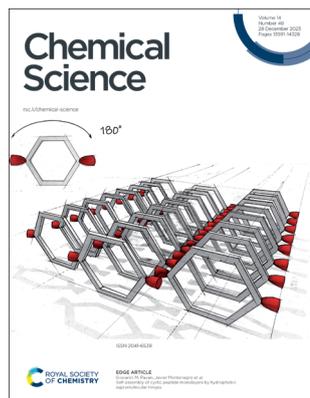


IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(48) 13991–14328 (2023)



Cover
See Giovanni M. Pavan, Javier Montenegro *et al.*, pp. 14074–14081. Image reproduced by permission of Beatriz Perez and Javier Montenegro from *Chem. Sci.*, 2023, 14, 14074.



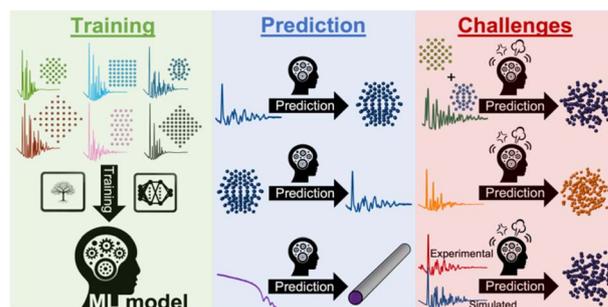
Inside cover
See Andrew Kellett, José Martínez-Costas, Miguel Vázquez López *et al.*, pp. 14082–14091. Image reproduced by permission of M. Eugenio Vázquez from *Chem. Sci.*, 2023, 14, 14082.

PERSPECTIVES

14003

Machine learning for analysis of experimental scattering and spectroscopy data in materials chemistry

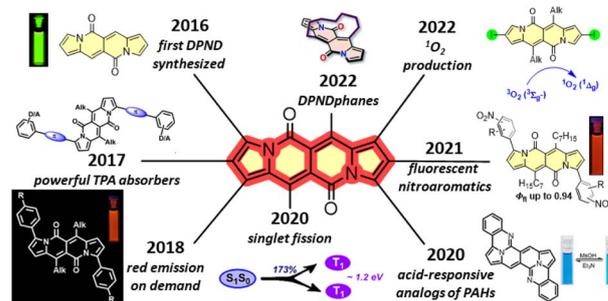
Andy S. Anker, Keith T. Butler, Raghavendra Selvan and Kirsten M. Ø. Jensen*



14020

Dipyrrolonaphthyridinedione – (still) a mysterious cross-conjugated chromophore

Bartłomiej Sadowski* and Daniel T. Gryko*



Chemical Science

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

D. Adams, University of Glasgow
A. Ajayaghosh, NIIST
R. Amaro, UC San Diego
A. Anastasaki, ETH Zürich
U.-P. Apfel, Ruhr-University Bochum
K. Asmis, Leipzig University
X. Bao, DICP-CAS
Z. Bao, Stanford University
D. N. Beratan, Duke University
G. Bernardes, University of Cambridge
F. Biedermann, KIT
D. Blackmond, Scripps Research Institute
E. Blasco, Heidelberg University
J. Bode, ETH Zurich
J. S. Brodbelt, UT Austin
C. Chang, UC Berkeley
C.-M. Che, University of Hong Kong
J. Chen, Nankai University
M. Cohen, OHSU
C. Coley, MIT
J. Cornella, MPIC
L. Cronin, University of Glasgow
J. Crowley, University of Otago
C. C. Cummins, MIT
V. Däschlein-Gessner, Ruhr University Bochum
M. Delbianco, MPICI
J. Dempsey, UNC Chapel Hill
W. Dichtel, Northwestern University
K. Domen, University of Tokyo
H. Duan, Tsinghua University
X. Feng, TU Dresden
B. Feringa, University of Groningen
J. Figueroa, UC San Diego
N. Frank, University of Nevada
M. Freitag, Newcastle University
S. Gao, Peking University
J. Gassensmith, UT Dallas
G. Gasser, PSL University
E. Gibson, Newcastle University
R. Gilliard, Jr., MIT
F. Glorius, WWU Münster
L. González, University of Vienna
D. Graham, University of Strathclyde
V. Grassian, UC San Diego
A. Grimaud, Collège de France/CNRS
T. Gulder, Leipzig University
W. Gutekunst, Georgia Tech
C. Hackenberger, FMP Berlin
I. Hamachi, Kyoto University
G. Han, Brandeis University
B. Han, CAS

