

Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(26) 9861–10250 (2024)



Cover

See Mikhail V. Polynski, Valentine P. Ananikov *et al.*, pp. 9977–9986. Image reproduced by permission of Olga Chentsova and Christina Rulina from *Chem. Sci.*, 2024, **15**, 9977. Cover artwork by Olga Chentsova and Christina Rulina.



Inside cover

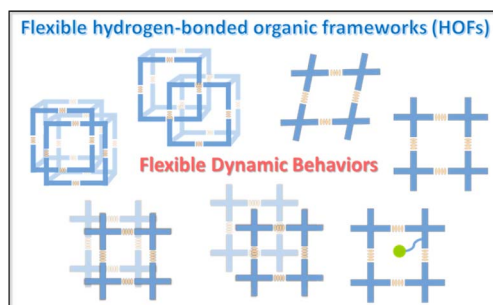
See Michael C. Biewer, Mihaela C. Stefan *et al.*, pp. 9987–10001. Image reproduced by permission of Mihaela C. Stefan from *Chem. Sci.*, 2024, **15**, 9987. Artwork generated with Adobe Firefly.

PERSPECTIVES

9874

Flexible hydrogen-bonded organic frameworks (HOFs): opportunities and challenges

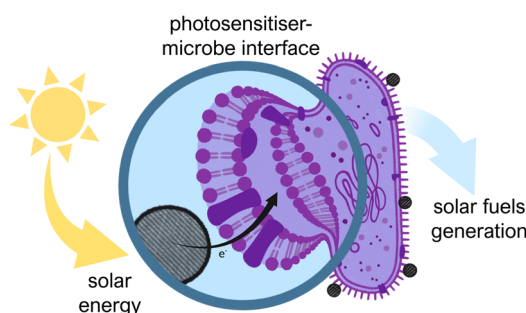
Jiantang Li* and Banglin Chen*



9893

Engineering of bespoke photosensitiser–microbe interfaces for enhanced semi-artificial photosynthesis

Imogen L. Bishara Robertson, Huijie Zhang, Erwin Reisner, Julea N. Butt and Lars J. C. Jeuken*



ChemComm

**Uncover new possibilities
with outstanding
preliminary research**

**Original discoveries, fuelling
every step of scientific progress**

rsc.li/chemcomm

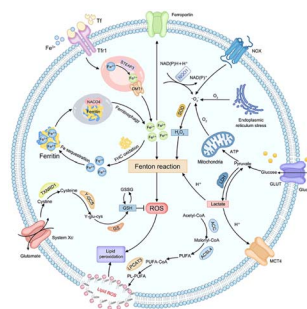
**Fundamental questions
Elemental answers**

PERSPECTIVES

9915

Current progress in the regulation of endogenous molecules for enhanced chemodynamic therapy

Jun Wang, Yina Liu, Tingting Cui,* Huanghao Yang* and Lisen Lin*

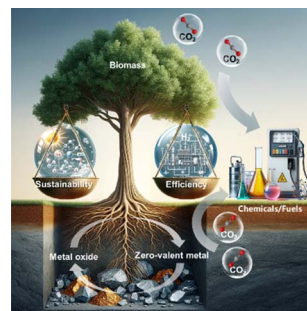


REVIEWS

9927

Recent advances in CO₂ reduction with renewable reductants under hydrothermal conditions: towards efficient and net carbon benefit CO₂ conversion

Zien Tang, Xu Liu, Yang Yang* and Fangming Jin*



9949

Electrocatalysis in deep eutectic solvents: from fundamental properties to applications

