

# Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(21) 5531–5812 (2023)



### Cover

See Selvan Demir *et al.*, pp. 5577–5592.  
Image reproduced by permission of Selvan Demir from *Chem. Sci.*, 2023, **14**, 5577.



### Inside cover

See Jatish Kumar *et al.*, pp. 5593–5601.  
Image reproduced by permission of Jatish Kumar from *Chem. Sci.*, 2023, **14**, 5593.

## COMMENTARY

5542

### A focus on aromaticity: fuzzier than ever before?

Henrik Ottosson

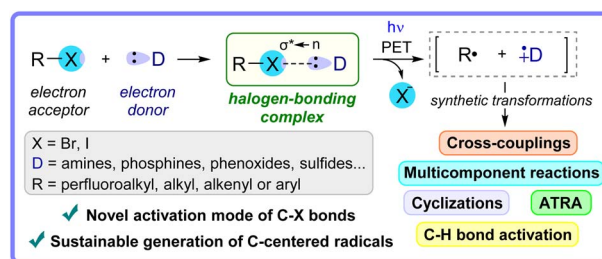


## REVIEW

5545

### Shining light on halogen-bonding complexes: a catalyst-free activation mode of carbon–halogen bonds for the generation of carbon-centered radicals

Helena F. Piedra, Carlos Valdés and Manuel Plaza\*



## Editorial Staff

### Executive Editor

May Copsey

### Deputy Editor

Samantha Apps

### Senior Editor

James Moore

### Scientific Editors

Ellis Crawford, Jingtao Huang, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

### Editorial Assistant

Karina Webster

### Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail [chemicalscience@rsc.org](mailto:chemicalscience@rsc.org)

For pre-submission queries please contact May Copsey, Executive Editor. E-mail [chemicalscience-rsc@rsc.org](mailto:chemicalscience-rsc@rsc.org)

Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email [orders@rsc.org](mailto:orders@rsc.org) to register your interest or contact Royal Society of Chemistry 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](mailto:orders@rsc.org)

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](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

# Chemical Science

[rsc.li/chemical-science](http://rsc.li/chemical-science)

## Editorial Board

### Editor-in-Chief

Andrew Cooper, University of Liverpool

### Associate Editors

Vincent Artero, CEA-Grenoble  
Luis M. Campos, Columbia University  
Michelle Chang, University of California, Berkeley  
Lin X. Chen, Northwestern University  
Graeme Day, University of Southampton  
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

Vy Dong, University of California, Irvine  
François Gabbai, Texas A&M University  
Subi George, JNCASR  
Jinlong Gong, Tianjin University  
Stephen Goldup, University of Birmingham  
Zaiping Guo, University of Adelaide  
Christopher A. Hunter, University of Cambridge  
Malika Jefferies-EL, Boston University  
Ning Jiao, Peking University  
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University  
Maja Köhn, University of Freiburg  
Yi-Tao Long, Nanjing University  
Gabriel Merino, CINVESTAV Merida  
James K. McCusker, Michigan State University  
Thomas Meade, Northwestern University  
Paolo Melchiorre, University of Bologna  
Carsten Schultz, Oregon Health & Science University  
Dmitri Talapin, The University of Chicago  
Toshiharu Teranishi, Kyoto University  
Andrei Yudin, University of Toronto