M. Hariharan, IISER-TVM
C. Haynes, University of Minnesota
J. Heemstra, WUSTL
T. Heine, DTU
P. Holland, Yale University
K. E. Jelfs, Imperial College London
X. Jiang, Aramco
Y. Jung, SNU
S. Kath-Schorr, University of Cologne
T. Kato, University of Tokyo
C. Kelly, Janseen Research/J&J
R. Klausen, Johns Hopkins University
Y. Krishnan, University of Chicago
M. Kuimova, Imperial College London
K. Lancaster, Cornell University
A.-L. Lee, Heriot-Watt University
D. Leonori, University of Manchester
X. Li, University of Washington
Y. Li, Jilin University
M. H. Lim, KAIST
J. Lloret-Fillol, ICIQ
B. Lotsch, Max Planck Institute
X. W. Lou, NTU
K. Maeda, Tokyo Tech
S. Maeda, Hokkaido University
D. Maiti, IIT Bombay
L. Malins, ANU
S. Mandal, IISER Kolkata
T. Martinez, Stanford University
C. Martínez-Huitle, UFRN
E. Matson, Rochester University
J. L. Medina-Franco, UNAM
V. Moliner, INAM, Jaume I University
W. Nam, Ewha Womans University
T. Noël, University of Amsterdam
A. Obermeyer, Columbia University
M. Oestreich, TU Berlin
D. O'Hagan, University of St Andrews
T. Ooi, Nagoya University
R. O'Reilly, University of Birmingham
S. Ott, Uppsala University
H. Ottosson, Uppsala University
Z. Ouyang, Tsinghua University
X. Pan, DICP-CAS
S. Patil, SSCU-IISC
E. Pentzer, Texas A&M University
S. Peter, JNCASR
W. Piers, University of Calgary
N. Plumeré, Ruhr-University Bochum
S. Qiao, University of Adelaide
V. Rai, IISER Bhopal

S. Rasmussen, North Dakota State University
J. Read de Alaniz, UC Santa Barbara
E. Reisner, University of Cambridge
A. Rentmeister, WWU Münster
J. Rinehart, UC San Diego
A. Roitberg, University of Florida
H. Sardon, UPV-EHU
R. Sarpong, UC Berkeley
G. Schultz, Northwestern University
D. Schult, Merck
D. Seferos, University of Toronto
R. Sessoli, University of Florence
H. Shafaat, UCLA
T. Snaddon, Indiana University
M. Solà, University of Girona
G. Soler-Illia, UNSAM
D. Spring, University of Cambridge
B. Sumerlin, University of Florida
R. B. Sunoj, IIT Bombay
Y. Surendranath, MIT
M. Tada, Nagoya University
T. Tahara, RIKEN
Z. Tang, NCSNT
S. Teichert, DESY
C. Thomas, Ohio State University
H. Tian, ECUST
Z.-Q. Tian, Xiamen University
A. Tkatchenko, University of Luxembourg
H. Tran, University of Toronto
T. Uemura, University of Tokyo
C. Vanderwal, UC Irvine
L. Venkataraman, Columbia University
G. Vilé, Politecnico di Milano
A. Wakamiya, Kyoto University
L.-S. Wang, Brown University
C. Wang, Peking University
E. Weerapana, Boston College
J. Weinstein, University of Sheffield
T. Welton, Imperial College London
A. Wendlandt, MIT
C. Williams, University of Oxford
V. Yam, University of Hong Kong
N. Yanai, Kyushu University
S. Q. Yao, National University of Singapore
A. Zarkin, UFPR
L. Zhang, ECNU
T. Zhang, TIPC-CAS
J. Zhang, University of Cambridge
Z.-J. Zhao, Tianjin University
B. Zhong Tang, CUHK-Shenzhen
Q.-L. Zhou, Nankai University