Hengan Wang, Xinchun Kang* and Buxing Han*

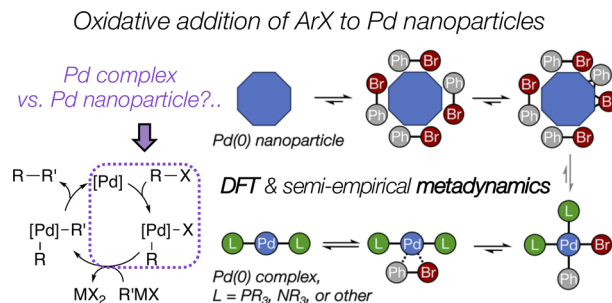


EDGE ARTICLES

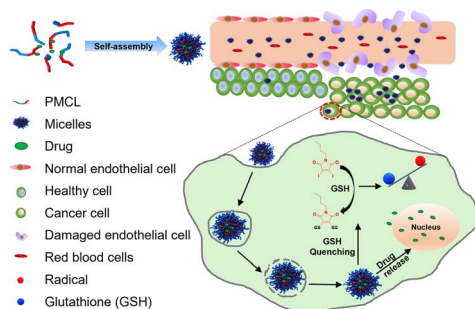
9977

Computational analysis of R–X oxidative addition to Pd nanoparticles

Mikhail V. Polynski,* Yulia S. Vlasova, Yaroslav V. Solovov, Sergey M. Kozlov and Valentine P. Ananikov*



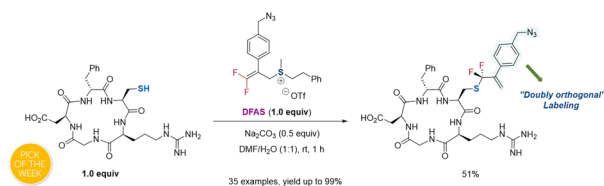
9987



Maleimide functionalized polycaprolactone micelles for glutathione quenching and doxorubicin delivery

Godwin K. Babanyinah, Abhi Bhadrar, Himanshu Polara, Hanghang Wang, Tejas Shah, Michael C. Biewer* and Mihaela C. Stefan*

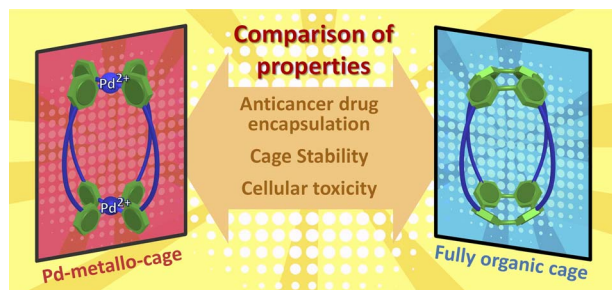
10002



Site-selective *S*-gem-difluoroallylation of unprotected peptides with 3,3-difluoroallyl sulfonium salts

Jin-Xiu Ren, Minqi Zhou, Xiao-Tian Feng, Hai-Yang Zhao, Xia-Ping Fu and Xingang Zhang*

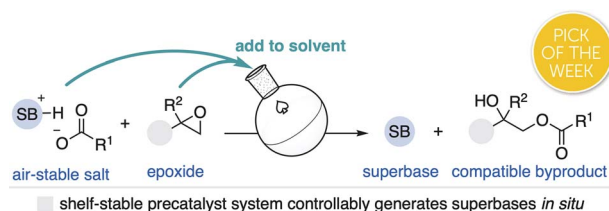
10010



Comparing organic and metallo-organic hydrazone molecular cages as potential carriers for doxorubicin delivery

Giovanni Montà-González, David Bastante-Rodríguez, Alba García-Fernández, Paul J. Lusby, Ramón Martínez-Máñez* and Vicente Martí-Centelles*

10018



A strategy for the controllable generation of organic superbases from benchtop-stable salts

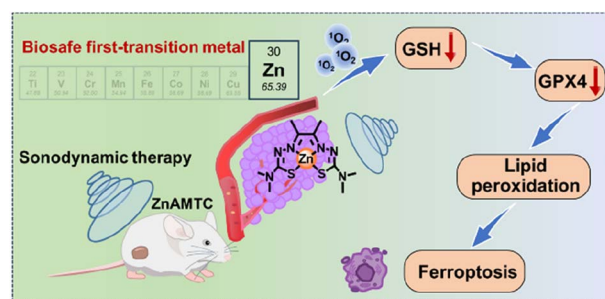
Stephen J. Sujansky, Garrett A. Hoteling and Jeffrey S. Bandar*



