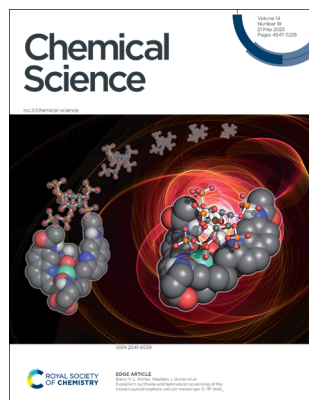
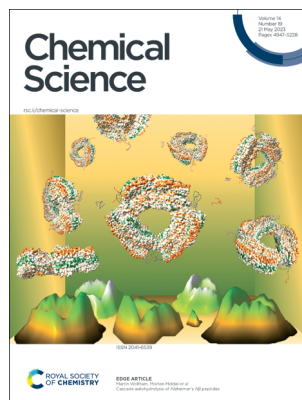


IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(19) 4947–5228 (2023)



Cover
See Barry V. L. Potter, Stephen J. Butler *et al.*, pp. 4979–4985. Image reproduced by permission of Stephen Butler and Felix Plasser from *Chem. Sci.*, 2023, 14, 4979.



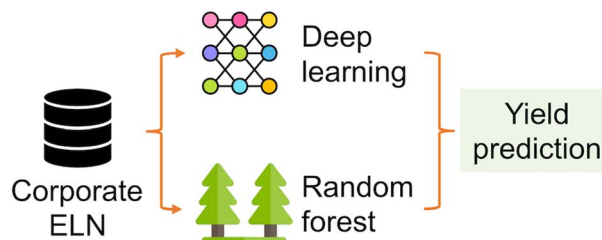
Inside cover
See Martin Wolfram, Morten Meldal *et al.*, pp. 4986–4996. Image reproduced by permission of Morten Meldal from *Chem. Sci.*, 2023, 14, 4986.

COMMENTARY

4958

A focus on the use of real-world datasets for yield prediction

Latimah Bustillo and Tiago Rodrigues*

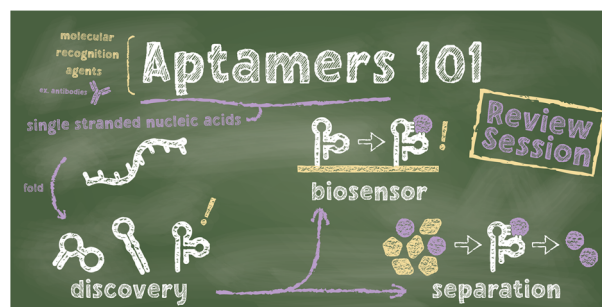


REVIEW

4961

Aptamers 101: aptamer discovery and *in vitro* applications in biosensors and separations

Lucy F. Yang, Melissa Ling, Nataly Kacherovsky and Suzie H. Pun*



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

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

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

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
R. Graham Cooks, 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 Minciola, 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 Martín
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 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

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.

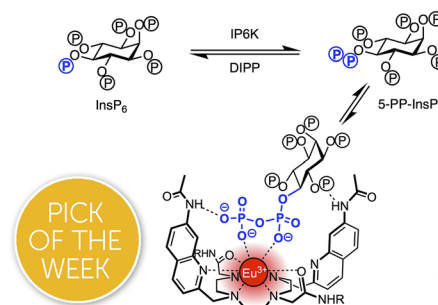
Registered charity number: 207890



4979

Expedient synthesis and luminescence sensing of the inositol pyrophosphate cellular messenger 5-PP-InsP₅

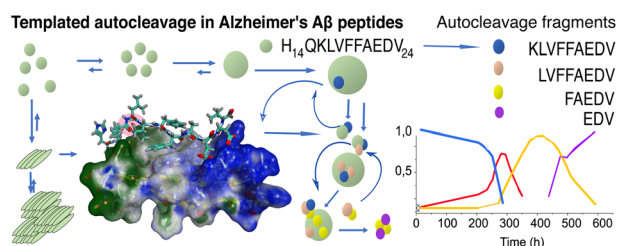
Megan L. Shipton, Fathima A. Jamion, Simon Wheeler, Andrew M. Riley, Felix Plasser, Barry V. L. Potter* and Stephen J. Butler*