Editorial Staff

Executive Editor

May Copsy

Deputy Editor

Samantha Apps

Senior Editor

James Moore

Scientific Editors

Ellis Crawford, 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

For pre-submission queries please contact May Copsy, Executive Editor. E-mail 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 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

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

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

Authors may reproduce/publish 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

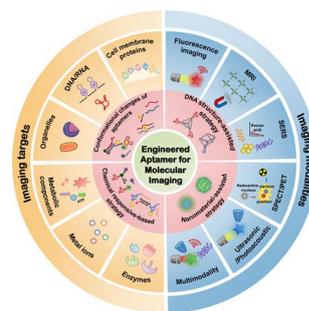


REVIEWS

14039

Engineered aptamers for molecular imaging

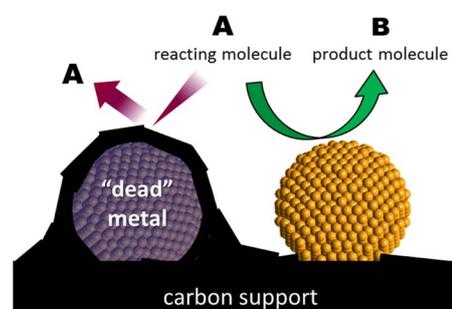
Bingqian Lin,* Feng Xiao, Jinting Jiang, Zhengjia Zhao and Xiang Zhou



14062

The phenomenon of “dead” metal in heterogeneous catalysis: opportunities for increasing the efficiency of carbon-supported metal catalysts

Roman M. Mironenko, Dmitry B. Eremin and Valentine P. Ananikov*

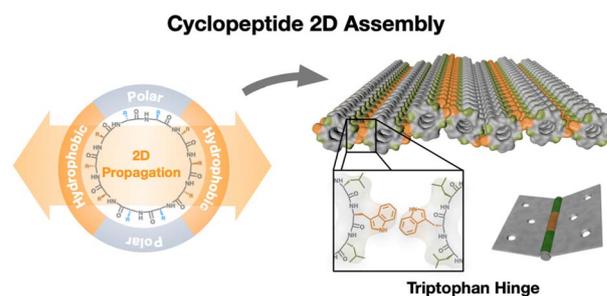


EDGE ARTICLES

14074

Self-assembly of cyclic peptide monolayers by hydrophobic supramolecular hinges

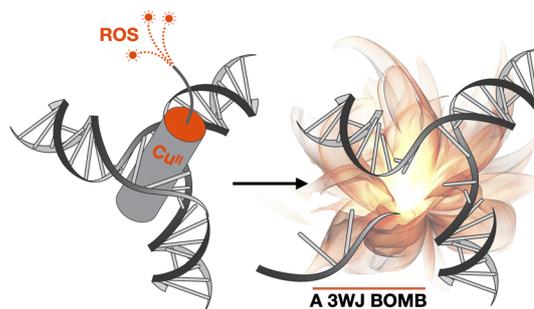
Ignacio Insua, Annalisa Cardellini, Sandra Díaz, Julian Bergueiro, Riccardo Capelli, Giovanni M. Pavan* and Javier Montenegro*



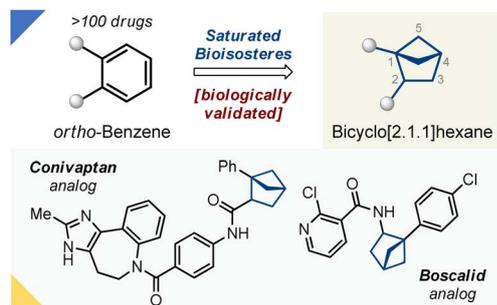
14082

A copper(II) peptide helicate selectively cleaves DNA replication foci in mammalian cells