## Advisory Board

Dave Adams, University of Glasgow  
Ayyappanpillai Ajayaghosh, NIIST  
Ulf-Peter Apfel, Ruhr-University Bochum  
Polly Arnold, University of California, Berkeley  
Xinhe Bao, Dalian Institute of Chemical Physics  
Zhenan Bao, Stanford University  
Gonçalo Bernardes, University of Cambridge  
Frank Biedermann, Karlsruhe Institute of Technology  
Donna Blackmond, Scripps Research Institute  
Jeffrey Bode, ETH Zurich  
Jennifer S. Brodbelt, University of Texas at Austin, USA  
Christopher Chang, University of California, Berkeley  
Chi-Ming Che, University of Hong Kong  
Jun Chen, Nankai University  
R. Graham Cooks, Purdue University  
Christophe Copéret, ETH Zurich  
Eugenio Coronado, University of Valencia  
Leroy Cronin, University of Glasgow  
James Crowley, University of Otago  
Christopher C. Cummins, Massachusetts Institute of Technology  
Ben Davis, University of Oxford  
Jillian Dempsey, University of North Carolina at Chapel Hill  
Kazunari Domen, University of Tokyo  
James Durrant, Imperial College London  
Xinlang Feng, TU Dresden  
Ben Feringa, University of Groningen  
Makoto Fujita, University of Tokyo  
Phillip Gale, University of Technology Sydney  
Song Gao, Peking University  
Jeremiah Gassensmith, University of Texas at Dallas  
Elizabeth Gibson, Newcastle University  
Ryan Gilmour, WWU Münster  
Hubert Girault, EPFL  
Frank Glorius, WWU Münster  
Leticia González, University of Vienna  
Duncan Graham, University of Strathclyde

Vicki Grassian, University of California, San Diego  
Alexis Grimaud, Boston College  
Christian Hackenberger, FMP Berlin  
Buxing Han, Chinese Academy of Sciences  
Christy Haynes, University of Minnesota  
Patrick Holland, Yale University  
Kim Jelfs, Imperial College London  
Yousung Jung, KAIST  
Stephanie Kath-Schorr, University of Cologne  
Takashi Kato, University of Tokyo  
Christopher Kelly, Janssen Research & Development  
Jérôme Lacour, University of Geneva  
Ai-Lan Lee, Heriot-Watt University  
Daniele Leonori, RWTH Aachen University  
Chao-Jun Li, McGill University  
Yi Li, Jilin University  
Mi Hee Lim, KAIST  
Wenbin Lin, University of Chicago  
Kopin Liu, Academia Sinica  
Watson Loh, UNICAMP  
Bettina Lotsch, Max Planck Institute  
Xiong Wen (David) Lou, Nanyang Technological University  
Kazuhiko Maeda, Tokyo Institute of Technology  
Satoshi Maeda, Hokkaido University  
Swadhin Mandal, IISER Kolkata  
Ellen Matson, University of Rochester  
Scott Miller, Yale University  
Daniel Mindiola, University of Pennsylvania  
Wonwoo Nam, Ewha Womans University  
Jonathan Nitschke, University of Cambridge  
Allie Obermeyer, Columbia University  
Martin Oestreich, Technical University of Berlin  
Takashi Ooi, Nagoya University  
Rachel O'Reilly, University of Birmingham  
Oleg Ozerov, Texas A&M University  
Xiulian Pan, Dalian Institute of Chemical Physics  
Nicolas Plummer, Technical University of

Munich  
Rasmita Raval, University of Liverpool  
Erwin Reisner, University of Cambridge  
Andrea Rentmeister, WWU Münster  
Jeffrey Rinehart, University of California, San Diego  
Stuart Rowan, University of Chicago  
Richmond Sarpong, University of California, Berkeley  
Danielle Schultz, Merck  
Dwight Seferos, University of Toronto  
Oliver Seitz, Humboldt University of Berlin  
Roberta Sessoli, University of Florence  
Kay Severin, Federal Polytechnic School of Lausanne  
Mikiko Sodeoka, RIKEN  
Galo Soler-Illia, Universidad Nacional de San Martin  
David Spring, University of Cambridge  
Brian Stoltz, California Institute of Technology  
Brent Sumerlin, University of Florida  
Raghavan B. Sunoj, IIT Bombay  
Yogesh Surendranath, MIT  
Mizuki Tada, Nagoya University  
Ben Zhong Tang, The Hong Kong University of Science and Technology  
Zhiyong Tang, National Center for Nanoscience and Nanotechnology  
Christine Thomas, Ohio State University  
He Tian, East China University of Science & Technology  
Zhong-Qun Tian, Xiamen University  
F. Dean Toste, University of California, Berkeley  
Takashi Uemura, University of Tokyo  
Jan van Hest, Radboud University  
Latha Venkataraman, Columbia University  
Chu Wang, Peking University  
Julia Weinstein, University of Sheffield  
Tom Welton, Imperial College London  
Charlotte Williams, University of Oxford  
Vivian Yam, University of Hong Kong  
Qi-Lin Zhou, Nankai University  
Jenny Zhang, University of Cambridge

