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ISSN 2041-6539 CODEN CSHCBM 14(41) 11285–11584 (2023)

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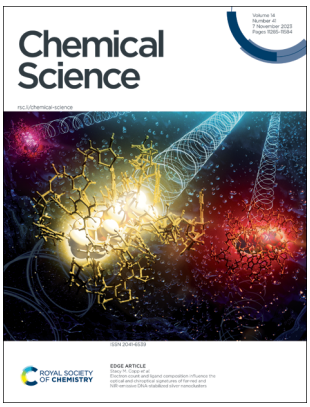

Inside cover
See Stacy M. Copp *et al.*, pp. 11340–11350. Image reproduced by permission of Stacy M. Copp from *Chem. Sci.*, 2023, **14**, 11340.

COMMENTARY

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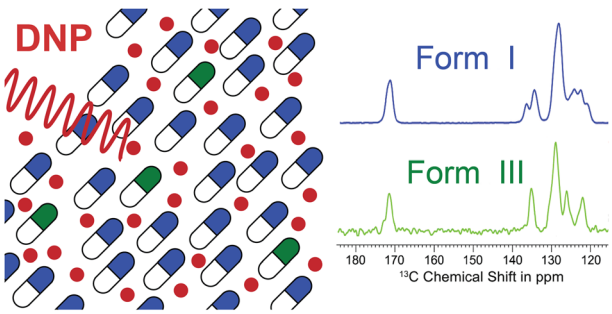
A focus on detection of polymorphs by dynamic nuclear polarization solid-state nuclear magnetic resonance spectroscopy

Yunhua Chen, Jiashan Mi and Aaron J. Rossini*

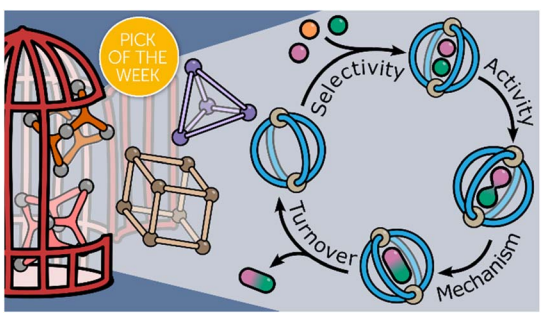


PERSPECTIVE

11300

Picking the lock of coordination cage catalysis

Tomasz K. Piskorz, Vicente Martí-Centelles, Rebecca L. Spicer, Fernanda Duarte* and Paul J. Lusby*



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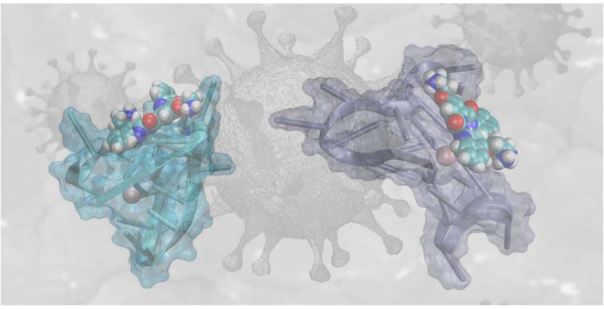
Resolving a guanine-quadruplex structure in the SARS-CoV-2 genome through circular dichroism and multiscale molecular modeling

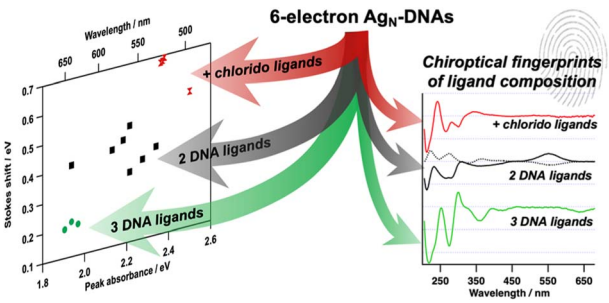
Luisa D'Anna, Tom Miclot, Emmanuelle Bignon, Ugo Perricone, Giampaolo Barone,* Antonio Monari* and Alessio Terenzi*



11340

Electron count and ligand composition influence the optical and chiroptical signatures of far-red and NIR-emissive DNA-stabilized silver nanoclusters

