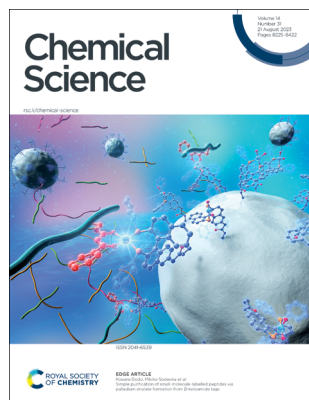


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(31) 8225–8422 (2023)



**Cover**  
See Kosuke Dodo, Mikiko Sodeoka *et al.*, pp. 8249–8254.  
Image reproduced by permission of Kosuke Dodo and Mikiko Sodeoka from *Chem. Sci.*, 2023, 14, 8249.



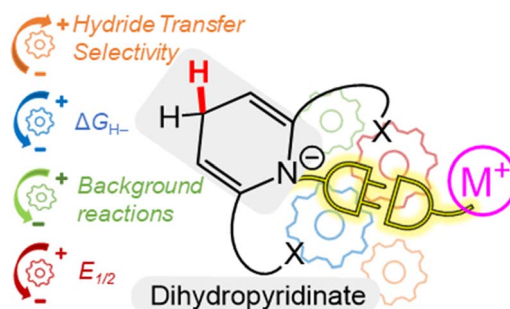
**Inside cover**  
See Bina Fu, Xueming Yang, Kaijun Yuan *et al.*, pp. 8255–8261.  
Image reproduced by permission of Kaijun Yuan from *Chem. Sci.*, 2023, 14, 8255.

## PERSPECTIVE

8234

### Metallated dihydropyridinates: prospects in hydride transfer and (electro)catalysis

Leo W. T. Parsons and Louise A. Berben\*

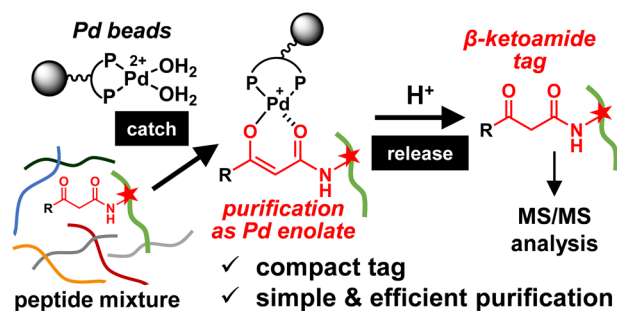


## EDGE ARTICLES

8249

### Simple purification of small-molecule-labelled peptides *via* palladium enolate formation from $\beta$ -ketoamide tags

Kenji Hayamizu, Kota Koike, Kosuke Dodo,\*  
Miwako Asanuma, Hiromichi Egami and Mikiko Sodeoka\*



## Editorial Staff

### Executive Editor

May Copsy

### 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 Copsy, 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

François Gabbai, Texas A&M University  
Subi George, JNCASR  
Ryan Gilmour, WWU Münster  
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  
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 Plumeré, 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 Sumriner, University of Florida  
Raghavan B. Sunoj, IIT Bombay  
Yogesh Surendranath, MIT  
Mizuki Tada, Nagoya University  
Ben Zhong Tang, The Chinese University of Hong Kong  
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.

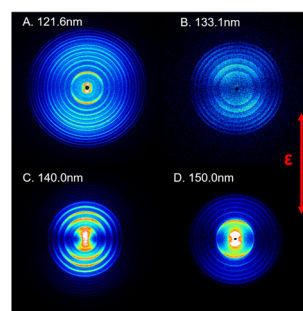
Registered charity number: 207890



8255

### Vacuum ultraviolet photodissociation of sulfur dioxide and its implications for oxygen production in the early Earth's atmosphere

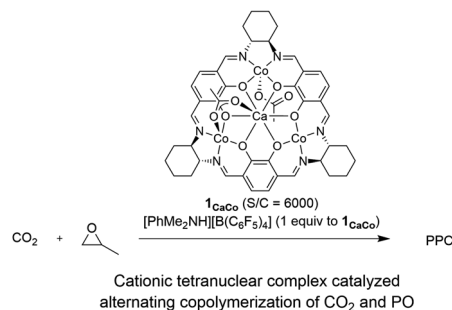
Yao Chang, Yanlin Fu, Zhichao Chen, Zijie Luo, Yaru Zhao, Zhenxing Li, Weiqing Zhang, Guorong Wu, Bina Fu,\* Dong H. Zhang, Michael N. R. Ashfold, Xueming Yang\* and Kaijun Yuan\*



