

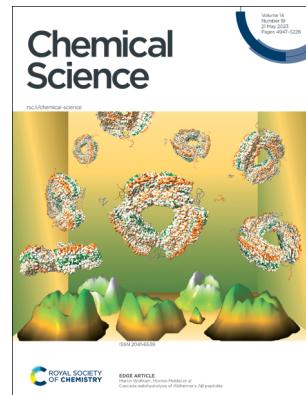
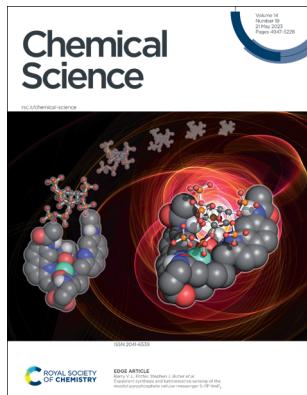
# Chemical Science

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

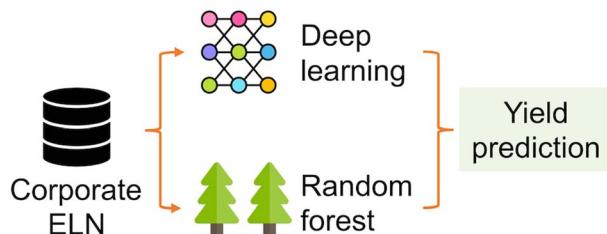


## COMMENTARY

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

Latimah Bustillo and Tiago Rodrigues\*

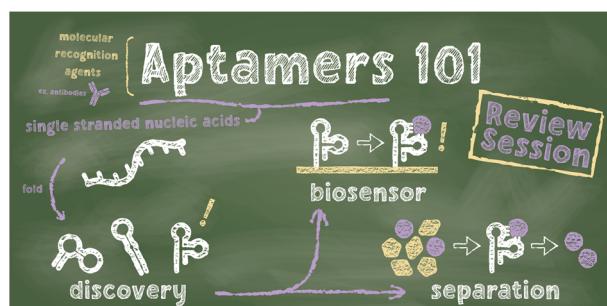


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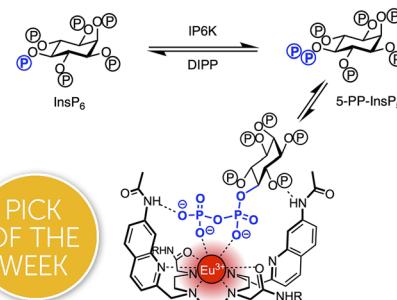


## EDGE ARTICLES

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**Expedient synthesis and luminescence sensing of the inositol pyrophosphate cellular messenger 5-PP-  
InsP<sub>5</sub>**

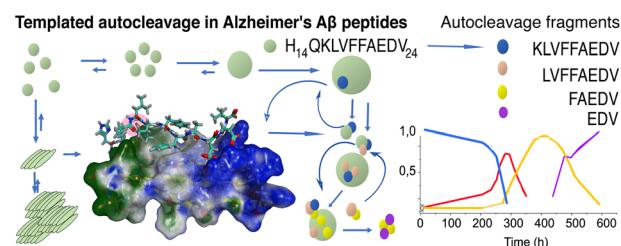
Megan L. Shipton, Fathima A. Jamion, Simon Wheeler,  
Andrew M. Riley, Felix Plasser, Barry V. L. Potter\*  
and Stephen J. Butler\*

PICK  
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WEEK

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**Cascade autohydrolysis of Alzheimer's A $\beta$  peptides**

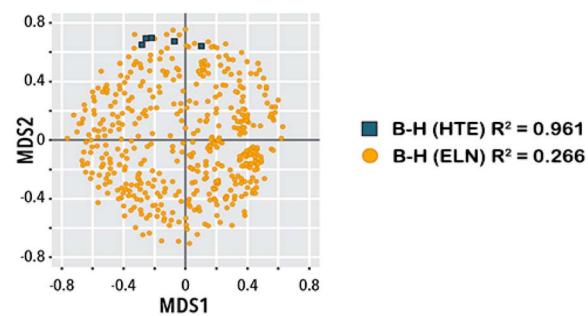
Martin Wolfram,\* Manish K. Tiwari, Tue Hassenkam,  
Ming Li, Morten J. Bjerrum and Morten Meldal\*