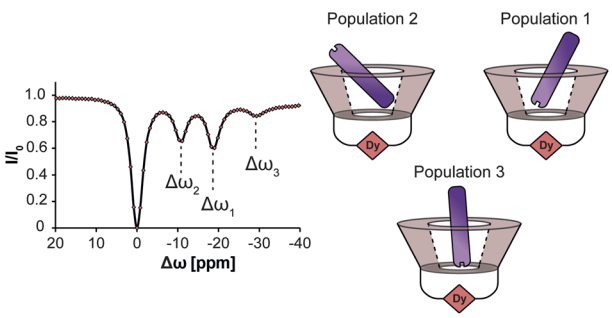
Rweetuparna Guha, Anna Gonzàlez-Rosell, Malak Rafik, Nery Arevalos, Benjamin B. Katz and Stacy M. Copp*



11351

NMR exchange dynamics studies of metal-capped cyclodextrins reveal multiple populations of host–guest complexes in solution

Elad Goren, Mark A. Iron, Yael Diskin-Posner, Alla Falkovich, Liat Avram and Amnon Bar-Shir*



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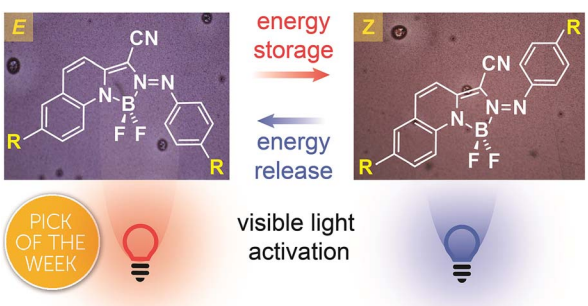
Visible light activated energy storage in solid-state Azo-BF_2 switches

Qianfeng Qiu, Qingkai Qi, Junichi Usuba, Karina Lee, Ivan Aprahamian* and Grace G. D. Han*



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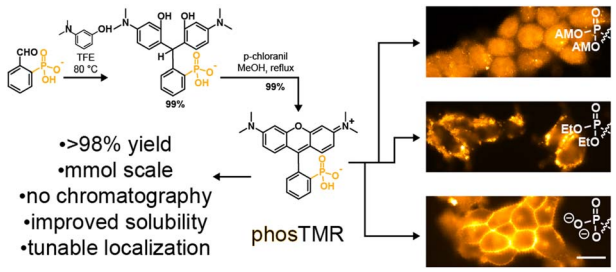

Mild and scalable synthesis of phosphonorhodamines

Joshua L. Turnbull, Ryan P. Golden, Brittany R. Benlian, Katharine M. Henn, Soren M. Lipman and Evan W. Miller*

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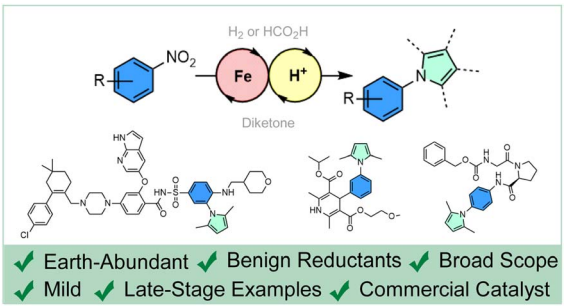

Applying green chemistry principles to iron catalysis: mild and selective domino synthesis of pyrroles from nitroarenes

Johannes Fessler, Kathrin Junge* and Matthias Beller*

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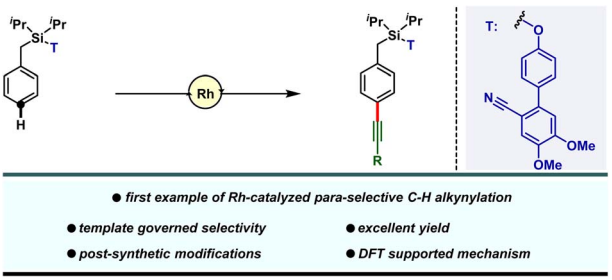

Directing group assisted *para*-selective C–H alkynylation of unbiased arenes enabled by rhodium catalysis

Uttam Dutta, Gaurav Prakash, Kirti Devi, Kongkona Borah, Xinglong Zhang* and Debabrata Maiti*