Ana Alcalde-Ordóñez, Natalia Barreiro-Piñeiro, Brionna McGormann, Jacobo Gómez-González, David Bouzada, Francisco Rivadulla, M. Eugenio Vázquez, Andrew Kellett,* José Martínez-Costas* and Miguel Vázquez López*



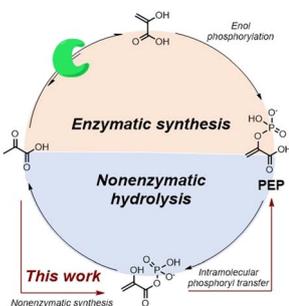
14092



1,2-Disubstituted bicyclo[2.1.1]hexanes as saturated bioisosteres of *ortho*-substituted benzene

Aleksandr Denisenko, Pavel Garbuz, Yelyzaveta Makovetska, Oleh Shablykin, Dmytro Lesyk, Galeb Al-Maali, Rodion Korzh, Iryna V. Sadkova and Pavel K. Mykhailiuk*

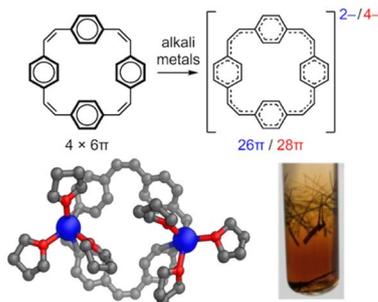
14100



A single phosphorylation mechanism in early metabolism – the case of phosphoenolpyruvate

Joris Zimmermann, Robert J. Mayer and Joseph Moran*

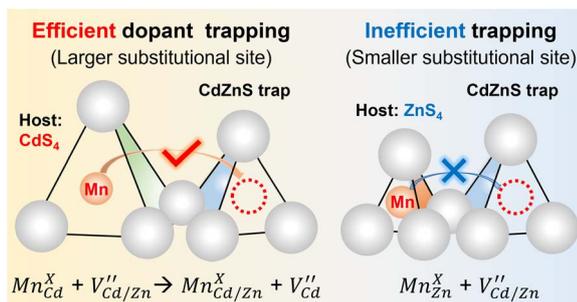
14109



Crystallographic evidence for global aromaticity in the di-anion and tetra-anion of a cyclophane hydrocarbon

Wojciech Stawski, Yikun Zhu, Zheng Wei, Marina A. Petrukhina* and Harry L. Anderson*

14115



Inserting an "atomic trap" for directional dopant migration in core/multi-shell quantum dots

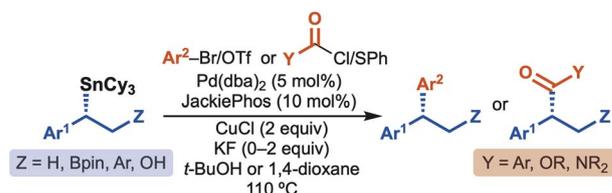
Chun Chu, Elan Hofman, Chengpeng Gao, Shuya Li, Hanjie Lin, Walker MacSwain, John M. Franck, Robert W. Meulenber, Arindam Chakraborty and Weiwei Zheng*



14124

A general approach to stereospecific Pd-catalyzed cross-coupling reactions of benzylic stereocenters

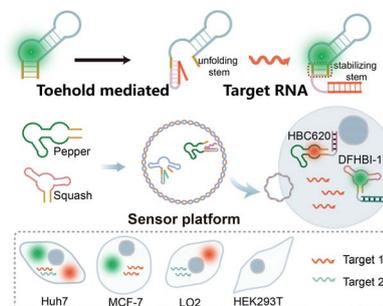
Meruyert Binayeva, Xinghua Ma,
Pejman Ghaemimohammadi and Mark R. Biscoe*



14131

A universal orthogonal imaging platform for living-cell RNA detection using fluorogenic RNA aptamers