4997

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

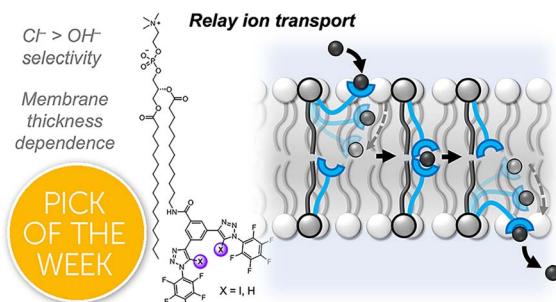
Mandana Saebi, Bozhao Nan, John E. Herr,  
Jessica Wahlers, Zhichun Guo, Andrzej M. Zurański,  
Thierry Kogej, Per-Ola Norrby, Abigail G. Doyle, Nitesh  
V. Chawla\* and Olaf Wiest\*



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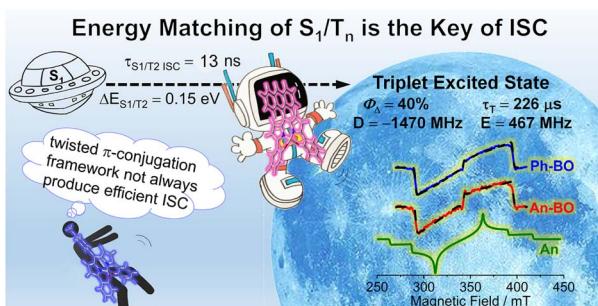
**Halogen bonding relay and mobile anion  
transporters with kinetically controlled chloride  
selectivity**

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

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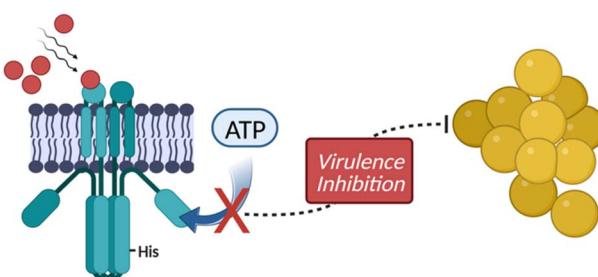
5014



### 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\*

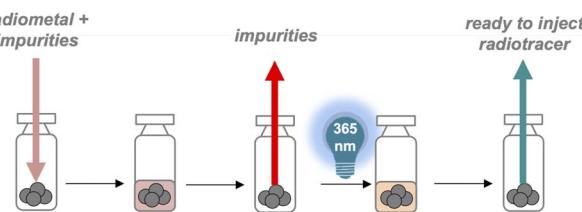
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### Targeting multidrug resistant *Staphylococcus* infections with bacterial histidine kinase inhibitors

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

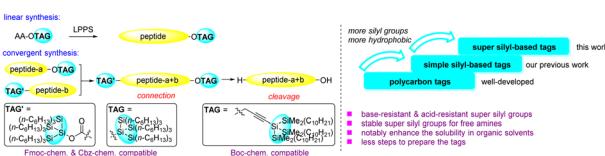
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### Radiometallation and photo-triggered release of ready-to-inject radiopharmaceuticals from the solid phase

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

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

An Wu\* and Hisashi Yamamoto\*

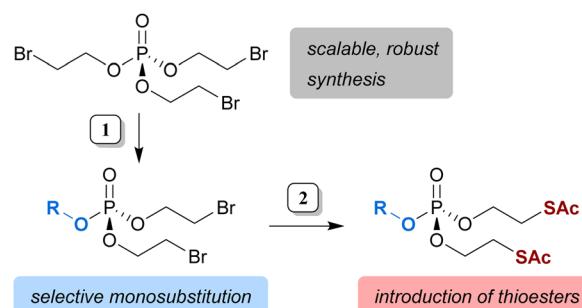


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**Synthesis of biolabile thioalkyl-protected phosphates from an easily accessible phosphotriester precursor**