4986

Cascade autohydrolysis of Alzheimer's Aβ peptides

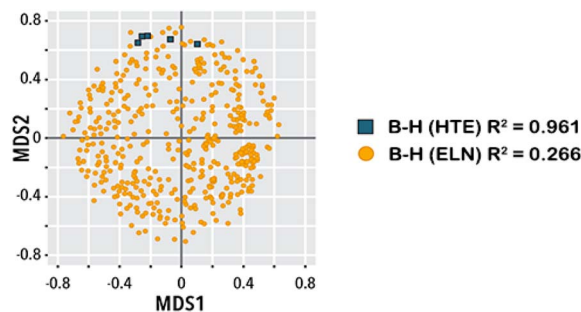
Martin Wolfram,* Manish K. Tiwari, Tue Hassenkam, Ming Li, Morten J. Bjerrum and Morten Meldal*



4997

On the use of real-world datasets for reaction yield prediction

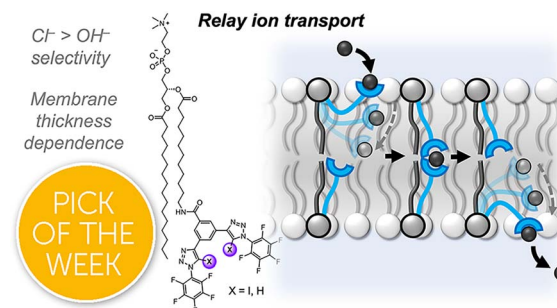
Mandana Saebi, Bozhao Nan, John E. Herr, Jessica Wahlers, Zhichun Guo, Andrzej M. Zurański, Thierry Kogej, Per-Ola Norrby, Abigail G. Doyle, Nitesh V. Chawla* and Olaf Wiest*



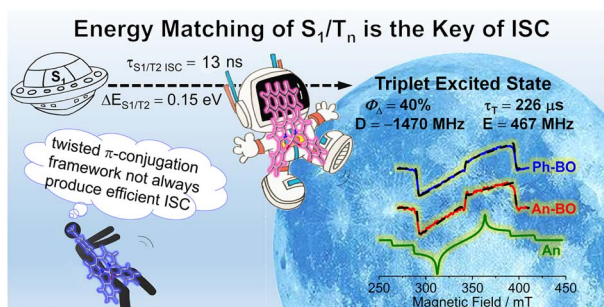
5006

Halogen bonding relay and mobile anion transporters with kinetically controlled chloride selectivity

Toby G. Johnson, Andrew Docker, Amir Sadeghi-Kelishadi and Matthew J. Langton*



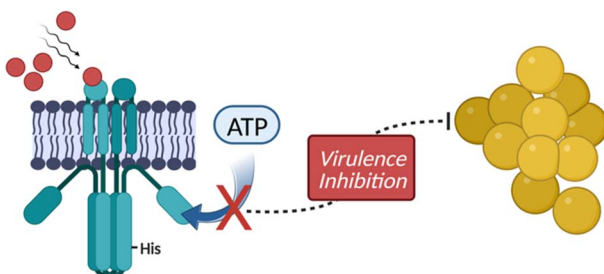
5014



Origin of intersystem crossing in highly distorted organic molecules: a case study with red light-absorbing *N,N,O,O*-boron-chelated Bodipys

Xue Zhang, Andrey A. Sukhanov, Xi Liu, Maria Taddei, Jianzhang Zhao,* Anthony Harriman,* Violeta K. Voronkova,* Yan Wan,* Bernhard Dick* and Mariangela Di Donato*

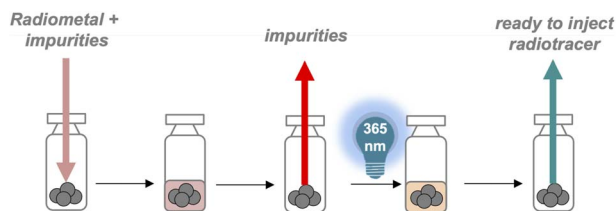
5028



Targeting multidrug resistant *Staphylococcus* infections with bacterial histidine kinase inhibitors