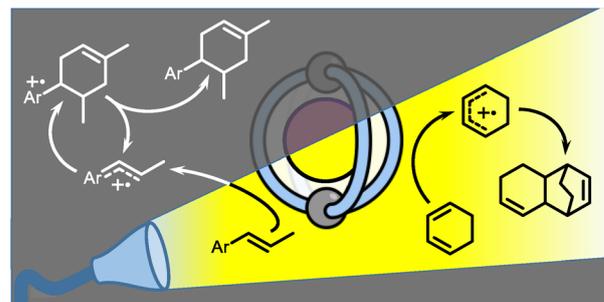
Peng Yin, Mingmin Ge, Shiyi Xie, Li Zhang, Shi Kuang*
and Zhou Nie*



14140

Exo-cage catalysis and initiation derived from photo-activating host-guest encapsulation

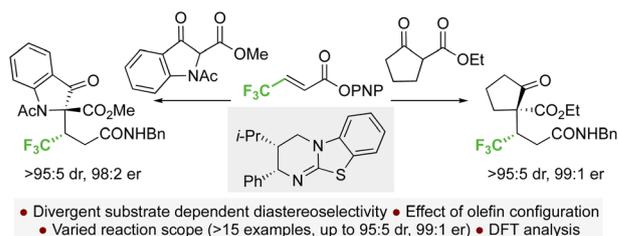
Rebecca L. Spicer, Helen M. O'Connor, Yael Ben-Tal,
Hang Zhou, Patrick J. Boaler, Fraser C. Milne, Euan
K. Brechin,* Guy. C. Lloyd-Jones* and Paul J. Lusby*



14146

Understanding divergent substrate stereoselectivity in the isothiurea-catalysed conjugate addition of cyclic α -substituted β -ketoesters to α,β -unsaturated aryl esters

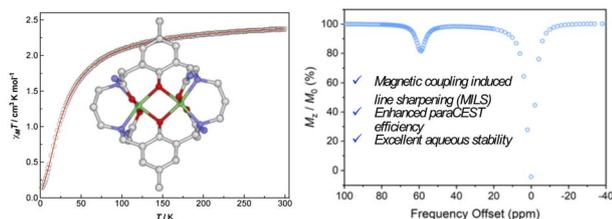
Ding Yuan, Alister S. Goodfellow, Kevin Kasten,
Zhuan Duan, Tengfei Kang, David B. Cordes, Aidan
P. McKay, Michael Bühl,* Gregory R. Boyce* and Andrew
D. Smith*



- Divergent substrate dependent diastereoselectivity
- Effect of olefin configuration
- Varied reaction scope (>15 examples, up to 95:5 dr, 99:1 er)
- DFT analysis



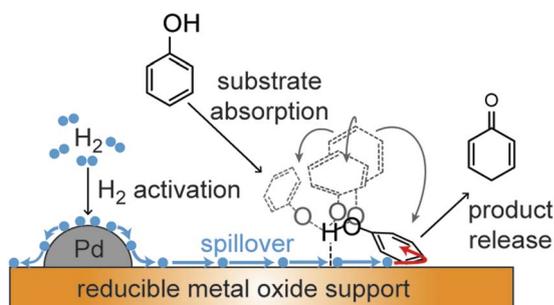
14157



Improving the potential of paraCEST through magnetic-coupling induced line sharpening

Xin Guo, Lei Zhang, Jiesheng Hu, Balázs Szilágyi, Meng Yu,* Shizhen Chen,* Gyula Tircsó, Xin Zhou and Jun Tao*

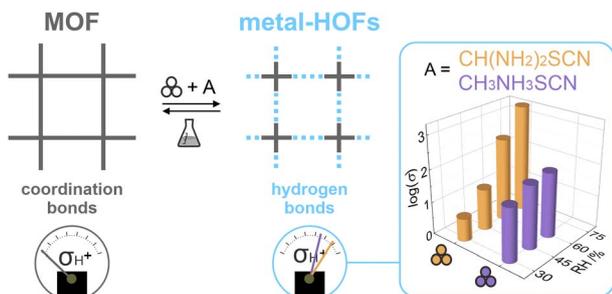
14166



Hydrogen spillover and substrate–support hydrogen bonding mediate hydrogenation of phenol catalyzed by palladium on reducible metal oxides

