ORGANIC CHEMISTRY

FRONTIERS

rsc.li/frontiers-organic

IN THIS ISSUE

ISSN 2052-4129 CODEN OCFRA8 10(8) 1869-2116 (2023)



Cover

See Hideto Ito, Kenichiro Itami et al., pp. 1880-1889.

Image reproduced by permission of Dr. Issey Takahashi from Org. Chem. Front., 2023, 10, 1880.

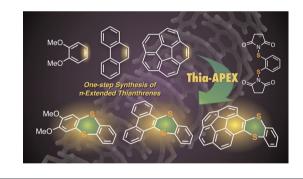
The artwork was created by Dr Issey Takahashi (Nagoya University).

RESEARCH ARTICLES

1880

One-step synthesis of polycyclic thianthrenes from unfunctionalized aromatics by thia-APEX reactions

Kou P. Kawahara, Hideto Ito* and Kenichiro Itami*



1890

Copper(ı)-catalyzed multicomponent interrupted click reaction: modular synthesis of triazole sulfides from elemental sulfur

Pengfei Sun, Weiguo Wang, Jilong Lai, Huang Yan, Chen-Ho Tung and Zhenghu Xu*



EDITORIAL STAFF

Executive Editor

Wenjun Liu

Deputy Editor

Kailin Deng

Development Editor

Cheng Du

Editorial Production Manager

Helen Saxton

Senior Publishing Editor

Becky Webb

Publishing Editors

Kirstine Anderson, Matthew Bown, Laura Cooper, Emily Cuffin-Munday, Hannah Fielding, Clare Fitzgerald, Anoushka Handa, Claire Harding, Alan Holder, Rosie Rothwell, Donna Smith, Laura Smith

Assistant Editors

Jie Gao, Yu Zhang

Publisher

Jeanne Andres

For queries about submitted papers, please contact Helen Saxton, Editorial Production Manager, in the first instance. E-mail: OrgChemFrontiersPROD@rsc.org

For pre-submission queries please contact Wenjun Liu,

Executive Editor. Email: OrgChemFrontiersED@rsc.org

Organic Chemistry Frontiers (electronic: ISSN 2052-4129) is published 24 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 OWE.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail orders@rsc.org

2023 Annual (electronic) subscription price: £2,182; USS3,492. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

ORGANIC CHEMISTRY

FRONTIFRS

An international, high impact journal for cutting-edge researches from all disciplines of organic chemistry.





rsc.li/frontiers-organic

Published in collaboration with the Chinese Chemical Society and Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences

Editorial Board

Editor-in-Chief

Shengming Ma, Shanghai Institute of Organic Chemistry, China

Associate Editors

Arjan W. Kleij, Institute of Chemical Research of Catalonia, Spain Chulbom Lee, Seoul National University, Korea

Bill Morandi, ETH Zurich, Switzerland

Jennifer M. Schomaker, University of Guy

Wisconsin-Madison, USA Frank Würthner, University of Würzburg, Germany

Pei-Qiang Huang, Xiamen University, China Qian Zhang, Northeast Normal University, China

Members

Guy Bertrand, University of California, San Diego, USA Nicolai Cramer, EPFL, Switzerland

Louis Fensterbank, Sorbonne Université, France Lichang Wang, Southern Illinois University.

Dan Yang, Westlake University, China

Advisory Board

Ayyappanpillai Ajayaghosh, National Institute for Interdisciplinary Science and Technology, India

Lutz Ackermann, Georg-August-Universitat Gottingen, Germany

Marco Bandini, University of Bologna, Italy Matthias Beller, University of Rostock, Germany

Akkattu T. Biju, Indian Institute of Science, India

Xi Chen, University of California-Davis, USA Yiyun Chen, Shanghai Institute of Organic Chemistry, China

Yonggui Robin Chi, Nanyang Technological University, Singapore Stuart Conway, University of Oxford, UK Shuanhu Gao, East China Normal

University, China Véronique Gouverneur, University of Oxford, Frank Glorius, Westfälische Wilhelms-Universität Münster, Germany Zhenhua Gu, University of Science and Technology of China, China Masayuki Inoue, The University of Tokyo, Japan

Guochen Jia, Hong Kong University of Science & Technology, China Michael Kerr, University of Western Ontario, Canada

Ohyun Kwon, University of California, Los Angeles, USA Rai-Shung Liu, National Tsing Hua

University, Hsinchu Sanzhong Luo, Tsinghua University, China Cristina Nevado, University of Zurich,