Adeline Espinasse, Manibarsha Goswami, Junshu Yang, Onanong Vorasin, Yinduo Ji* and Erin E. Carlson*

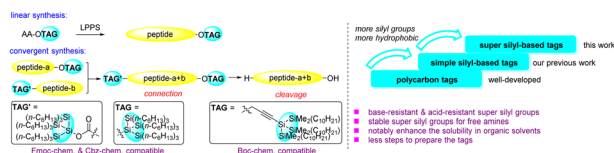
5038



Radiometallation and photo-triggered release of ready-to-inject radiopharmaceuticals from the solid phase

Dariusz Śmitowicz, Shawn Eisenberg, Shin Hye Ahn, Angus J. Koller, Philip P. Lampkin and Eszter Boros*

5051



Super silyl-based stable protecting groups for both the C- and N-terminals of peptides: applied as effective hydrophobic tags in liquid-phase peptide synthesis

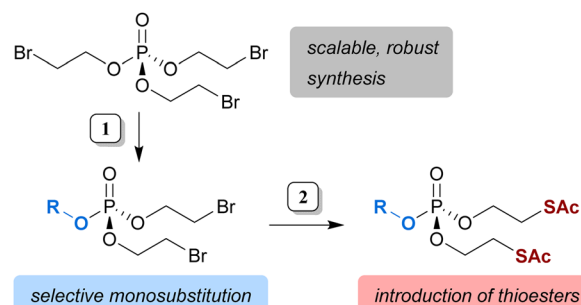
An Wu* and Hisashi Yamamoto*



5062

Synthesis of biolabile thioalkyl-protected phosphates from an easily accessible phosphotriester precursor

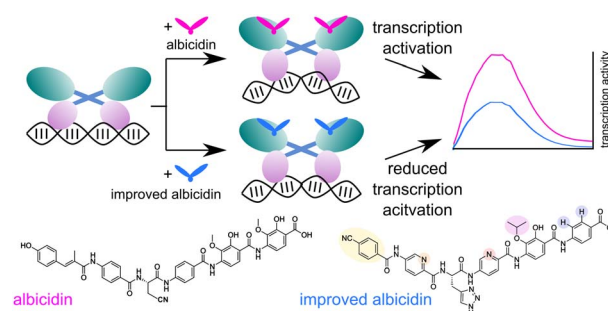
Lloyd D. Murphy, Kathryn E. Huxley, Ava Wilding, Cyane Robinson, Quentin P. O. Foucart and Lianne I. Willems*



5069

Transcription activation by the resistance protein AlbA as a tool to evaluate derivatives of the antibiotic albicidin

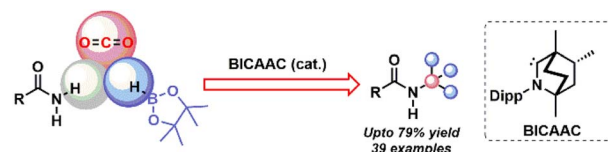
Simone Kosol, Lida Rostock, Jonas Barsig, Theresa Tabarelli, Kay Hommernick, Marcel Kulike, Tobias Eulberg, Maria Seidel, Iraj Behroz, Leonardo Kleebauer, Stefan Grätz, Andi Mainz and Roderich D. Süssmuth*



5079

Bicyclic (alkyl)(amino)carbene (BICAAC) in a dual role: activation of primary amides and CO₂ towards catalytic N-methylation

Nimisha Gautam, Ratan Logdi, Sreejyothi P., Antara Roy, Ashwani K. Tiwari* and Swadhin K. Mandal*

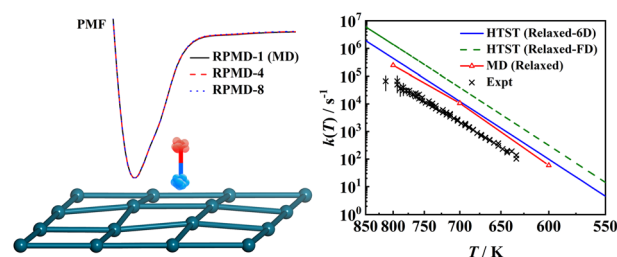


- first catalytic report
- metal-free condition
- diversification of drug and bioactive molecules
- BICAAC as dual activator
- 1 atm of CO₂
- mechanistic study (NMR, DFT)