Yeongseo An, Puranjan Chatterjee, Pranjali Naik, Sayak Banerjee, Wenyu Huang, Igor I. Slowing and Vincenzo Venditti*

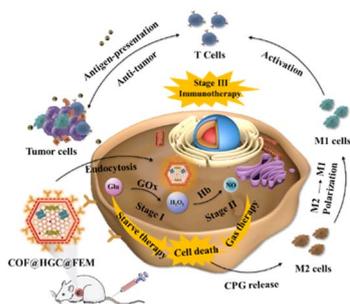
14176



From non-conductive MOF to proton-conducting metal-HOFs: a new class of reversible transformations induced by solvent-free mechanochemistry

Magdalena Lupa-Myszkowska, Marcin Oszajka and Dariusz Matoga*

14182



An erythrocyte membrane-camouflaged fluorescent covalent organic framework for starving/nitric oxide/immunotherapy of triple-negative breast cancer

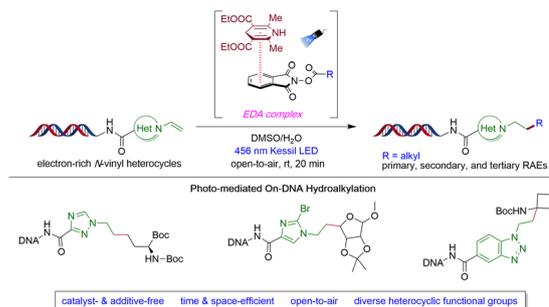
Fang Yuan, Cuiling Zhang,* Xianzhu Luo, Shasha Cheng, Yingxin Zhu and Yuezhong Xian*



14193

On-DNA hydroalkylation of *N*-vinyl heterocycles via photoinduced EDA-complex activation

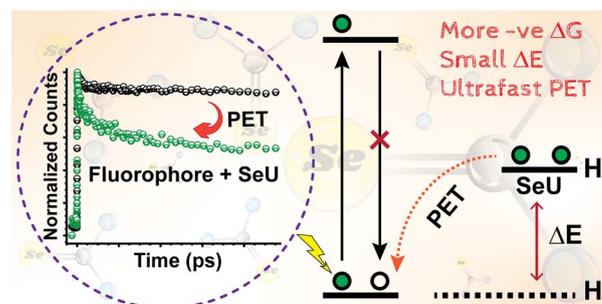
Mohammed Sharique, Bianca Matsuo, Albert Granados, Saegun Kim, Mahwish Arshad, Hyunjung Oh, Victoria E. Wu, Minxue Huang, Adam Csakai, Lisa A. Marcaurelle and Gary A. Molander*



14200

Critical assessment of selenourea as an efficient small molecule fluorescence quenching probe to monitor protein dynamics

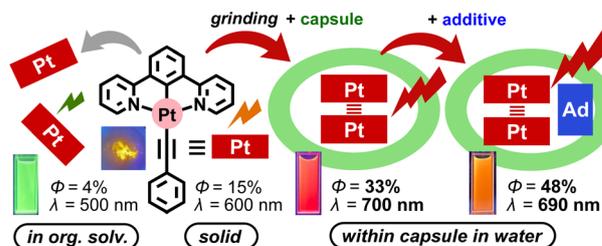
Subhrakant Jena, Kiran Devi Tulsian, Rudhi Ranjan Sahoo, Saiprakash Rout, Akshay Kumar Sahu and Himansu S. Biswal*



14211

Solution-state mechanochromic luminescence of Pt(II)-complexes displayed within micellar aromatic capsules

