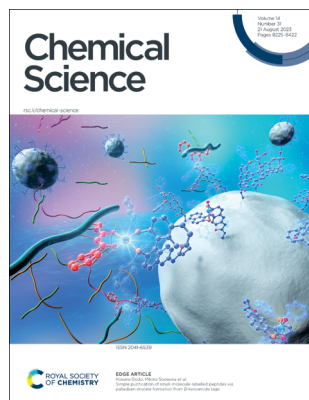


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ISSN 2041-6539 CODEN CSHCBM 14(31) 8225–8422 (2023)



Cover

See Kosuke Dodo, Mikiko Sodeoka *et al.*, pp. 8249–8254.
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Inside cover

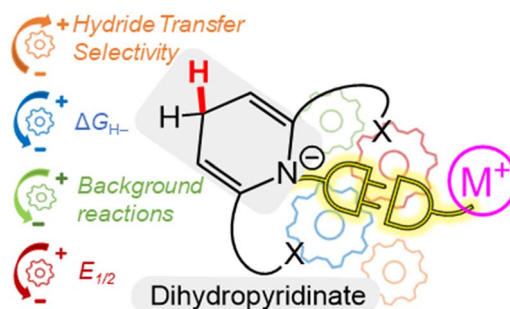
See Bina Fu, Xueming Yang, Kaijun Yuan *et al.*, pp. 8255–8261.
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PERSPECTIVE

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Metallated dihydropyridinates: prospects in hydride transfer and (electro)catalysis

Leo W. T. Parsons and Louise A. Berben*

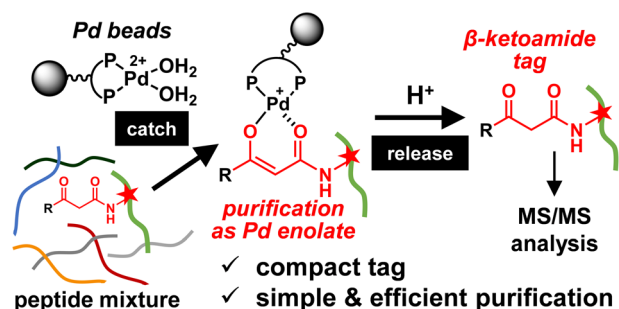


EDGE ARTICLES

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Simple purification of small-molecule-labelled peptides via palladium enolate formation from β -ketoamide tags

Kenji Hayamizu, Kota Koike, Kosuke Dodo,*
Miwako Asanuma, Hiromichi Egami and Mikiko Sodeoka*



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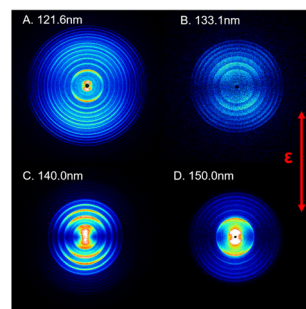
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Vacuum ultraviolet photodissociation of sulfur dioxide and its implications for oxygen production in the early Earth's atmosphere

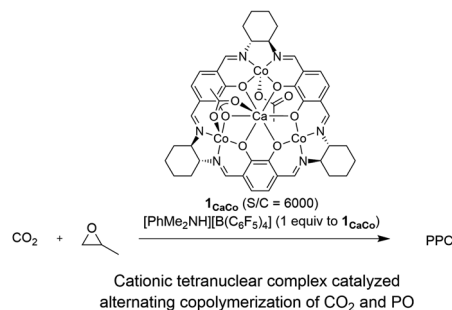
Yao Chang, Yanlin Fu, Zhichao Chen, Zijie Luo, Yarui Zhao, Zhenxing Li, Weiqing Zhang, Guorong Wu, Bina Fu,^{*} Dong H. Zhang, Michael N. R. Ashfold, Xueming Yang^{*} and Kaijun Yuan^{*}



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Cationic tetranuclear macrocyclic CaCo_3 complexes as highly active catalysts for alternating copolymerization of propylene oxide and carbon dioxide

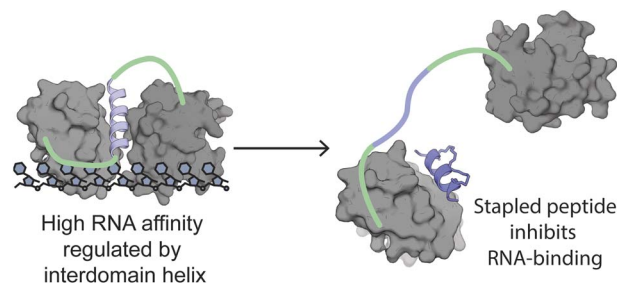
Haruki Nagae, Saki Matsushiro, Jun Okuda^{*} and Kazushi Mashima^{*}



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Rationally designed stapled peptides allosterically inhibit PTBP1–RNA-binding