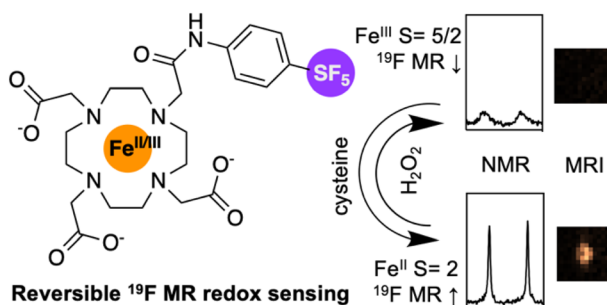
5087

First-principles surface reaction rates by ring polymer molecular dynamics and neural network potential: role of anharmonicity and lattice motion

Chen Li, Yongle Li* and Bin Jiang*



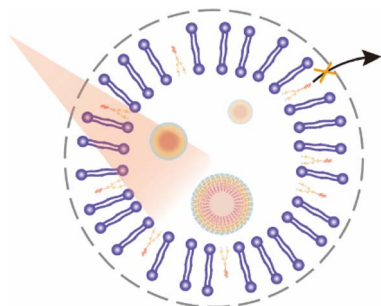
5099



An Fe complex for ^{19}F magnetic resonance-based reversible redox sensing and multicolor imaging

Rahul T. Kadakia, Raphael T. Ryan, Daniel J. Cooke and Emily L. Que*

5106

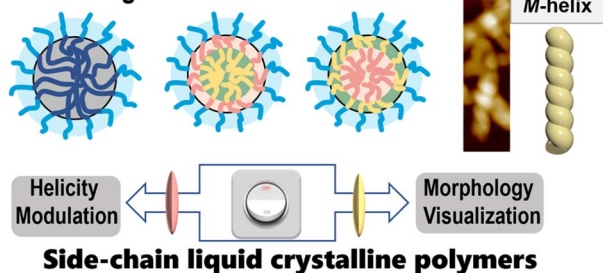


A self-assembled nanophotosensitizer targets lysosomes and induces lysosomal membrane permeabilization to enhance photodynamic therapy

Youyou Li, Wenbo Han, Deyan Gong, Taokun Luo, Yingjie Fan, Jianming Mao, Wenwu Qin and Wenbin Lin*

5116

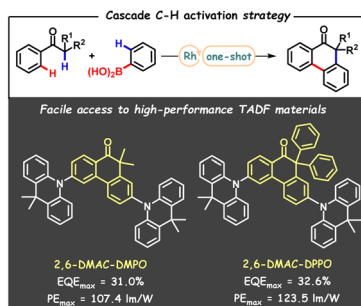
Controlling the Chiral Communication



Conformationally supramolecular chirality prevails over configurational point chirality in side-chain liquid crystalline polymers

Xiaoxiao Cheng, Yijing Gan, Gong Zhang, Qingping Song,* Zhengbiao Zhang* and Wei Zhang*

5125



Molecular engineering of locked alkyl aryl carbonyl-based thermally activated delayed fluorescence emitters via a cascade C–H activation process

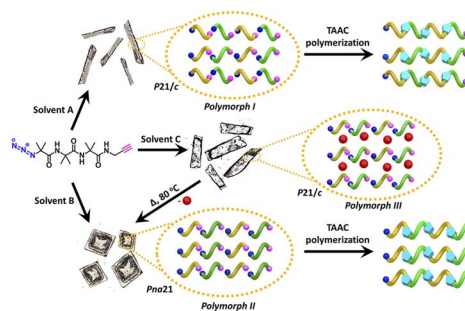
Yunxi Zhang, Zhengmei Huang, Yudong Yang, Jiahui Liu, Yang Tian, Zhengyang Bin* and Jingsong You*