Yoshihisa Hashimoto, Yuri Katagiri, Yuya Tanaka* and Michito Yoshizawa*

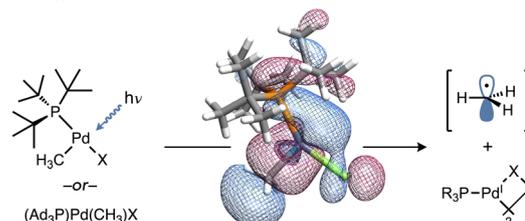


14217

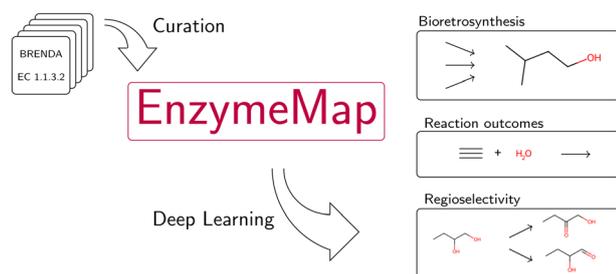
Visible light-induced palladium–carbon bond weakening in catalytically relevant T-shaped complexes

Peter M. Waddell, Lei Tian, Anthony R. Scavuzzo, Lalu Venigalla, Gregory D. Scholes and Brad P. Carrow*

low energy d-σ* transition · redirects ubiquitous Pd(II) into SET pathways



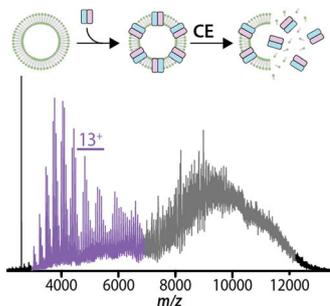
14229



EnzymeMap: curation, validation and data-driven prediction of enzymatic reactions

Esther Heid,^{*} Daniel Probst, William H. Green and Georg K. H. Madsen

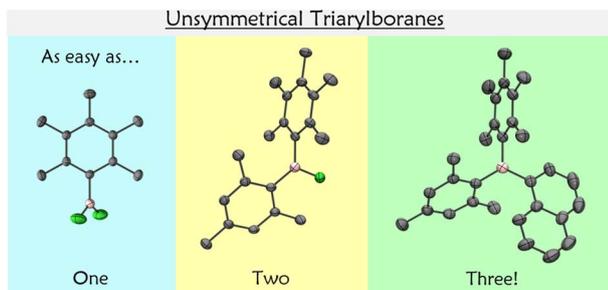
14243



Native mass spectrometry of proteoliposomes containing integral and peripheral membrane proteins

Yun Zhu, Sangho D. Yun, Tianqi Zhang, Jing-Yuan Chang, Lauren Stover and Arthur Laganowsky^{*}

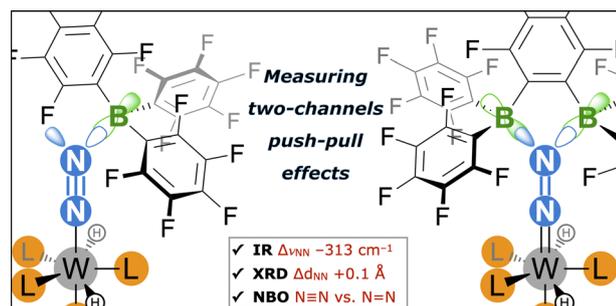
14256



Rapid, iterative syntheses of unsymmetrical di- and triarylboranes from crystalline aryl difluoroboranes

Douglas Turnbull and Marc-André Légaré^{*}

14262



An orbitally adapted push-pull template for N_2 activation and reduction to diazene-diide

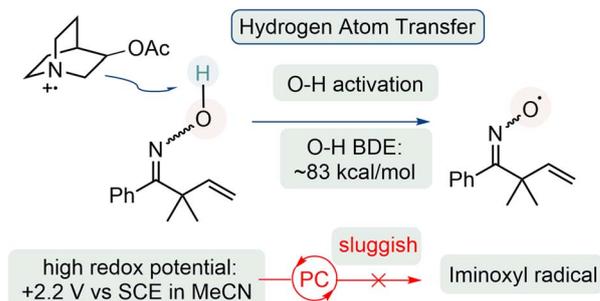
David Specklin, Marie-Christine Boegli, Anaïs Coffinet, Léon Escomel, Laure Vendier, Mary Grellier and Antoine Simonneau^{*}