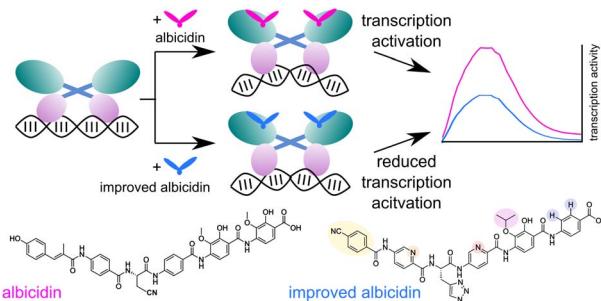
Lloyd D. Murphy, Kathryn E. Huxley, Ava Wilding, Cyane Robinson, Quentin P. O. Foucart and Lianne I. Willems\*



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

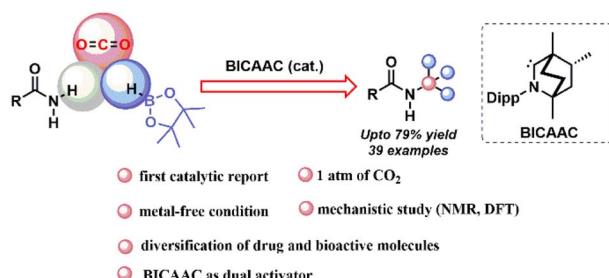
Simone Kosol, Lida Rostock, Jonas Barsig, Theresa Tabarelli, Kay Hommernick, Marcel Kulike, Tobias Eulberg, Maria Seidel, Iraj Behroz, Leonardo Kleebauer, Stefan Grätz, Andi Mainz and Roderich D. Süssmuth\*



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**Bicyclic (alkyl)(amino)carbene (BICAAC) in a dual role: activation of primary amides and CO<sub>2</sub> towards catalytic N-methylation**

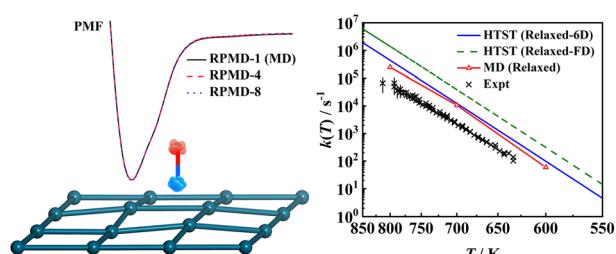
Nimisha Gautam, Ratan Logdi, Sreejyothi P., Antara Roy, Ashwani K. Tiwari\* and Swadhin K. Mandal\*



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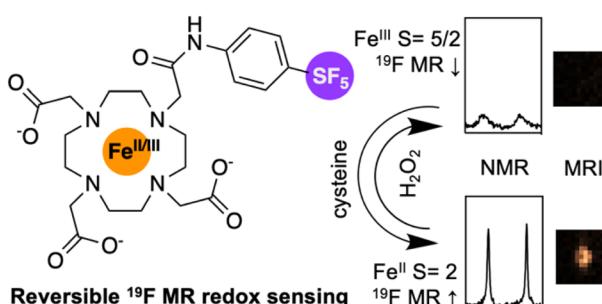
**First-principles surface reaction rates by ring polymer molecular dynamics and neural network potential: role of anharmonicity and lattice motion**

Chen Li, Yongle Li\* and Bin Jiang\*



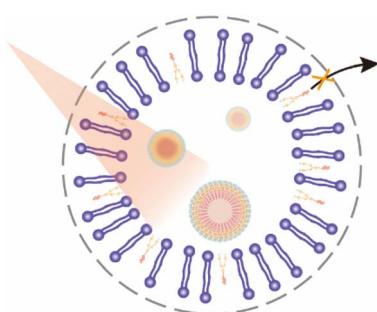
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**An Fe complex for  $^{19}\text{F}$  magnetic resonance-based reversible redox sensing and multicolor imaging**