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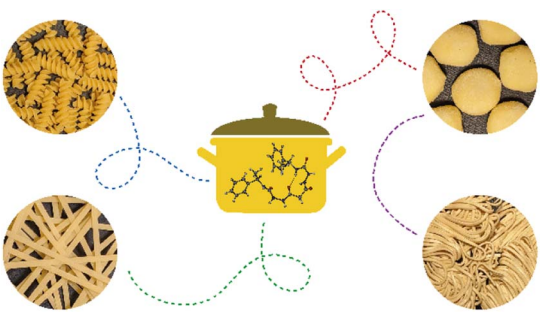

Pathway complexity in fibre assembly: from liquid crystals to hyper-helical gelmorphs

Rafael Contreras-Montoya, James P. Smith, Stephen C. Boothroyd, Juan A. Aguilar, Marzieh Mirzamani, Martin A. Screen, Dmitry S. Yufit, Mark Robertson, Lilin He, Shuo Qian, Harshita Kumari and Jonathan W. Steed*

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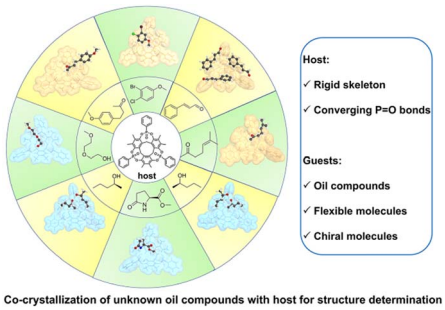
Host–guest system of a phosphorylated macrocycle assisting structure determination of oily molecules in single-crystal form

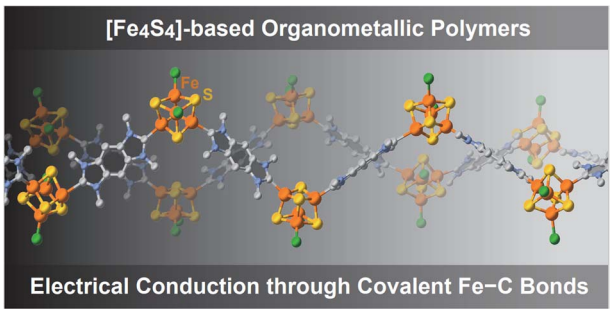
Jianmin Jiao, Heng Li, Wang Xie, Yue Zhao, Chen Lin,* Juli Jiang* and Leyong Wang*



11410

Electrically conductive [Fe_4S_4]-based organometallic polymers

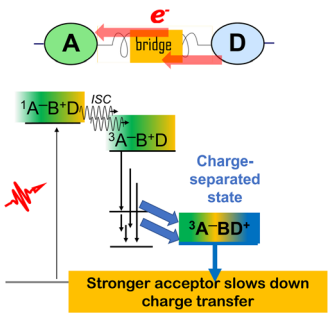
Kentaro Kadota, Tianyang Chen, Eoghan L. Gormley, Christopher H. Hendon, Mircea Dincă and Carl K. Brozek*



11417

A stronger acceptor decreases the rates of charge transfer: ultrafast dynamics and on/off switching of charge separation in organometallic donor–bridge–acceptor systems

Alexander J. Auty, Paul A. Scattergood, Theo Keane, Tao Cheng, Guanzhi Wu, Heather Carson, James Shipp, Andrew Sadler, Thomas Roseveare, Igor V. Sazanovich, Anthony J. H. M. Meijer,* Dimitri Chekulaev, Paul I. P. Elliot, Mike Towrie and Julia A. Weinstein*



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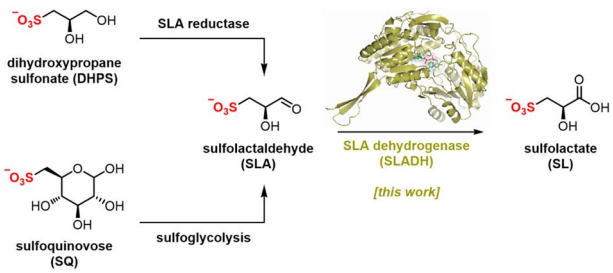
Molecular basis of sulfolactate synthesis by sulfolactaldehyde dehydrogenase from *Rhizobium leguminosarum*

Jinling Li, Mahima Sharma, Richard Meek, Amani Alhifthi, Zachary Armstrong, Niccolay Madiedo Soler, Mihwa Lee, Ethan D. Goddard-Borger, James N. Blaza, Gideon J. Davies* and Spencer J. Williams*