5132

Rational design and topochemical synthesis of polymorphs of a polymer

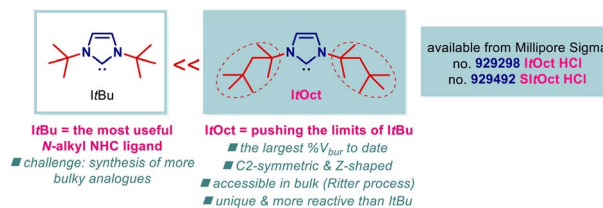
Vignesh Athiyarath, Liby Ann Mathew, Yakai Zhao, Ravichandran Khazeber, Upadrasta Ramamurty and Kana M. Sureshan*



5141

ItOct (ItOctyl) – pushing the limits of ItBu: highly hindered electron-rich N-aliphatic N-heterocyclic carbenes

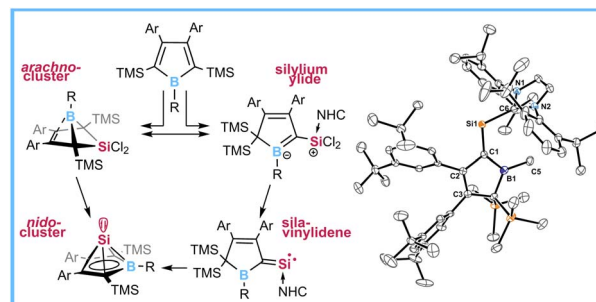
Md. Mahbubur Rahman, Guangrong Meng, Elwira Bisz, Błażej Dziuk, Roger Lalancette, Roman Szostak and Michal Szostak*



5148

A donor-supported silavinylidene and silylium ylides: boroles as a flexible platform for versatile Si(II) chemistry

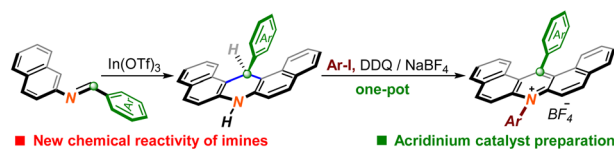
Julijan Sarcevic, Tobias Heitkemper, Paul Niklas Ruth, Leonard Naß, Maximilian Kubis, Dietmar Stalke and Christian P. Sindlinger*



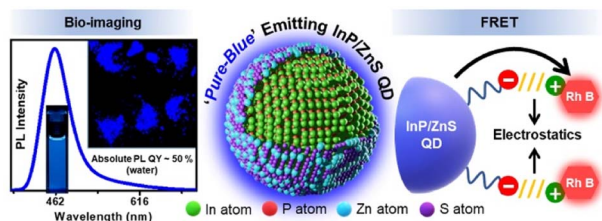
5160

In(OTf)₃-catalyzed reorganization/cycloaddition of two imine units and subsequent modular assembly of acridinium photocatalysts

Jiang Nan,* Guanjie Huang, Shilei Liu, Jing Wang, Yangmin Ma and Xinjun Luan*



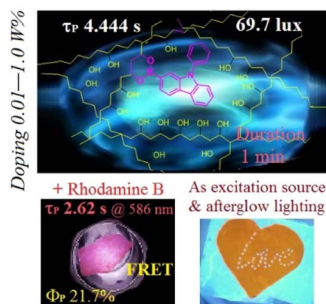
5167



Blue-emitting InP quantum dots participate in an efficient resonance energy transfer process in water

Pradyut Roy, Mishika Virmani and Pramod P. Pillai*

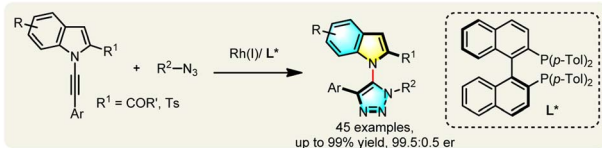
5177



Rational molecular and doping strategies to obtain organic polymers with ultralong RTP