Christoph Schalley, Freie Universität Berlin, Germany Daniel Seidel, University of Florida, USA Feng Shi, Jiangsu Normal University, China Yian Shi, Colorado State University, USA Vinod K. Singh, ITT Kanpur, India Wenjun Tang, Shanghai Institute of Organic

Chemistry, China Yong Tang, Shanghai Institute of Organic

Chemistry, China
Chen-Ho Tung, Technical Institute
of Physics and Chemistry, CAS, China
Tao Ve Peking University (Shenzhen) Ch

Tao Ye, Peking University (Shenzhen), China Tomoki Ogoshi, Kanazawa University, Japan Zhaohui Wang, Institute of Chemistry , CAS, China

Lizhu Wu, Technical Institute of Physics and Chemistry, CAS, China Xingang Zhang, Shanghai Institute of Organic Chemistry, China

Information for Authors

Full details on how to submit material for publication in Organic Chemistry Frontiers are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made via the journal's homepage: rsc.li/frontiers-organic

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)-Reproduced by permission of the Royal Society of Chemistry.

This journal is \circledcirc the Partner Organisations 2023 . Apart from fair dealing for the purposes of research or private

study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

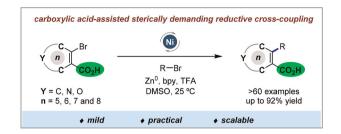
Registered charity number: 207890



1897

Carboxylic acid-assisted sterically demanding reductive cross-coupling between cycloalkenyl and alkyl bromides

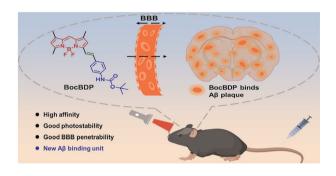
Jinglin An. Xue Zhou, Yifan Zhang, Zhenfei Ye. Qianyou Guo, Hao Song, Zhenlei Song, * Xiao-Yu Liu and Yong Qin*



1903

A BODIPY-based probe for amyloid-β imaging in vivo

Mingguang Zhu, Guoyang Zhang, Ziwei Hu, Chaofeng Zhu, Yixiang Chen, Tony D. James,* Lijun Ma* and Zhuo Wang*



1910

Asymmetric synthesis of 7-membered-ring-bridged 3,4-fused tricyclic indoles via Friedel-Crafts alkylation/annulation

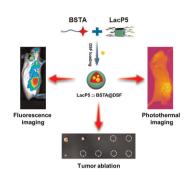
Bai-Yu Xue, Chen-Ying Hou, Xiao-Bing Wang, Ming-Sheng Xie* and Hai-Ming Guo*

1915

Synthesis of α -amino acid derived (1,2,3-triazol-4-yl)-picolinamide (tzpa) ligands and their corresponding luminescent Tb(III) complexes

Isabel N. Hegarty, Chris S. Hawes and Thorfinnur Gunnlaugsson*

1927



A supramolecular near-infrared nanophotosensitizer from host-guest complex of lactose-capped pillar[5] arene with aza-BODIPY derivative for tumor eradication

Jiaxuan Li, Xiaomeng Lv, Jiahui Li, Wenjuan Jin, Zelong Chen, Yafei Wen, Zhichao Pei and Yuxin Pei*

1936

Synthesis of quinol-type heterobiaryls *via* an acid-catalyzed heteroannulation of alkynes and *o*-aminobenzaldehydes

Qing-Song Jian, Bo-Bo Gou, Shao-Jie Wang, Huai-Ri Sun, Atif Sharif, Yong-Qiang Wang, Ling Zhou* and Jie Chen*

1942



Transition metal-free, photocatalytic arylation and dioxygenation for vicinal diketone synthesis using alkynes and arene diazonium salts

Baoli Zhao, Xiaoting Yin, Haifeng Li, Kai Cheng* and Jie-Ping Wan*

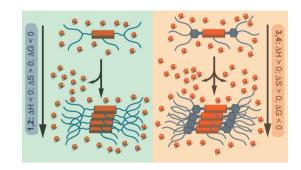
A DFT study of Ni-catalyzed (3 + 3)-annulation between donor–acceptor cyclopropanes and diaziridines

Song-Shan Dai, Xiao-jiao Yang, Ran Fang,* Alexander M. Kirillov and Lizi Yang*

1959

Thermodynamics of the self-assembly of *N*-annulated perylene bisimides in water. Disentangling the enthalpic and entropic contributions

Manuel A. Martínez, Daniel Aranda, Enrique Ortí, Juan Aragó* and Luis Sánchez*



1968

Photochemical difluoromethylation of alkynes: synthesis of CF₂H-substituted seven-membered dioxodibenzothiazepines and dibenzazepines