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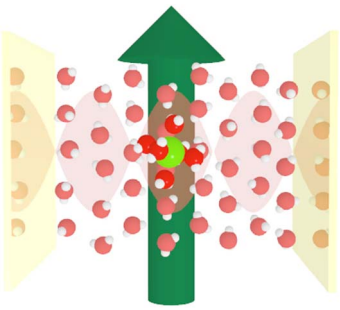

Unlimiting ionic conduction: manipulating hydration dynamics through vibrational strong coupling of water

Tomohiro Fukushima,* Soushi Yoshimitsu and Kei Murakoshi*

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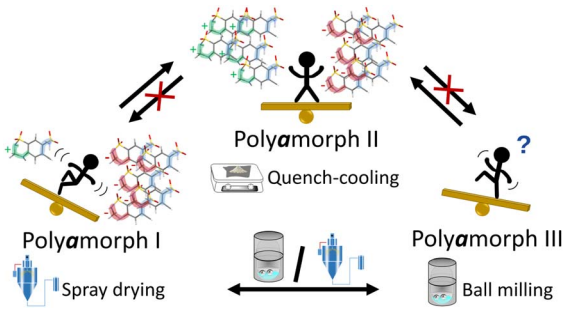

Unveiling polyamorphism and polyamorphic interconversions in pharmaceuticals: the peculiar case of hydrochlorothiazide

Inês C. B. Martins,* Anders S. Larsen, Anders Ø. Madsen, Olivia Aalling Frederiksen, Alexandra Correia, Kirsten M. Ø. Jensen, Henrik S. Jeppesen and Thomas Rades*

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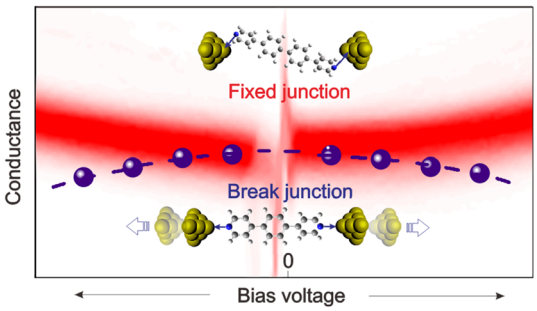

Regulating the orientation of a single coordinate bond by the synergistic action of mechanical forces and electric field

Wei Zhang, Zhibin Zhao, Min Tan, Adila Adijiang, Shurong Zhong, Xiaona Xu, Tianran Zhao, Emusani Ramya, Lu Sun, Xueyan Zhao, Zhiqiang Fan* and Dong Xiang*

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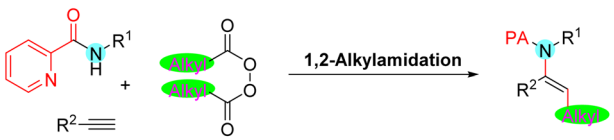

- Coordinating activation strategy enables 1,2-alkylamidation of alkynes
- Formation of β-alkylated enamides
- Easily accessible starting materials
- Broad substrate scope and good functional group tolerance
- Late-stage functionalization

Coordinating activation strategy enables 1,2-alkylamidation of alkynes

Jing Ren, Junhua Xu, Xiangxiang Kong, Jinlong Li and Kaizhi Li*

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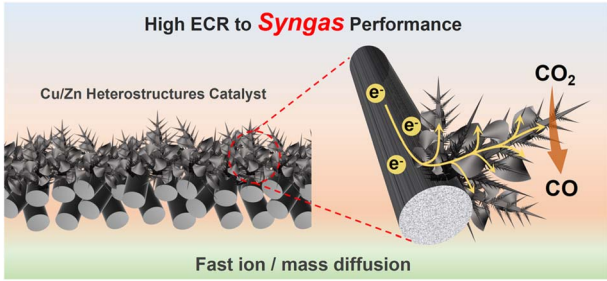
Ultra-fast synthesis of three-dimensional porous Cu/Zn heterostructures for enhanced carbon dioxide electroreduction

Shuaiqiang Jia, Qinggong Zhu,* Shitao Han, Jianxin Zhai, Mengke Dong, Wei Xia, Xueqing Xing, Haihong Wu,* Mingyuan He and Buxing Han*