10027

Facile synthesis of a hydrazone-based zinc(II) complex for ferroptosis-augmented sonodynamic therapy

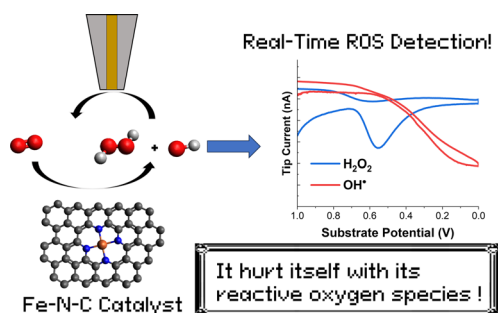
Dan Li, Minghui Fan, Haobing Wang, Yongjie Zhu, Bole Yu, Pingyu Zhang* and Huaiyi Huang*



10036

Real-time investigation of reactive oxygen species and radicals evolved from operating Fe–N–C electrocatalysts during the ORR: potential dependence, impact on degradation, and structural comparisons

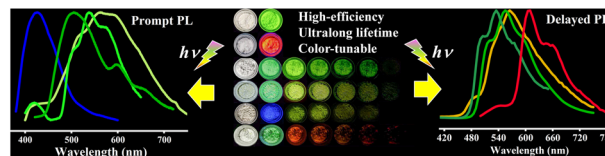
Seth T. Putnam and Joaquín Rodríguez-López*



10046

High-efficiency color-tunable ultralong room-temperature phosphorescence from organic–inorganic metal halides *via* synergistic inter/intramolecular interactions

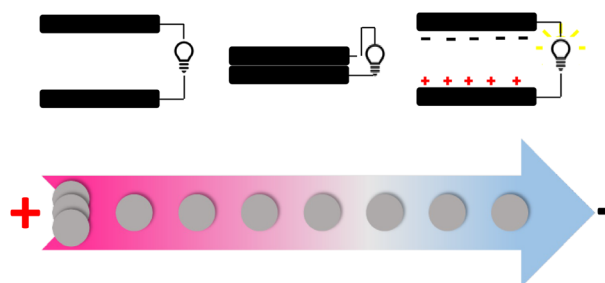
Lei Zhou, Kailei Li, Yuanyuan Chang, Yuan Yao, Yuqi Peng, Ming Li and Rongxing He*



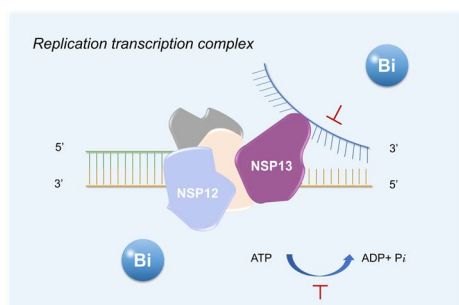
10056

Triboelectric behaviour of selected zeolitic-imidazolate frameworks: exploring chemical, morphological and topological influences

Ben Slater and Jin-Chong Tan*



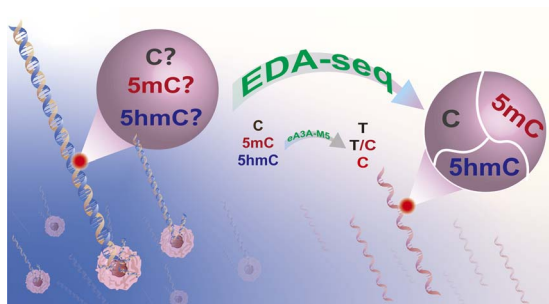
10065



Mechanistic insights into bismuth(III) inhibition of SARS-CoV-2 helicase

Xueying Wei, Chun-Lung Chan, Ying Zhou, Kaiming Tang, Jingxin Chen, Suyu Wang, Jasper Fuk-Woo Chan, Shuofeng Yuan, Hongyan Li and Hongzhe Sun*

