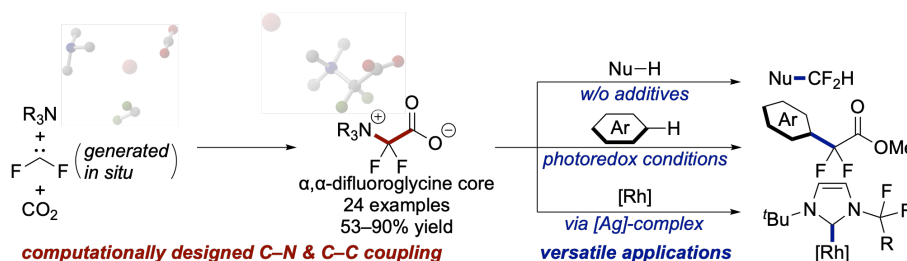
J. Org. Chem. **2022**, *87*, 6769–6780.



10. “Synthesis of Difluoroglycine Derivatives from Amines, Difluorocarbene, and CO₂: Computational Design, Scope, and Applications”

Hiroki Hayashi, Hideaki Takano, Hitomi Katsuyama, Yu Harabuchi, Satoshi Maeda, Tsuyoshi Mita

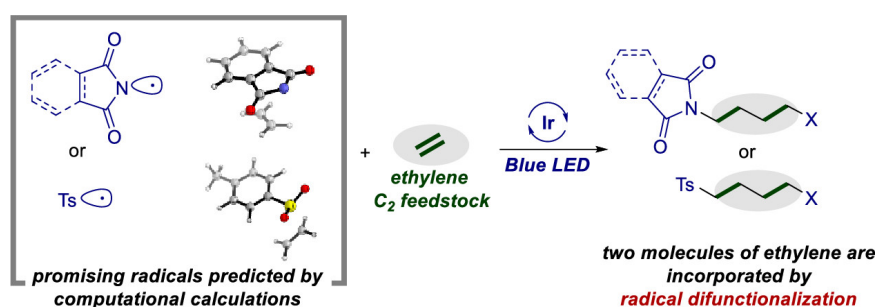
Chem. Eur. J. **2021**, 27, 10040–10047.



11. “Radical Difunctionalization of Gaseous Ethylene Guided by Quantum Chemical Calculations: Selective Incorporation of Two Molecules of Ethylene”

Hideaki Takano, Yong You, **Hiroki Hayashi**, Yu Harabuchi, Satoshi Maeda, Tsuyoshi Mita

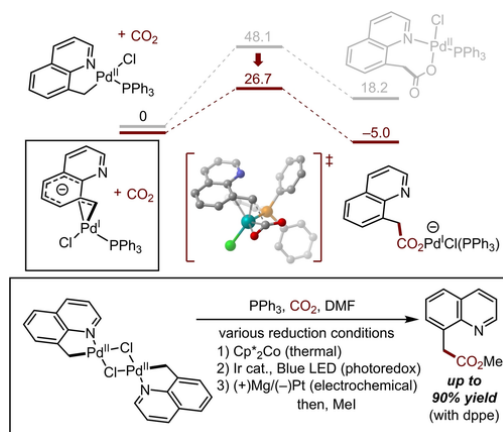
ACS Omega. **2021**, 6, 33846–33854.



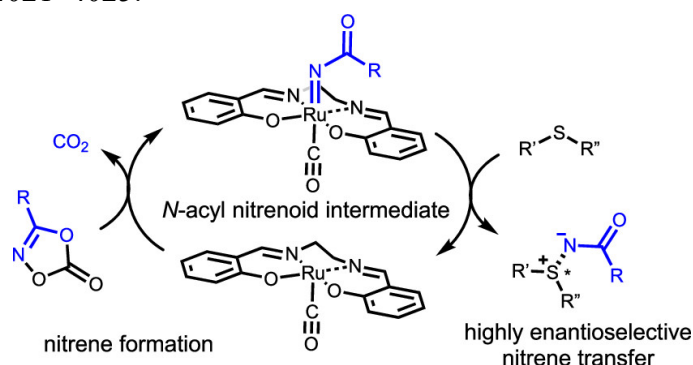
12. “Carboxylation of a Palladacycle Formed via C(sp³)–H Activation: Theory-Driven Reaction Design”