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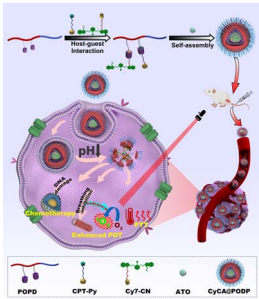
A supramolecular nanoplatform for imaging-guided phototherapies *via* hypoxia tumour microenvironment remodeling

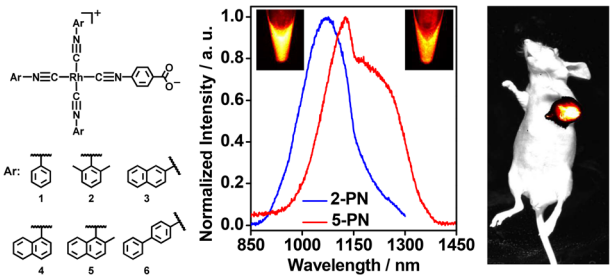
Weijie Zhou, Suwen Chen, Yingjie Ouyang, Baoxuan Huang, Hongman Zhang, Weian Zhang* and Jia Tian*



11490

Synthesis, supramolecular aggregation, and NIR-II phosphorescence of isocyanorhodium(I) zwitterions

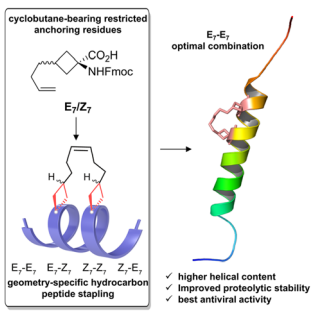
Wenxuan Wei, Jun Wang,* Xiaomei Kang, Haoquan Li, Qun He, Guanjun Chang and Weifeng Bu*



11499

Cyclobutane-bearing restricted anchoring residues enabled geometry-specific hydrocarbon peptide stapling

Baobao Chen, Chao Liu, Wei Cong, Fei Gao, Yan Zou, Li Su, Lei Liu, Alexander Hillisch, Lutz Lehmann, Donald Bierer, Xiang Li* and Hong-Gang Hu*



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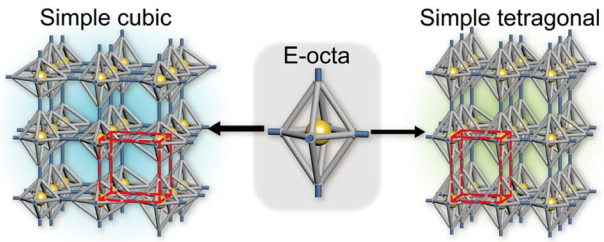
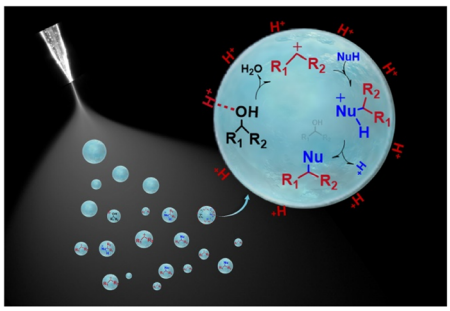


Geometry guided crystallization of anisotropic DNA origami shapes

Shujing Huang, Min Ji, Yong Wang and Ye Tian*

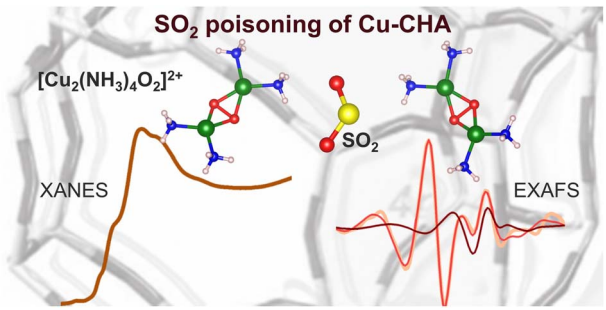
11515



Ultrafast C–C and C–N bond formation reactions in water microdroplets facilitated by the spontaneous generation of carbocations