14271

O–H bond activation of β,γ -unsaturated oximes via hydrogen atom transfer (HAT) and photoredox dual catalysis

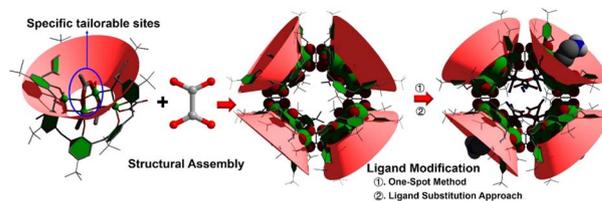
Liang Yi, Chen Zhu, Xiangyu Chen, Huifeng Yue, Tengfei Ji, Yiqiao Ma, Yuanyuan Cao, Rajesh Kancharla and Magnus Rueping*



14280

Atomically accurate site-specific ligand tailoring of highly acid- and alkali-resistant Ti(IV)-based metallamacrocycle for enhanced CO₂ photoreduction

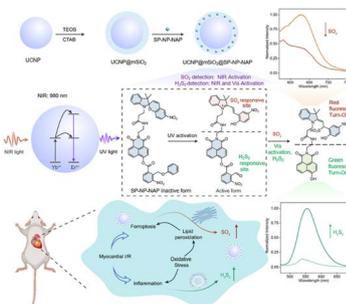
Yi-Qi Tian, Lin-Fang Dai, Wen-Lei Mu, Wei-Dong Yu, Jun Yan* and Chao Liu*



14290

A near-infrared light-activated nanoprobe for simultaneous detection of hydrogen polysulfide and sulfur dioxide in myocardial ischemia–reperfusion injury

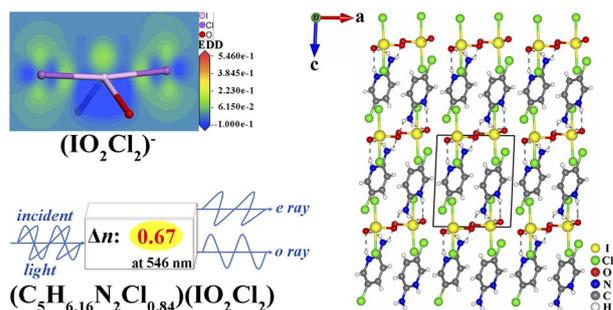
Xianzhu Luo, Cuiling Zhang,* Chenyang Yue, Yuelin Jiang, Fei Yang and Yuezhong Xian*



14302

(C₅H_{6.16}N₂Cl_{0.84})(IO₂Cl₂): a birefringent crystal featuring unprecedented (IO₂Cl₂)⁻ anions and π -conjugated organic cations

Qian-Qian Chen, Chun-Li Hu, Ming-Zhi Zhang and Jiang-Gao Mao*



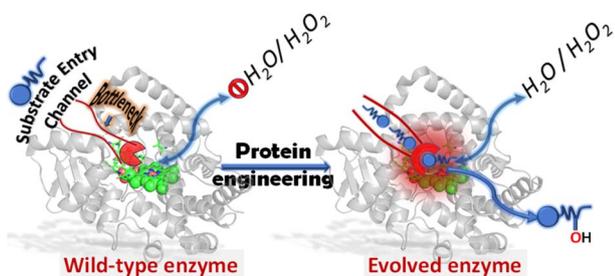
14308



Optimizing copper nanoparticles with a carbon shell for enhanced electrochemical CO₂ reduction to ethanol

Ting Yao, Wei Xia,* Shitao Han, Shuaiqiang Jia, Xue Dong, Min Wang, Jiapeng Jiao, Dawei Zhou, Jiahao Yang, Xueqing Xing, Chunjun Chen, Mingyuan He, Haihong Wu* and Buxing Han*

14316



Computationally guided bioengineering of the active site, substrate access pathway, and water channels of thermostable cytochrome P450, CYP175A1, for catalyzing the alkane hydroxylation reaction

Mohd Taher,* Kshatresh Dutta Dubey* and Shyamalava Mazumdar*