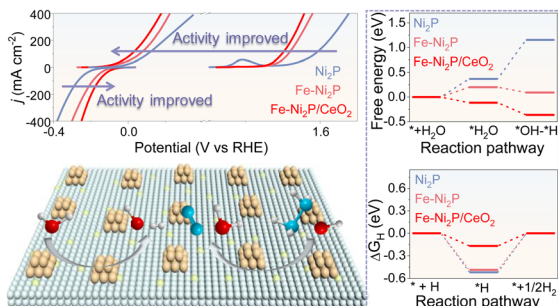
10073



Simultaneous detection of 5-methylcytosine and 5-hydroxymethylcytosine at specific genomic loci by engineered deaminase-assisted sequencing

Neng-Bin Xie, Min Wang, Tong-Tong Ji, Xia Guo, Fang-Yin Gang, Ying Hao, Li Zeng, Ya-Fen Wang, Yu-Qi Feng and Bi-Feng Yuan*

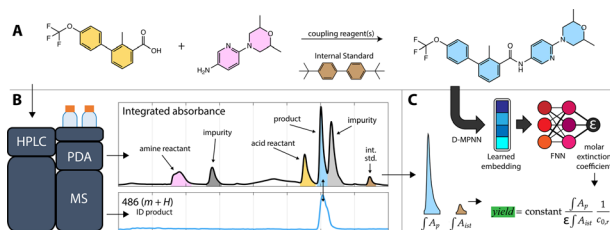
10084



Dual-strategy engineered nickel phosphide for achieving efficient hydrazine-assisted hydrogen production in seawater

Rui-Qing Li,* Songyun Guo, Xiaojun Wang, Xiaoyu Wan, Shuixiang Xie, Yu Liu, Changming Wang, Guangyu Zhang, Jun Cao,* Jiamu Dai, Mingzheng Ge and Wei Zhang*

10092



Calibration-free reaction yield quantification by HPLC with a machine-learning model of extinction coefficients

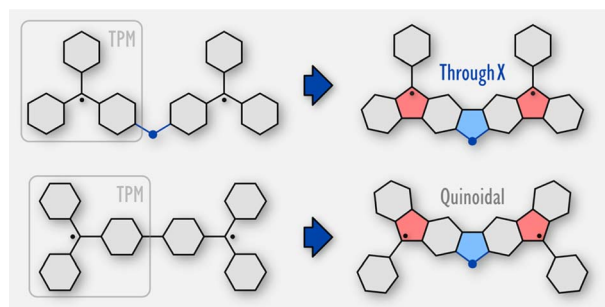
Matthew A. McDonald, Brent A. Koscher, Richard B. Canty and Klavs F. Jensen*



10101

Difluorenoheteroles: topological control of π conjugation in diradicaloids and mixed-valence radical ions

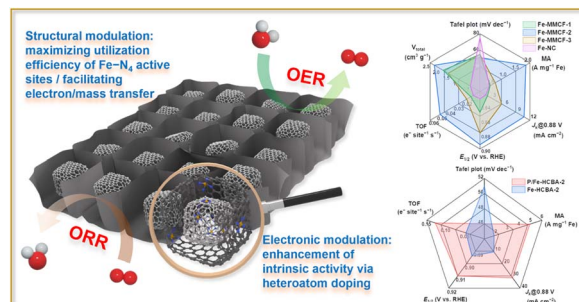
Bibek Prajapati, Tendai Kwenda, Tadeusz Lis, Piotr J. Chmielewski, Carlos J. Gómez-García, Marcin A. Majewski and Marcin Stępień*



10110

2D arrays of hollow carbon nanoboxes: outward contraction-induced hollowing mechanism in Fe–N–C catalysts

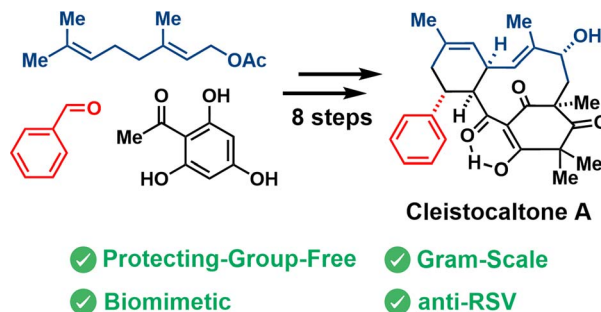
Xiaokai Song, Xiaoke Wang, Jiamin Wei,* Shenghua Zhou, Haifeng Wang, Jiali Lou, Yaqi Zhang, Yuhai Liu, Luyao Zou, Yingji Zhao, Xiaoqian Wei, Sameh M. Osman, Xiaopeng Li* and Yusuke Yamauchi*