Ting Wang, Zheng Li, Hang Gao, Jun Hu,* Hong-Yuan Chen and Jing-Juan Xu*

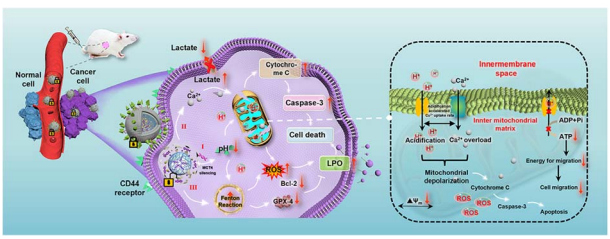
11521



Elucidating the reaction mechanism of SO_2 with Cu-CHA catalysts for NH_3-SCR by X-ray absorption spectroscopy

Anastasia Yu. Molokova, Reza K. Abasabadi, Elisa Borfecchia, Olivier Mathon, Silvia Bordiga, Fei Wen, Gloria Berlier, Ton V. W. Janssens* and Kirill A. Lomachenko*

11532



Synergistically remodulating H^+/Ca^{2+} gradients to induce mitochondrial depolarization for enhanced synergistic cancer therapy

Xiaoni Wang, Xiyang Ge, Xiaowen Guan, Jin Ouyang and Na Na*

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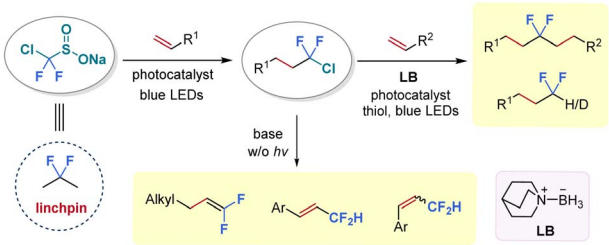
Programmable synthesis of difluorinated hydrocarbons from alkenes through a photocatalytic linchpin strategy

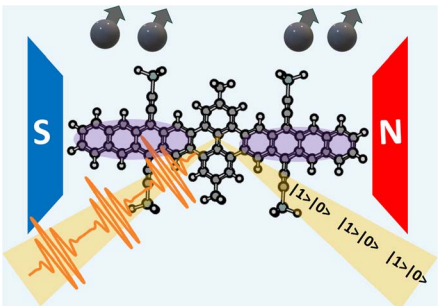
Zhi-Qi Zhang, Cheng-Qiang Wang, Long-Ji Li, Jared L. Piper, Zhi-Hui Peng,* Jun-An Ma,* Fa-Guang Zhang* and Jie Wu*



11554

Multiexciton quintet state populations in a rigid pyrene-bridged parallel tetracene dimer

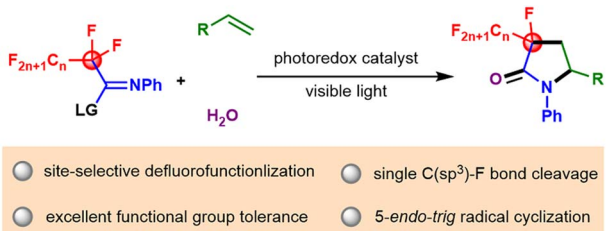
Liang-Chun Lin, Tanner Smith, Qianxiang Ai, Brandon K. Rugg, Chad Risko, John E. Anthony, Niels H. Damrauer and Justin C. Johnson*



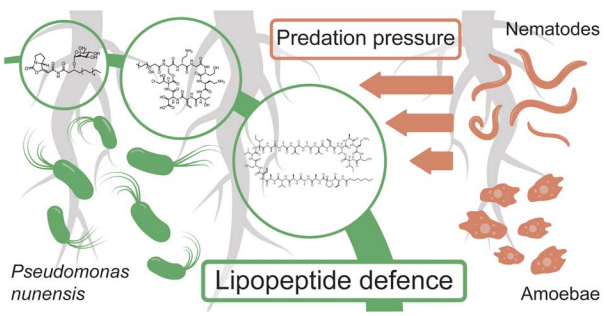
11566

Photocatalytic redox-neutral selective single C(sp^3)–F bond activation of perfluoroalkyl iminosulfides with alkenes and water

Tao Wang, Yuan-Yuan Zong, Tao Huang, Xiao-Ling Jin, Li-Zhu Wu and Qiang Liu*



11573

Nonribosomal peptides protect *Pseudomonas nunensis* 4A2e from amoebal and nematodal predation

Sebastian Pflanze, Ruchira Mukherji, Anan Ibrahim, Markus Günther, Sebastian Götze, Somak Chowdhury, Lisa Reimer, Lars Regestein and Pierre Stallforth*