Wataru Kanna, Yu Harabuchi, Hideaki Takano, **Hiroki Hayashi**, Satoshi Maeda, Tsuyoshi Mita

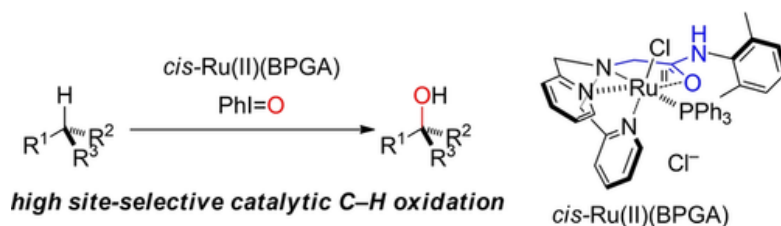
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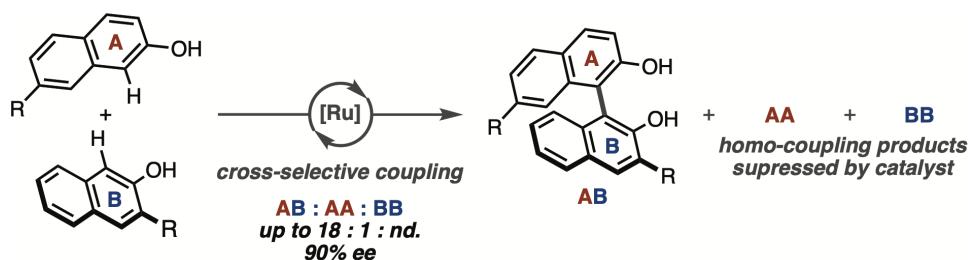
13. “Ruthenium-Catalyzed Asymmetric N-Acyl Nitrene Transfer Reaction: Imidation of Sulfide”
Masaki Yoshitake, **Hiroki Hayashi**, Tatsuya Uchida
Org. Lett. **2020**, 22, 4021–4025.



14. “Non-Heme-Type Ruthenium Catalyzed Chemo- and Site-Selective C–H Oxidation”
Daiki Doiuchi, Tatsuya Nakamura, **Hiroki Hayashi**, Tatsuya Uchida
Chem. Asian J. **2020**, 15, 762–765.



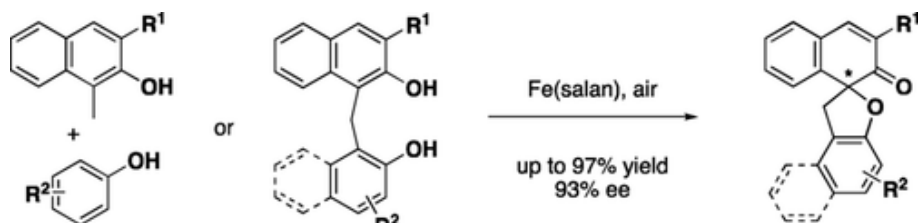
15. “Ruthenium-Catalyzed Cross-Selective Asymmetric Oxidative Cross-Coupling of Arenols”
Hiroki Hayashi, Takamasa Ueno, Chungsik Kim, Tatsuya Uchida
Org. Lett. **2020**, 22, 1469–1474.



16. “Iron-Catalyzed Asymmetric Inter- and Intramolecular Aerobic Oxidative Dearomatizing Spirocyclization of 2-Naphthols”

Takuya Oguma, Daiki Doiuchi, Chisaki Fujitomo, Chungsik Kim, **Hiroki Hayashi**, Tatsuya Uchida, Tsutomu Katsuki

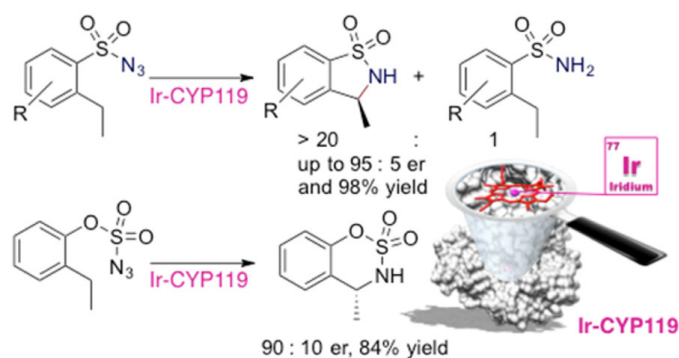
Asian J. Org. Chem. **2019**, 9, 404–415.