8262

### Cationic tetranuclear macrocyclic $\text{CaCO}_3$ complexes as highly active catalysts for alternating copolymerization of propylene oxide and carbon dioxide

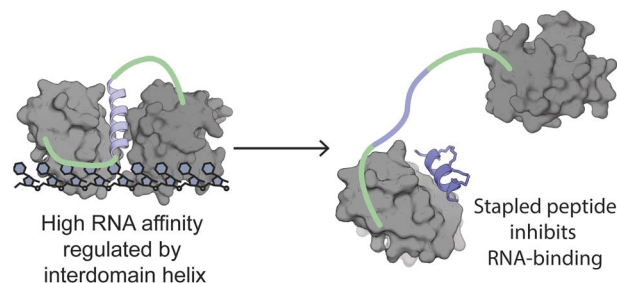
Haruki Nagae, Saki Matsushiro, Jun Okuda\* and Kazushi Mashima\*



8269

### Rationally designed stapled peptides allosterically inhibit PTBP1–RNA-binding

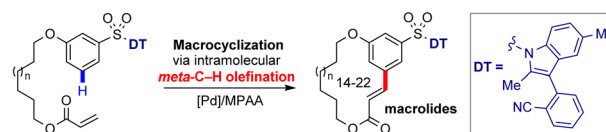
Stefan Schmeing, Gulshan Amrahova, Katrin Bigler, Jen-Yao Chang, Joseph Openy, Sunit Pal, Laura Posada, Raphael Gasper and Peter 't Hart\*



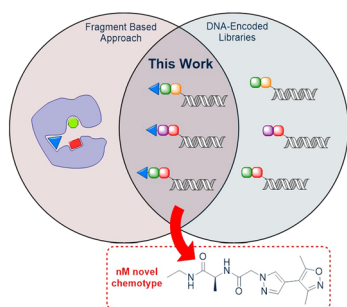
8279

### Macrocyclization via remote *meta*-selective C–H olefination using a practical indolyl template

Pengfei Zhang, Zhiwei Jiang, Zhoulong Fan, Guoshuai Li, Qingxue Ma, Jun Huang, Jinghong Tang, Xiaohua Xu,\* Jin-Quan Yu\* and Zhong Jin\*



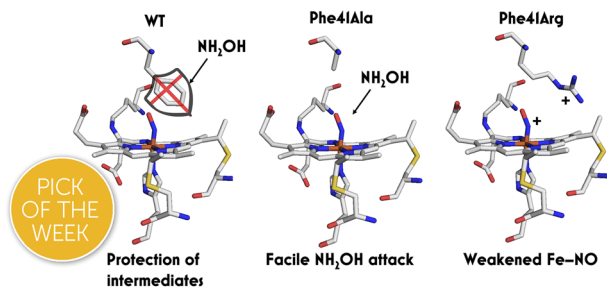
8288



### Fragment expansion with NUDELs – poised DNA-encoded libraries

Catherine L. A. Salvini, Benoit Darlot, Jack Davison, Mathew P. Martin, Susan J. Tudhope, Shannon Turberville, Akane Kawamura, Martin E. M. Noble, Stephen R. Wedge, James J. Crawford and Michael J. Waring\*