Xiaoyu Chen, Yang Geng, Bo Liu, Yu Zhu, Dapeng Zou,* Yangjie Wu* and Yusheng Wu*

1975

Preparation of benzoyl fluorides and benzoic acids from phenols *via* a dearomatization—rearomatization strategy

Meixian Yang, Xinyue Huang, Wenjun Miao, Lan Yi, Jiajing Cai, Zhenghuan Zhao, Jia He* and Dachuan Qiu*

$$R_1$$
 R_2 R_3 t -BuOK, DMF R_1 R_1 R_2 R_3 t -BuOK, DMF R_1 R_2 R_3 R_4 R_4 R_5 R_5 R_6 R_7 R_8 R_8 R_8

1981

Visible-light-promoted defluorinated alkylation of trifluoromethyl alkenes initiated by radical [1,2]-Brook rearrangement: facile synthesis of *gem*-difluoro homoallylic alcohol derivatives

Tao Qin, Chunlu Xu, Ge Zhang* and Qian Zhang

1988

Quadruple cleavage of CICF₂COONa

Metal-free reaction conditions

Quadruple view of CICF₂COONa

y Metal-free reaction conditions

y to 90% yield

TBHP-promoted multicomponent reaction to access 2-aminobenzoxazinones using sodium chlorodifluoroacetate as the C1 synthon

Huijuan Li, Yongfeng Wang, Cheng Xu,* Jingwen Zou, Yaxuan Wu and Guodong Yin*

1994

$$\begin{array}{c} \textbf{One-pot} \\ \textbf{O} \\ \textbf{R}^2 \\ \textbf{N} \end{array} \overset{\textbf{1}) \ [IrCl(COE)_2]_2 \ (cat.),}{\underbrace{Et_2SiH_2, \ toluene, \ r.t.}} \\ \textbf{2) \ Acyl \ chloride, \ Et_3N, \ r.t.} \\ \begin{array}{c} \textbf{Bicyclic \ I} \\ \textbf{Bicyclic \ I} \end{array} \overset{\textbf{N}}{} \overset{\textbf{R}^3} \overset{\textbf{O}}{\underset{\textbf{R}^4}{}} \overset{\textbf{R}^3}{\underset{\textbf{O} \ \textbf{R}^2}{}} \\ \textbf{Monocyclic \ II} \end{array}$$

good compatibility

Broad substrate scope

- readily accessible reagents
- mild conditions scalable
- la, m=1, 32 examples, up to 97% yield lb. m=2, 12 examples, up to 89% yield
- II, 2 examples, 84% and 91% yield

One-pot synthesis of 1,3-oxazin-4-ones through an Ir-catalyzed mild formal condensation reaction of secondary amides with acyl chlorides

Si-Jia Yu, Jie Li, Jian-Liang Ye* and Pei-Qiang Huang*

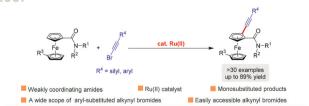
2002

■ Merging Ullmann coupling and ring-expansion reaction ■ Dicyclization using amidine hydrochlorides as a dual synthon
■ Simple catalytic system and Functional group tolerance ■ Formation of four C-N bonds and cleavage of one C-C bond

Merging Ullmann-type cyclization and ring-expansion: a facile assembly of pyrimidine-fused quinazolinones by copper catalysis

Zhen-Wei Sun, Na Luo, Xiang Zhang, Wen-Jun Tuo, Xiao-Qiang Hu* and Feng-Cheng Jia*

2007



Ru(II)-catalyzed C-H alkynylation of ferrocenes with bromoalkynes directed by carboxamide groups

Ru-Yuan Zhao, Jing Zhang, Rui-Han Niu, Jin-Heng Li* and Bo Sun*

2013

Transition-metal free oxidative carbocarboxylation of alkenes with formate in air

Pei Xu, Hui Xu, Sai Wang, Tian-Zi Hao, Si-Yi Yan, Dong Guo* and Xu Zhu*

- ✓ no organo (pseudo)halides needed
- ✓ transition-metals free
- ✓ air as a "green" oxidant
- ✓ high synthetic utility

2018

Visible-light-induced alkoxycarbonylation/cyclization of 1,7-enynes: synthesis of dihydropyranones containing all-carbon quaternary centers

Jian-Qiang Chen, Qi Chen, Baofu Chen* and Jie Wu*

2024

Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B₂pin₂ and alkyl iodides: a computational study

Xinyi Song, Hongli Wu, Jinjin Yang, Wentao Zhao* and Genping Huang*

2033

Palladium-catalyzed allylic allenylation of homoallyl alcohols with propargylic carbonates