## Information for Authors

Full details on how to submit material for publication in Chemical Science 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/chemical-science](http://rsc.li/chemical-science)

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 © The Royal Society of Chemistry 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



## PERSPECTIVE

5569

**Aromaticity: Quo Vadis**

Gabriel Merino,\* Miquel Solà,\* Israel Fernández,\*  
Cina Foroutan-Nejad,\* Paolo Lazzeretti,\*  
Gernot Frenking,\* Harry L. Anderson, Dage Sundholm,  
Fernando P. Cossio, Marina A. Petrukhina, Jishan Wu,  
Judy I. Wu and Albeiro Restrepo

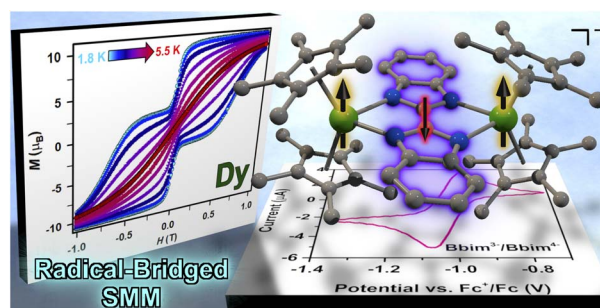


## EDGE ARTICLES

5577

**Magnetic hysteresis and large coercivity in bisbenzimidazole radical-bridged dilanthanide complexes**

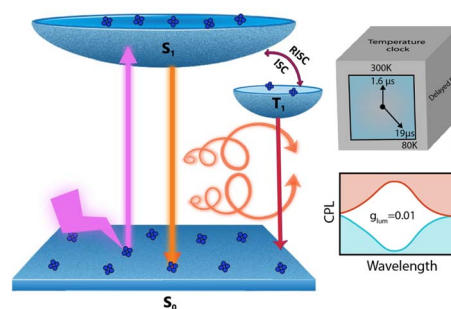
Florian Benner, Léo La Droitte, Olivier Cador,  
Boris Le Guennic and Selvan Demir\*



5593

**Delayed luminescence guided enhanced circularly polarized emission in atomically precise copper nanoclusters**

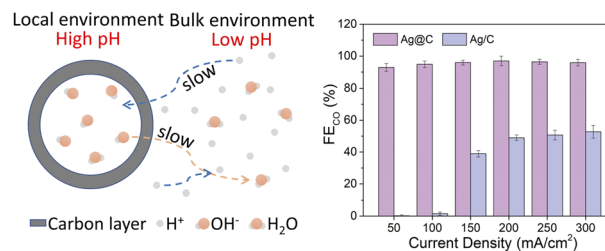
Camelia Dutta, Sonia Maniappan and Jatish Kumar\*



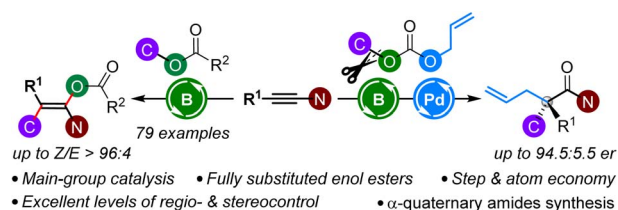
5602

**Confinement of an alkaline environment for electrocatalytic CO<sub>2</sub> reduction in acidic electrolytes**

Xiaozhi Li, Peng Zhang, Lili Zhang, Gong Zhang, Hui Gao,  
Zifan Pang, Jia Yu, Chunlei Pei, Tuo Wang  
and Jinlong Gong\*



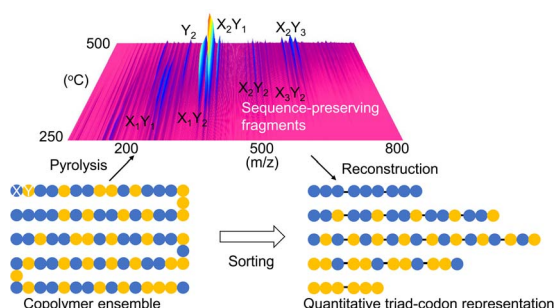
5608



### Atom-economic and stereoselective catalytic synthesis of fully substituted enol esters/carbonates of amides in acyclic systems enabled by boron Lewis acid catalysis