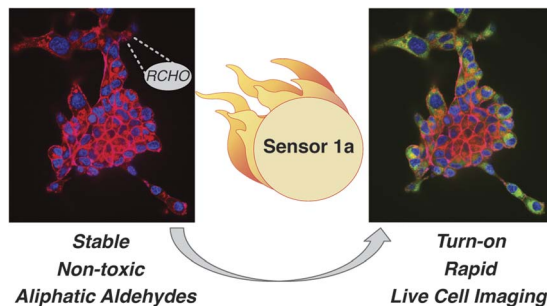
8295



### Outer coordination sphere influences on cofactor maturation and substrate oxidation by cytochrome P460

Melissa M. Bollmeyer, Sean H. Majer, Rachael E. Coleman and Kyle M. Lancaster\*

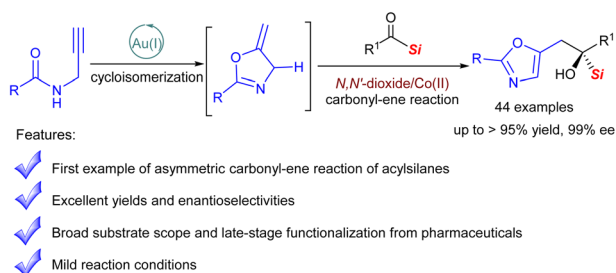
8305



### Chemical sensors for imaging total cellular aliphatic aldehydes in live cells

Rachel Wills, Jonathan Farhi, Patrick Czabala, Sophia Shahin, Jennifer M. Spangle and Monika Raj\*

8315



### Bimetallic tandem catalysis-enabled enantioselective cycloisomerization/carbonyl-ene reaction for construction of 5-oxazoylmethyl $\alpha$ -silyl alcohol

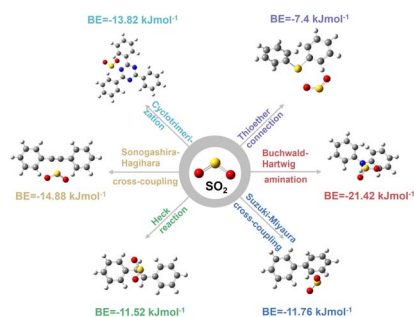
Xinpeng Sang, Yuhao Mo, Shiya Li, Xiaohua Liu, Weidi Cao\* and Xiaoming Feng\*



8321

### Feasible bottom-up development of conjugated microporous polymers (CMPs) for boosting the deep removal of sulfur dioxide

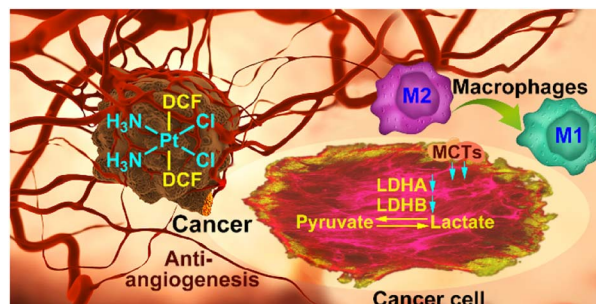
He Li, Hanqian Pan, Yijian Li, Shuaishuai Shang, Shihui Huang, Xili Cui,\* Jun Hu\* and Honglai Liu



8327

### Regulating tumor glycometabolism and the immune microenvironment by inhibiting lactate dehydrogenase with platinum(IV) complexes

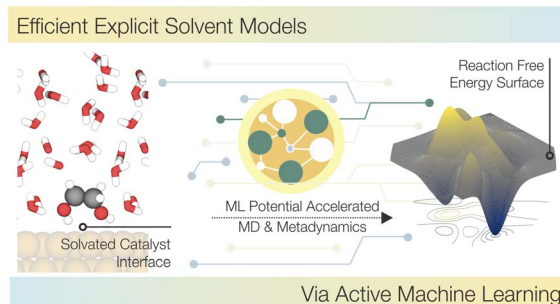
Suxing Jin, Enmao Yin, Chenyao Feng, Yuewen Sun, Tao Yang, Hao Yuan, Zijian Guo and Xiaoyong Wang\*



8338

### Accelerating explicit solvent models of heterogeneous catalysts with machine learning interatomic potentials

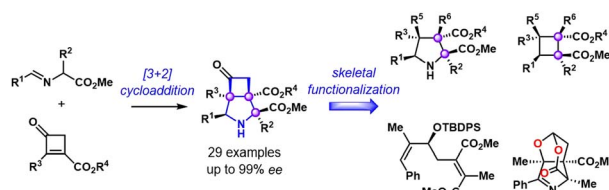
Benjamin W. J. Chen,\* Xinglong Zhang\* and Jia Zhang



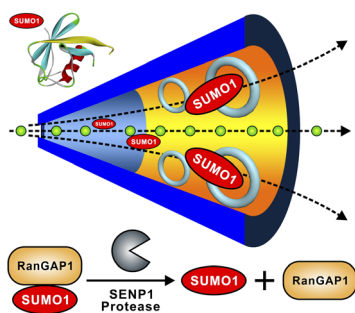
8355

### Enantioselective [3+2]-cycloaddition of 2,3-disubstituted cyclobutenones: vicinal quaternary stereocenters construction and skeletal functionalization