17. “Chemoselective, Enzymatic C–H Bond Amination Catalyzed by a Cytochrome P450 Containing an Ir(Me)-PIX Cofactor”

Paweł Dydio, Hanna M. Key, **Hiroki Hayashi**, Douglas S. Clark, John F. Hartwig

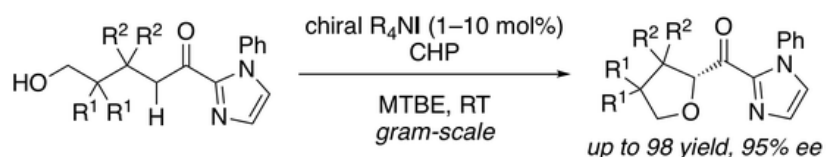
J. Am. Chem. Soc. **2017**, 139, 1750–1753.



18. “Chiral Ammonium Hypoiodite Salt-Catalyzed Enantioselective Oxidative Cycloetherification to 2-Acyl Tetrahydrofurans”

Muhammet Uyanik, **Hiroki Hayashi**, Hirokazu Iwata, Kazuaki Ishihara

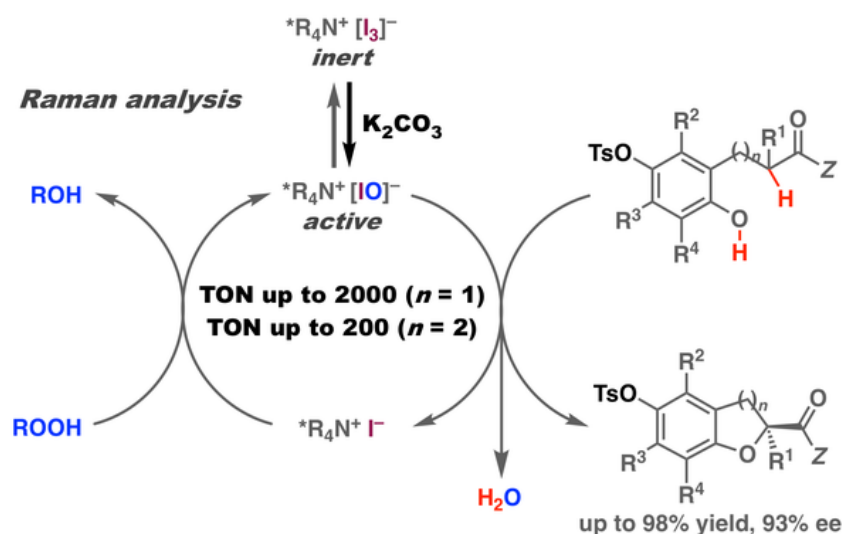
Chem. Lett. **2016**, 45, 353–355.



19. “High-Turnover Hypoiodite Catalysis for Asymmetric Synthesis of Tocopherols”

Muhammet Uyanik, **Hiroki Hayashi**, Kazuaki Ishihara

Science **2014**, 345, 291–294.



Review:

20. “Toward Ab Initio Reaction Discovery Using the Artificial Force Induced Reaction Method”

Satoshi Maeda, Yu Harabuchi, **Hiroki Hayashi**, Tsuyoshi Mita

Ann. Rev. Phys. Chem. **2022**, 74, 13.1-13.25.

21. “Nitrene Transfer Reactions for Asymmetric C–H Amination: Recent Development”

Hiroki Hayashi, Tatsuya Uchida

Eur. J. Org. Chem. **2020**, 8, 909–916.