Yuanjiu Xiao, Lei Tang, Tong-Tong Xu, Jiang-Yi-Hui Sheng, Zhongyan Zhou, Lei Yue, Guoqiang Wang,\* Martin Oestreich\* and Jian-Jun Feng\*

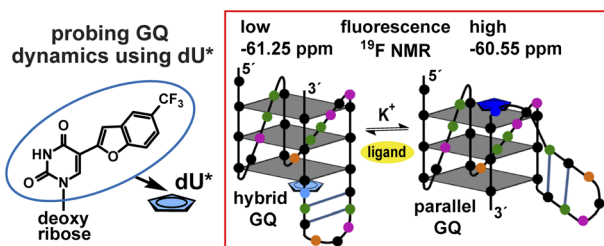
5619



### A data-driven sequencer that unveils latent "codons" in synthetic copolymers

Yusuke Hibi,\* Shiho Uesaka and Masanobu Naito\*

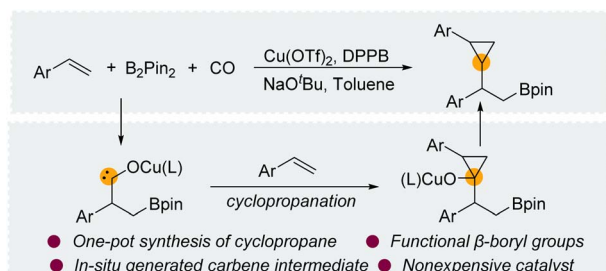
5627



### Probing juxtaposed G-quadruplex and hairpin motifs using a responsive nucleoside probe: a unique scaffold for chemotherapy

Saddam Y. Khatik, Sruthi Sudhakar, Satyajit Mishra, Jeet Kalia, P. I. Pradeepkumar and Seergazhi G. Srivatsan\*

5638



### Copper-catalyzed synthesis of $\beta$ -boryl cyclopropanes via 1,2-borocyclopropanation of aryl olefins with CO as the C1 source

Hui-Qing Geng and Xiao-Feng Wu\*

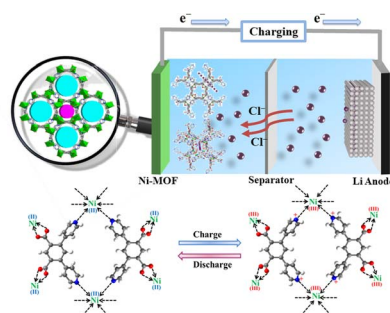




5643

### A nickel-based metal–organic framework as a new cathode for chloride ion batteries with superior cycling stability

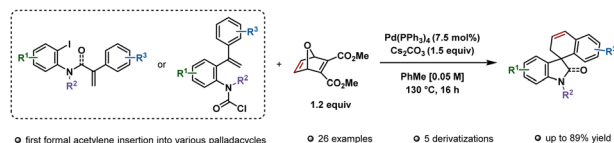
Qing Yin, Zhihao Song, Shuhan Yang, Gang-Ding Wang, Yanwei Sui,\* Jiqui Qi, Danyang Zhao, Lei Hou\* and Yong-Zhi Li\*



5650

### Synthesis of spirooxindoles via formal acetylene insertion into a common palladacycle intermediate

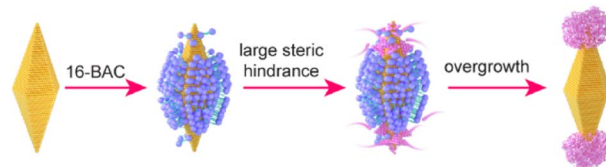
Xavier Abel-Snape, Colton E. Johnson, Bianca Imbriaco and Mark Lautens\*