10121

Synthesis and biological evaluation of cleistocaltone A, an inhibitor of respiratory syncytial virus (RSV)

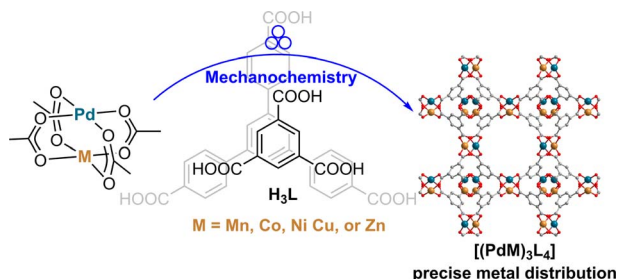
Lorenz Wiese, Sophie M. Kolbe, Manuela Weber, Martin Ludlow* and Mathias Christmann*



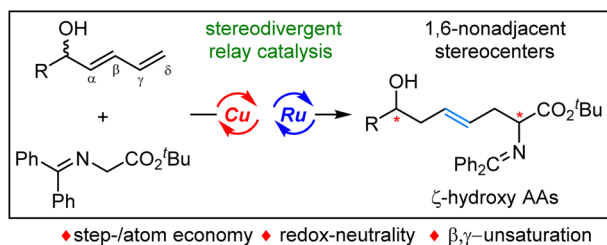
10126

Generic and facile mechanochemical access to versatile lattice-confined Pd(II)-based heterometallic sites

Zhuorigebatu Tegudeer, Jisue Moon, Joshua Wright, Milton Das, Gayan Rubasinghege, Wenqian Xu and Wen-Yang Gao*



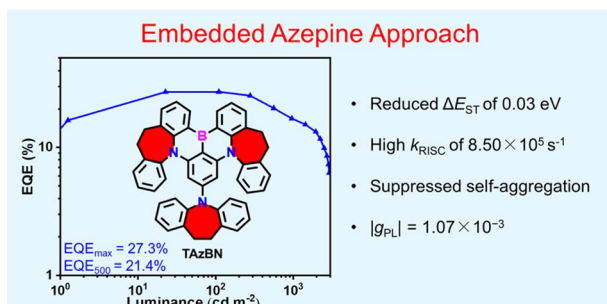
10135



Copper/ruthenium relay catalysis enables 1,6-double chiral inductions with stereodivergence

Hao-Ran Yang, Xiang Cheng, Xin Chang, Zuo-Fei Wang, Xiu-Qin Dong* and Chun-Jiang Wang*

10146



Elevating the upconversion performance of a multiple resonance thermally activated delayed fluorescence emitter *via* an embedded azepine approach

Yi-Kuan Chen, Jian Lei and Tien-Lin Wu*

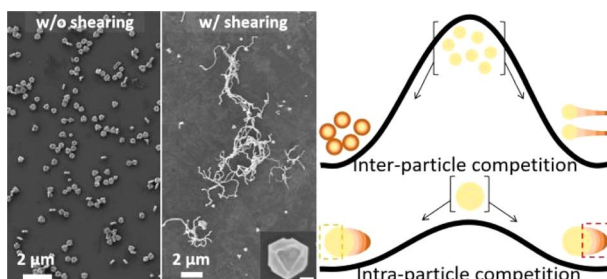
10155



Molecular bowls for inclusion complexation of toxic anticancer drug methotrexate

Pratik Karmakar, Tyler J. Finnegan, Darian C. Rostam, Sagarika Taneja, Sefa Uçar, Alexandar L. Hansen, Curtis E. Moore, Christopher M. Hadad, Kornkanya Pratunyot, Jon R. Parquette and Jovica D. Badjić*