Yuefa Zhang, Shiguo Zhang, Guanyu Liu, Qikun Sun, Shanfeng Xue* and Wenjun Yang*

5182

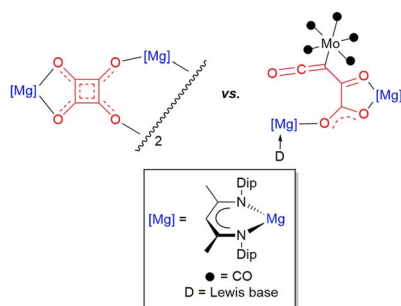


Asymmetric rhodium-catalyzed click cycloaddition to access C–N axially chiral *N*-triazolyl indoles

Li Zhou, Yankun Li, Shunian Li, Zhenwei Shi, Xue Zhang, Chen-Ho Tung and Zhenghu Xu*

- Atroposelective click reaction of internal alkynes
- Novel C–N axially chiral Indolyltriazole skeletons
- Broad scope with easily available Tol-BINAP ligands

5188



Molybdenum carbonyl assisted reductive tetramerization of CO by activated magnesium(i) compounds: squarate dianion vs. metallo-ketene formation

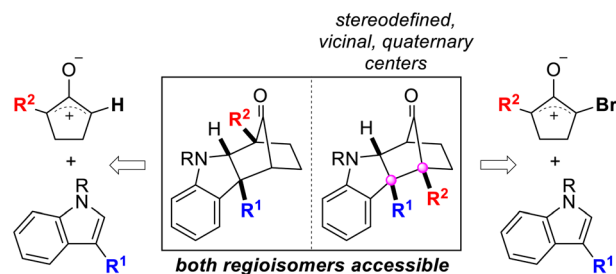
K. Yuvaraj, Jeremy C. Mullins, Thayalan Rajeshkumar, Iskander Douair, Laurent Maron* and Cameron Jones*



5196

Regiodivergent (3 + 2) annulation reactions of oxyallyl cations

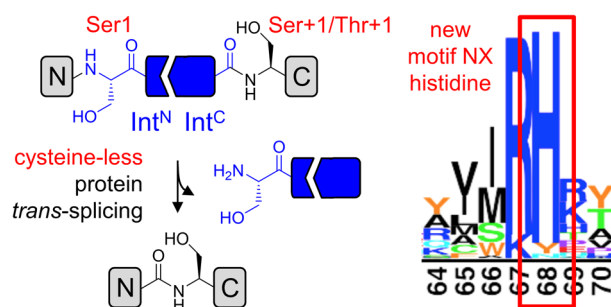
Zachary Protich, Leah L. Lowder, Russell P. Hughes* and Jimmy Wu*



5204

Structural and biochemical analysis of a novel atypically split intein reveals a conserved histidine specific to cysteine-less inteins

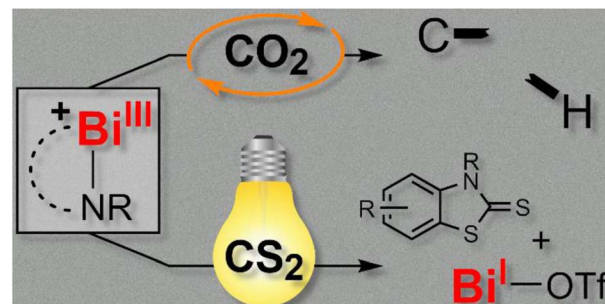
Tim Pasch, Alexander Schröder, Sabrina Kattelman, Miriam Eisenstein, Shmuel Pietrovski,* Daniel Kümmel* and Henning D. Mootz*



5214

Insertion of CO₂ and CS₂ into Bi–N bonds enables catalyzed CH-activation and light-induced bismuthinidene transfer

Kai Oberdorf, Anna Hanft, Xiulan Xie, F. Matthias Bickelhaupt, Jordi Poater* and Crispin Lichtenberg*



5220

A cheap metal catalyzed ring expansion/cross-coupling cascade: a new route to functionalized medium-sized and macrolactones

Shuai Liu, Pengchen Ma, Lu Zhang, Shenyu Shen, Hong-Jie Miao, Le Liu, K. N. Houk,* Xin-Hua Duan* and Li-Na Guo*