Licheng Lu and Ping Lu\*



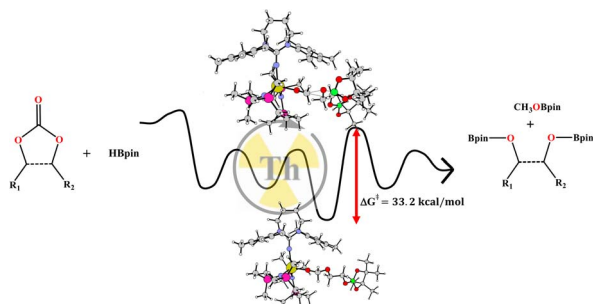
8360



### A highly sensitive nanochannel device for the detection of SUMO1 peptides

Yue Qin, Xiaoyu Zhang, Yanling Song, Bowen Zhong, Lu Liu, Dongdong Wang, Yahui Zhang, Wenqi Lu, Xinjia Zhao, Zhiqi Jia, Minmin Li, Lihua Zhang\* and Guangyan Qing\*

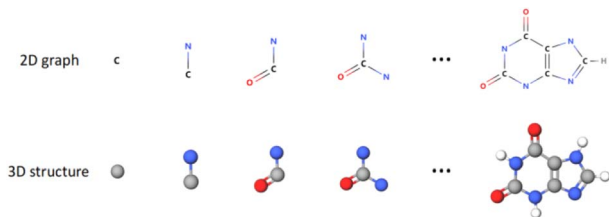
8369



### Catalytic regeneration of metal-hydrides from their corresponding metal-alkoxides via the hydroboration of carbonates to obtain methanol and diols

Hemanta Deka, Ida Ritacco, Natalia Fridman, Lucia Caporaso\* and Moris S. Eisen\*

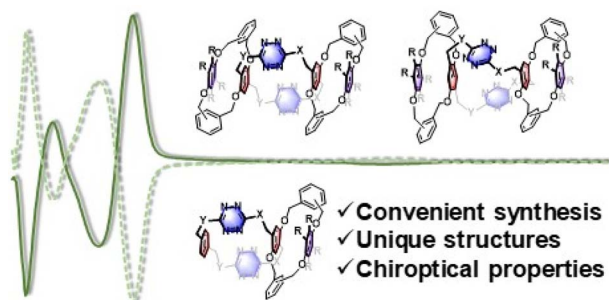
8380



### An equivariant generative framework for molecular graph-structure Co-design

Zaixi Zhang, Qi Liu,\* Chee-Kong Lee, Chang-Yu Hsieh and Enhong Chen

8393



### Tetrahomo corona[4]arene-based spirophanes: synthesis, structure, and properties

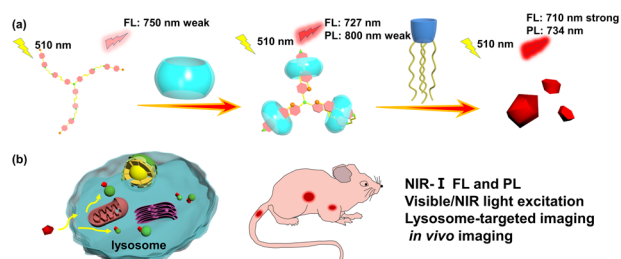
Shen-Yi Guo, Zhuo-Ang Zhang, Shuo Tong,\* Qing-Hui Guo, Ruimao Hua and Mei-Xiang Wang\*



8401

### Conformationally confined three-armed supramolecular folding for boosting near-infrared biological imaging

Hui-Juan Wang, Meng-Meng Zheng, Wen-Wen Xing, Yong-Xue Li, Yao-Yao Wang, Hongjie Zhu, Ying-Ming Zhang,\* Qilin Yu\* and Yu Liu\*



8408

### The H-NOX protein structure adapts to different mechanisms in sensors interacting with nitric oxide

Byung-Kuk Yoo, Sergei G. Kruglik, Jean-Christophe Lambry, Isabelle Lamarre, C. S. Raman, Pierre Nioche and Michel Negrerie\*