10164



Shearing-induced formation of Au nanowires

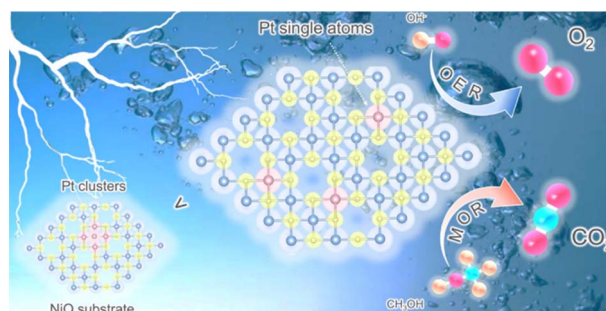
Yiwen Sun, An Su, Lecheng Zhao, Xiaobin Liu, Xueyang Liu, Yawen Wang* and Hongyu Chen*



10172

Tunable Pt–NiO interaction-induced efficient electrocatalytic water oxidation and methanol oxidation

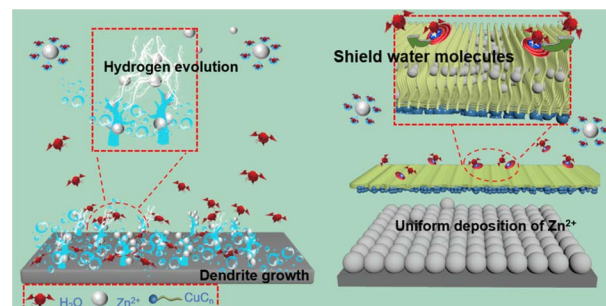
Fenglin Wang, Zhicheng Zheng, Dan Wu, Hao Wan,*
Gen Chen, Ning Zhang, Xiaohe Liu* and Renzhi Ma*



10182

Selectively “size-excluding” water molecules to enable a highly reversible zinc metal anode

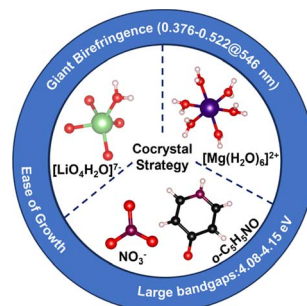
Xiaowei Shen, Wanhao Chen, Haocong Wang,
Lifang Zhang, Baojiu Hao, Changhao Zhu, Xiuzhen Yang,
Meizhu Sun, Jinqiu Zhou,* Xuejun Liu,* Chenglin Yan
and Tao Qian*



10193

Crystal clear: unveiling giant birefringence in organic–inorganic cocrystals

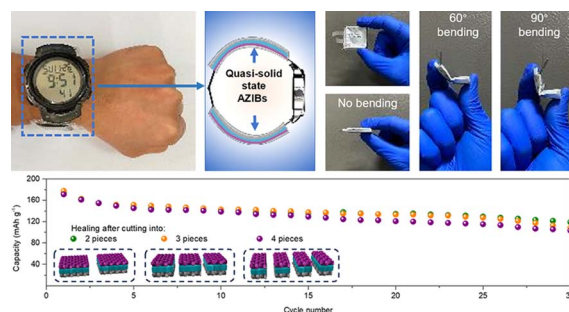
Yang Li and Kang Min Ok*



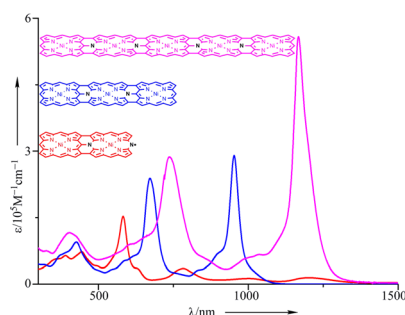
10200

A quasi-solid-state self-healing flexible zinc-ion battery using a dual-crosslinked hybrid hydrogel as the electrolyte and Prussian blue analogue as the cathode material