5656

### Steric hindrance-induced selective growth of rhodium on gold nanobipyramids for plasmon-enhanced nitrogen fixation

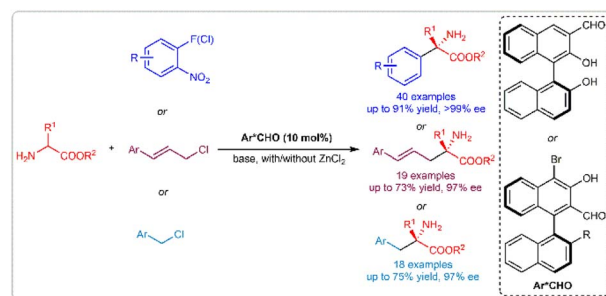
Henglei Jia, Fan Li, Yuanyuan Yang, Mengxuan Zhao, Jingzhao Li and Chun-yang Zhang\*



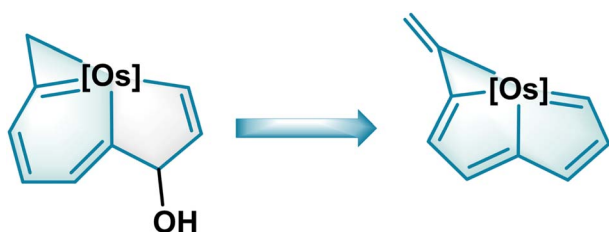
5665

### Chiral aldehyde catalysis enables direct asymmetric $\alpha$ -substitution reaction of N-protected amino acids with haloalkylcarbons

Hao-Ran Shen, Chao-Xing Li, Xin Jiang, Yao Lin, Jian-Hua Liu, Fang Zhu, Zhu-Lian Wu, Tian Cai, Wei Wen,\* Rong-Xing He and Qi-Xiang Guo\*



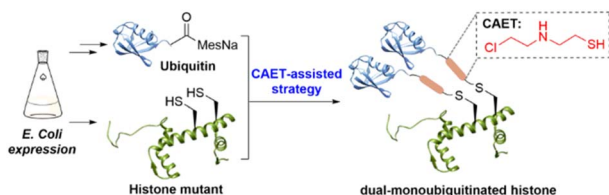
5672



### Reshaping aromatic frameworks: expansion of aromatic system drives metallabenzenoids to metallapentalenes

Qian Li, Jiawei Fei, Kaidong Ruan, Yuhui Hua, Dafa Chen, Ming Luo\* and Haiping Xia\*

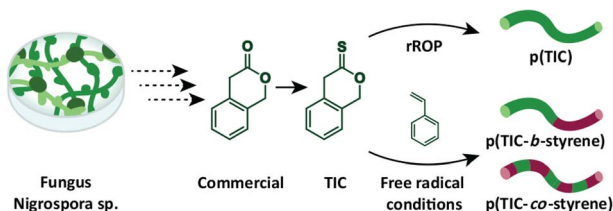
5681



### The expedient, CAET-assisted synthesis of dual-monoubiquitinated histone H3 enables evaluation of its interaction with DNMT1

Zichen Li, Zebin Tong, Qingyue Gong, Huasong Ai,\* Shuai Peng, Cong Chen, Guo-Chao Chu and Jia-Bin Li\*

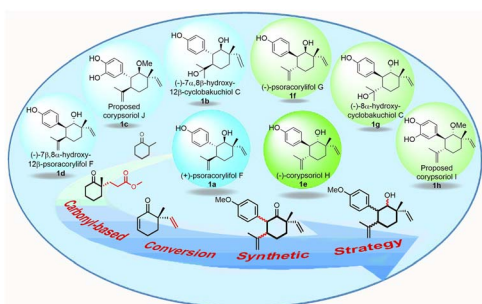
5689



### Radical ring-opening polymerization of sustainably-derived thionoisochromanone

Emily A. Prebihalo, Anna M. Luke, Yernaidu Reddi, Christopher J. LaSalle, Vijay M. Shah, Christopher J. Cramer and Theresa M. Reineke\*

5699



### Enantioselective total syntheses of six natural and two proposed meroterpenoids from *Psoralea corylifolia*

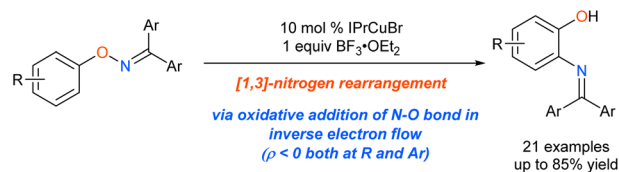
Xiao-Wei Chen, Zi-Chao Hou, Chi Chen, Ling-Hui Zhang, Meng-En Chen and Fu-Min Zhang\*