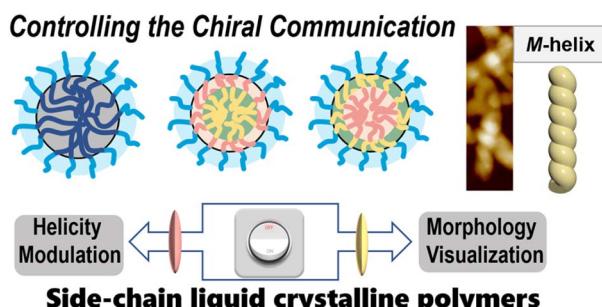
Rahul T. Kadakia, Raphael T. Ryan, Daniel J. Cooke and Emily L. Que\*

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

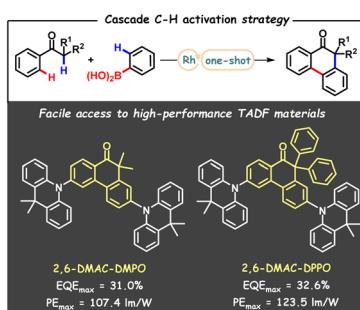
Youyou Li, Wenbo Han, Deyan Gong, Taokun Luo, Yingjie Fan, Jianming Mao, Wenwu Qin and Wenbin Lin\*

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**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\*

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**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\*

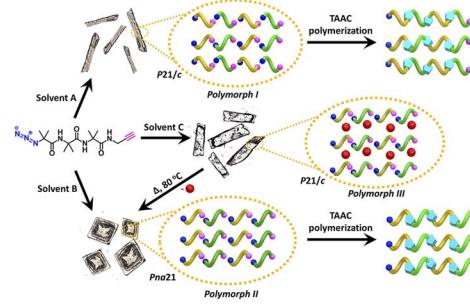


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**Rational design and topochemical synthesis of polymorphs of a polymer**

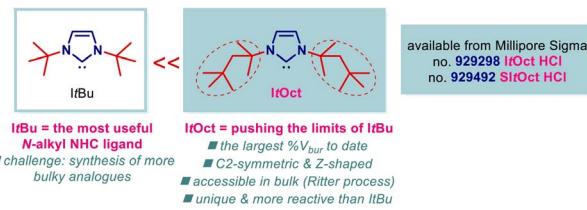
Vignesh Athiyarath, Liby Ann Mathew, Yakai Zhao, Ravichandran Khazeber, Upadrasta Ramamurthy and Kana M. Sureshan\*



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**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 Michał Szostak\*

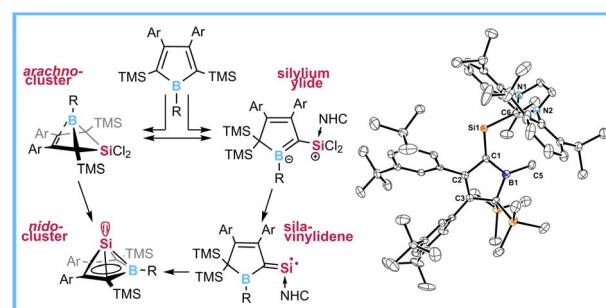


available from Millipore Sigma  
no. 929298 ItOct HCl  
no. 929492 SiItOct HCl

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**A donor-supported silavinylidene and silylum 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\*



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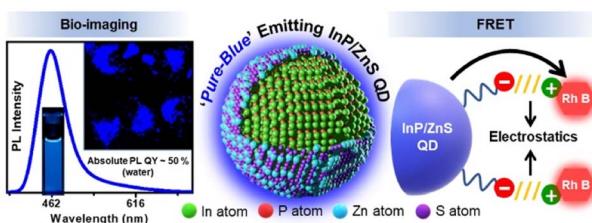
**In(OTf)<sub>3</sub>-catalyzed reorganization/cycloaddition of two imine units and subsequent modular assembly of acridinium photocatalysts**