Ping-Xin Zhou,* Murong Wang, Xiang Li, Xueyan Du, Xiaozhe Yang, Han Wang, Tangqiang Sun,* Feng Ren* and Yong-Min Liang

2039

$$R^{1} \xrightarrow{X} R^{2}$$

$$X = Br, Cl$$

$$V = N \text{ No noble metal catalyst}$$

$$R^{1} \xrightarrow{N} R^{2}$$

$$R^{2} \xrightarrow{N} R^{2}$$

$$R^{3} \xrightarrow{N} R^{3}$$

$$V = R^{2} \xrightarrow{N} R^{3}$$

$$R^{3} \xrightarrow{N} R^{3}$$

Indirect electrochemical reductive cyclization of o-halophenylacrylamides mediated by phenanthrene

Xue-Qi Zhou, Pei-Bo Chen, Qiang Xia, Ting-Kai Xiong, Xue-Jun Li, Ying-Ming Pan, Mu-Xue He* and Ying Liang*

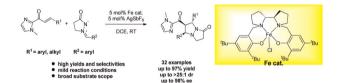
2045



Integration of CO₂ capture, activation, and conversion with a ternary acetylglucosyl 2-methylimidazolium modified Pd catalyst

Zhong-Gao Zhou,* Peng He, Jing Li, Jia Zhang, Guo-Hai Xu, Shi-Yong Zhang, Xiao-Xiao Deng, Zi-Yi Du, Guo-Tian Luo, Hong-Yu Zhen, Yi-Wang Chen and Chun-Ting He*

2054



Fe-BPsalan complex-catalyzed asymmetric 1,3-dipolar [3 + 2] cycloaddition reaction of N,N'-cyclic azomethine imines with α,β -unsaturated acyl imidazoles

Hao Lu, Kai-Ge Chen, Gong-Xin Li, Kun Zhan, Hao-Yang Wang, Zhen-Jiang Xu* and Chi-Ming Che*

2061

$$Ar^{1} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} R \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} R \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} R \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} Ar^{2} \stackrel{\bigcirc{}}{\underset{}} NH_{2} \stackrel{\bigcirc{}}{\underset{}} R \stackrel{\stackrel{}{\underset{}}{\underset{}} NH_{2} \stackrel{\stackrel{}}{\underset{}} R \stackrel{\stackrel{}}{\underset{}} NH_{2} \stackrel{\stackrel{}}{\underset{}} R \stackrel{\stackrel{}}{\underset{}} NH_{2} \stackrel{\stackrel{}}{\underset{}} R \stackrel{\stackrel{}}{\underset{}} N \stackrel{\stackrel{}}{\underset{}} N$$

- high chemoselectivity = inexpensive, abundant reagents
- broad scope operatinal-simplicity

Cation-controlled chemoselective synthesis of *N*-aroylureas and imides *via* amidation of *N*-Boc arylamides

Jiamin Wang, Sujuan Shuai, Lishe Gan, Yongxin Luo, Huimin Jin, Lingfeng Chen, Dong Zou, Guang Liang,* Patrick J. Walsh* and Jie Li*

2070

Construction of alkynyl and acyl disulfides directly through thiol-modification with N-alkynylthio phthalimides under acid catalysis

Yao-Nan Xue, Kai Feng, Jun Tian, Juan Zhang, Hong-Hong Chang and Wen-Chao Gao*

2075

Transition metal-free radical trans-hydroboration of alkynes with NHC-boranes via visible-light photoredox catalysis

Ding-Chang Li, Jia-Hao Zeng, Yu-Hang Yang and Zhuang-Ping Zhan*

$$R^{1} = R^{2} + \bigvee_{N}^{+} \stackrel{\stackrel{1}{\longrightarrow}}{BH_{3}} \frac{20 \text{ mol}\% \text{ 4-CF}_{3}\text{-PhSH}}{\text{rt, Blue LEDs}} + \bigvee_{R^{2}}^{R^{1}} \stackrel{H_{2}}{\overset{B}{\longrightarrow}} \stackrel{N^{+}}{\overset{B}{\longrightarrow}}$$

$$trans-hydroboration$$

★ metal-free photoredox catalysis ★ good regio- and stereoselectivity ★ high atom economy mild conditions

REVIEWS

2081

Transition metal-catalyzed alkynylation reactions via alkynyl carbon-carbon bond cleavage

Hairui Yuan, Qi Zhou and Jianbo Wang*

2095

Selective preparative 'oxidase phase' in sesquiterpenoids: the radical approach

Maria Kourgiantaki, Georgia G. Bagkavou, Christos I. Stathakis* and Alexandros L. Zografos*