Jiawei Long, Tianli Han, Xirong Lin, Yajun Zhu, Jinyun Liu*
and Junjie Niu*



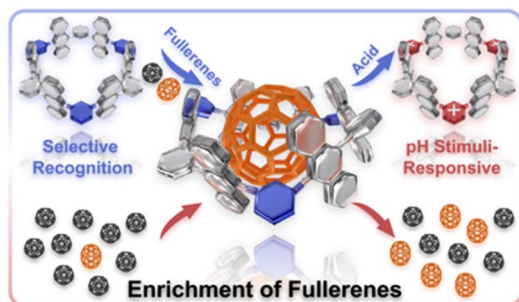
10207



Synthesis of Ni^{II} porphyrin–Ni^{II} 5,15-diazaporphyrin hybrid tapes

Lina Wang, Zian Liao, Peng Lin, Yingying Jia, Le Liu, Ling Xu, Mingbo Zhou, Bangshao Yin, Yutao Rao, Akito Nakai, Takayuki Tanaka, Daiki Shimizu, Atsuhiko Osuka and Jianxin Song*

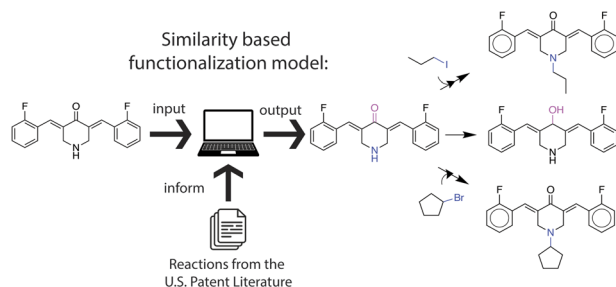
10214



Selective recognition and enrichment of C₇₀ over C₆₀ using an anthracene-based nanotube

Hao Nian, Song-Meng Wang, Yan-Fang Wang, Yu-Tao Zheng, Li-Shuo Zheng, Xiaoping Wang, Liu-Pan Yang,* Wei Jiang* and Liping Cao*

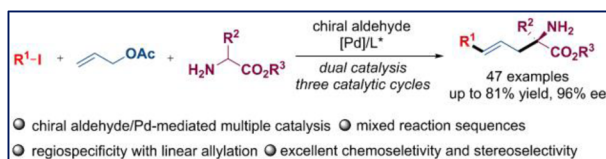
10221



Similarity based functionalization for enumeration of synthetically plausible chemical libraries surrounding a target

Karthik Sankaranarayanan* and Klavs F. Jensen*

10232



Asymmetric three-component Tsuji–Trost allylation reaction enabled by chiral aldehyde/palladium combined catalysis

Jian-Hua Liu, Wei Wen, Zhu-Lian Wu, Tian Cai, Yan-Min Huang* and Qi-Xiang Guo*

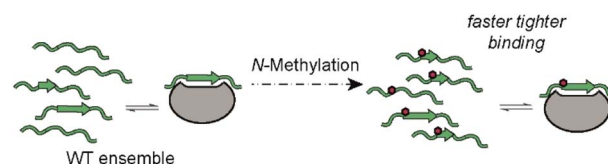


EDGE ARTICLES

10237

Understanding β -strand mediated protein–protein interactions: tuning binding behaviour of intrinsically disordered sequences by backbone modification

Emma E. Cawood, Emily Baker, Thomas A. Edwards, Derek N. Woolfson,^{*} Theodoros K. Karamanos^{*} and Andrew J. Wilson^{*}



CORRECTIONS

10246

Correction: Hydrogen bonding bolstered head-to-tail ligation of functional chromophores in a 0D SbF_3 ·glycine adduct for a short-wave ultraviolet nonlinear optical material

Zhiyong Bai, Jihyun Lee, Chun-Li Hu,^{*} Guohong Zou^{*} and Kang Min Ok^{*}

10247

Correction: An un-forgotten classic: the nitro-Mannich reaction between nitrones and silyl nitronates catalysed by $\text{B}(\text{C}_6\text{F}_5)_3$

Michael G. Guerzoni, Yara van Ingen, Rasool Babaahmadi, Thomas Wirth, Emma Richards^{*} and Rebecca L. Melen^{*}