5705

### Copper-catalyzed [1,3]-nitrogen rearrangement of O-aryl ketoximes via oxidative addition of N–O bond in inverse electron flow

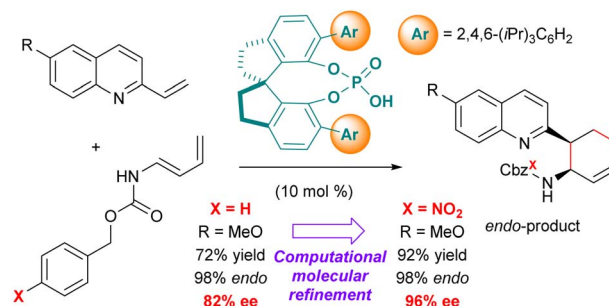
Mao Suzuki, Masahiro Terada and Itaru Nakamura\*



5712

### Computational molecular refinement to enhance enantioselectivity by reinforcing hydrogen bonding interactions in major reaction pathway

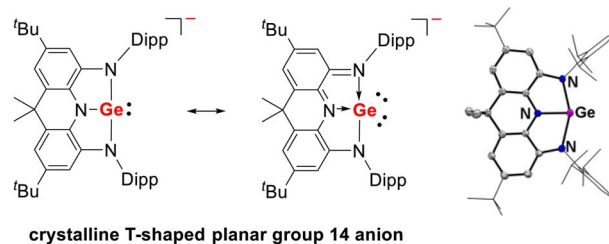
Taishi Nakanishi and Masahiro Terada\*



5722

### A crystalline T-shaped planar group 14 anion

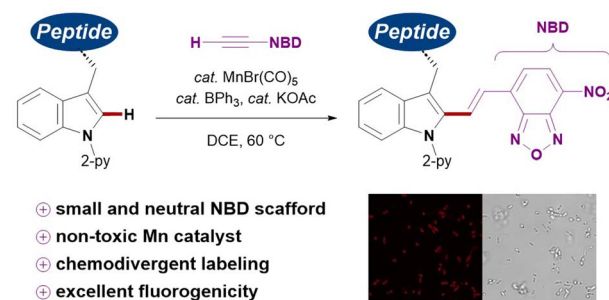
Xiaona Liu, Yuyang Dai, Manling Bao, Wenjuan Wang, Qianli Li, Chunmeng Liu, Xinping Wang\* and Yuanting Su\*



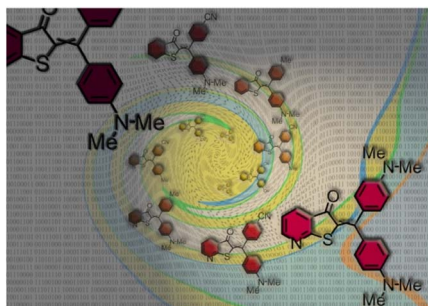
5728

### Late-stage peptide labeling with near-infrared fluorogenic nitrobenzodiazoles by manganese-catalyzed C–H activation

Tsuyoshi Oyama, Lorena Mendive-Tapia, Verity Cowell, Adelina Kopp, Marc Vendrell\* and Lutz Ackermann\*



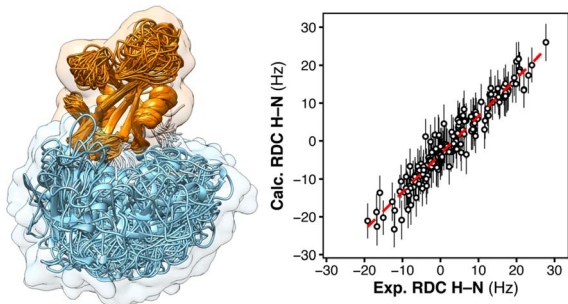
5734



### A cross-conjugation approach for high-performance diaryl-hemithioindigo photoswitches

Max Zitzmann, Frank Hampel and Henry Dube\*

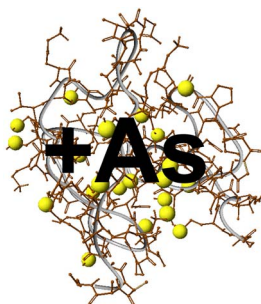
5743



### Experiment-guided molecular simulations define a heterogeneous structural ensemble for the *PTPN11* tandem SH2 domains