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



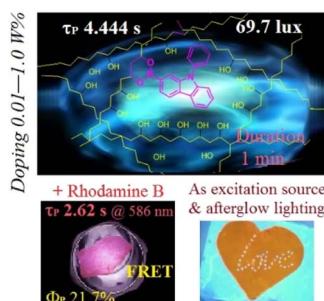
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**Blue-emitting InP quantum dots participate in an efficient resonance energy transfer process in water**

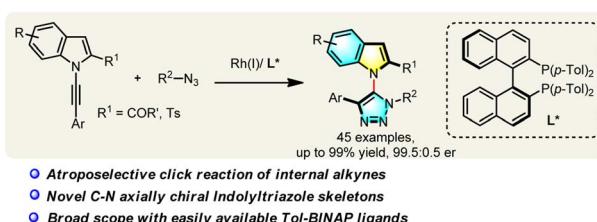
Pradyut Roy, Mishika Virmani and Pramod P. Pillai\*

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

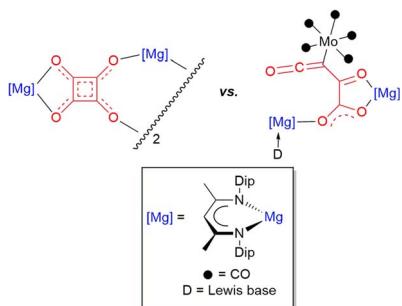
Yuefa Zhang, Shiguo Zhang, Guanyu Liu, Qikun Sun, Shanfeng Xue\* and Wenjun Yang\*

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**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\*

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

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

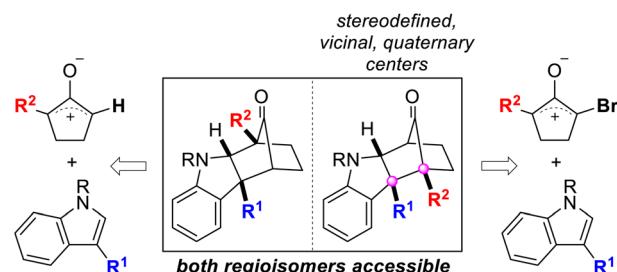


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**Regiodivergent (3 + 2) annulation reactions of oxyallyl cations**

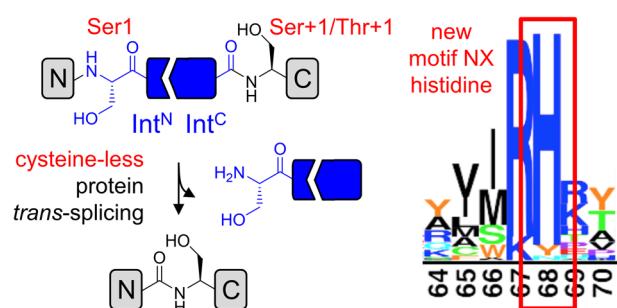
Zachary Protich, Leah L. Lowder, Russell P. Hughes\* and Jimmy Wu\*



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

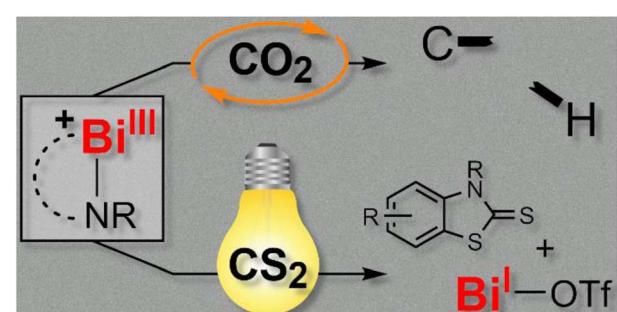
Tim Pasch, Alexander Schröder, Sabrina Kattelmann, Miriam Eisenstein, Shmuel Pietrokovski,\* Daniel Kümmel\* and Henning D. Mootz\*



5214

**Insertion of CO<sub>2</sub> and CS<sub>2</sub> 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\*



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**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\*