Michelangelo Marasco, John Kirkpatrick, Teresa Carlomagno, Jochen S. Hub and Massimiliano Anselmi\*

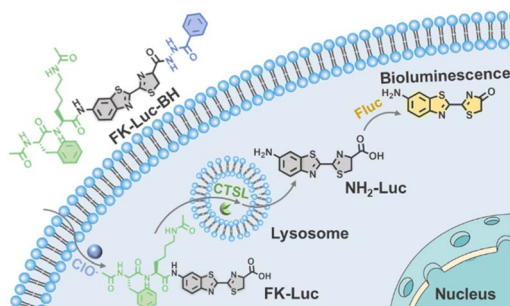
5756



### Arsenic binding to human metallothionein-3

Amelia T. Yuan and Martin J. Stillman\*

5768



### An AND-gate bioluminescent probe for precise tumor imaging

Chenchen Wang, Yajian Hong, Ling Dong, Hu Cheng, Duo Jin, Ronghua Zhao, Zian Yu and Yue Yuan\*

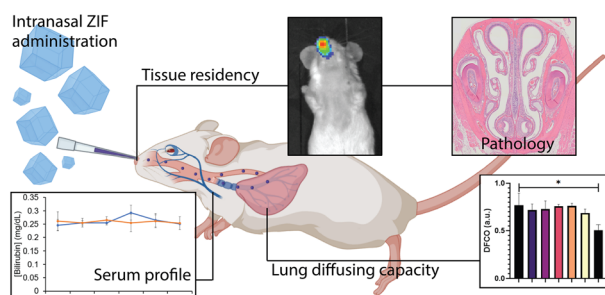




5774

### ***In vivo* biocompatibility of ZIF-8 for slow release via intranasal administration**

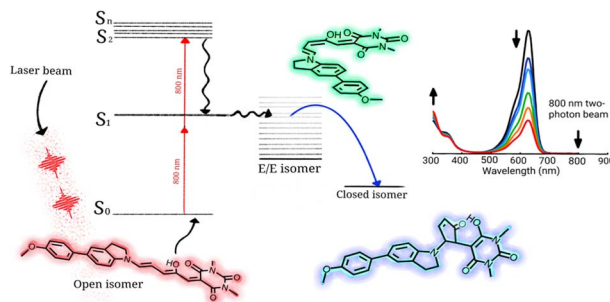
Sneha Kumari,\* Thomas S. Howlett, Ryanne N. Ehrman, Shailendra Koirala, Orikeda Trashi, Ikeda Trashi, Yalini H. Wijesundara and Jeremiah J. Gassensmith\*



5783

### **Two-photon isomerization properties of donor–acceptor Stenhouse adducts**

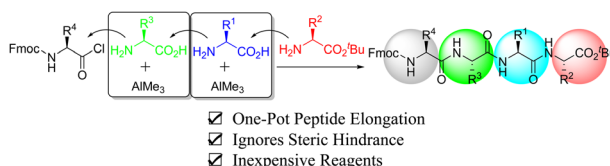
Francisco A. Reza-González, Emmanuel Villatoro, Mariana M. Reza, Jesús Jara-Cortés, Héctor García-Ortega, Edgard F. Blanco-Acuña, José G. López-Cortés, Nuria Esturau-Escofet, Alan Aguirre-Soto and Jorge Peon\*



5795

### **Trimethylaluminum-mediated one-pot peptide elongation**

Tomohiro Hattori\* and Hisashi Yamamoto\*



5802

### **Quantum chain amplification in nanocrystalline Dewar benzenes by intramolecular sensitization**

Edris Rivera, Indrajit Paul, Javier Fajardo, Jr and Miguel A. Garcia-Garibay\*