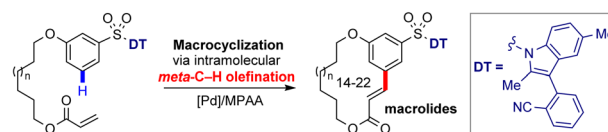
Stefan Schmeing, Gulshan Amrahova, Katrin Bigler, Jen-Yao Chang, Joseph Openy, Sunit Pal, Laura Posada, Raphael Gasper and Peter 't Hart^{*}



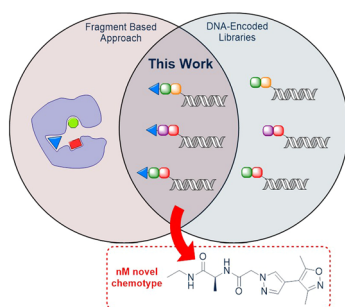
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Macrocyclization via remote *meta*-selective C–H olefination using a practical indolyl template

Pengfei Zhang, Zhiwei Jiang, Zhoulong Fan, Guoshuai Li, Qingxue Ma, Jun Huang, Jinghong Tang, Xiaohua Xu,^{*} Jin-Quan Yu^{*} and Zhong Jin^{*}



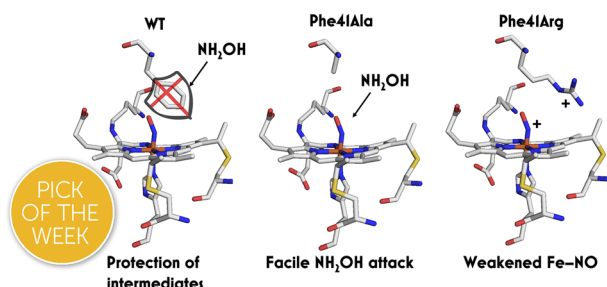
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Fragment expansion with NUDELs – poised DNA-encoded libraries

Catherine L. A. Salvini, Benoit Darlot, Jack Davison, Mathew P. Martin, Susan J. Tudhope, Shannon Turberville, Akane Kawamura, Martin E. M. Noble, Stephen R. Wedge, James J. Crawford and Michael J. Waring*

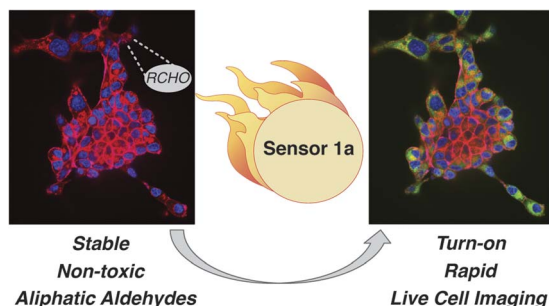
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Outer coordination sphere influences on cofactor maturation and substrate oxidation by cytochrome P460

Melissa M. Bollmeyer, Sean H. Majer, Rachael E. Coleman and Kyle M. Lancaster*

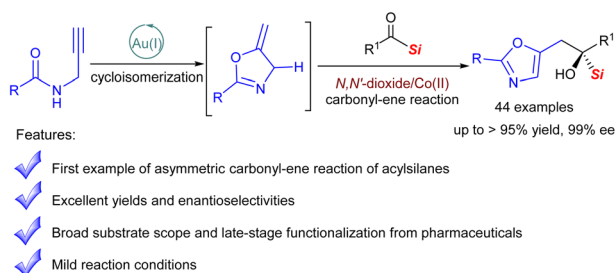
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Chemical sensors for imaging total cellular aliphatic aldehydes in live cells

Rachel Wills, Jonathan Farhi, Patrick Czabala, Sophia Shahin, Jennifer M. Spangle and Monika Raj*

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Bimetallic tandem catalysis-enabled enantioselective cycloisomerization/carbonyl-ene reaction for construction of 5-oxazoylmethyl α -silyl alcohol

Xinpeng Sang, Yuhao Mo, Shiya Li, Xiaohua Liu, Weidi Cao* and Xiaoming Feng*



Feasible bottom-up development of conjugated microporous polymers (CMPs) for boosting the deep removal of sulfur dioxide

Diagram illustrating the central role of SO_2 in various chemical reactions, showing the bond energy (BE) of the products:

- Top Left:** Reaction via *Cyclooligomerization* yields a product with $\text{BE} = -13.82 \text{ kJ mol}^{-1}$.
- Top Right:** Reaction via *Thioether condensation* yields a product with $\text{BE} = -7.4 \text{ kJ mol}^{-1}$.
- Middle Left:** Reaction via *Sonogashira-Hagihara cross-coupling* yields a product with $\text{BE} = -14.88 \text{ kJ mol}^{-1}$.
- Middle Right:** Reaction via *Buchwald-Hartwig amination* yields a product with $\text{BE} = -21.42 \text{ kJ mol}^{-1}$.
- Bottom Left:** Reaction via *Hock reaction* yields a product with $\text{BE} = -11.52 \text{ kJ mol}^{-1}$.
- Bottom Right:** Reaction via *Suzuki-Miyaura cross-coupling* yields a product with $\text{BE} = -11.76 \text{ kJ mol}^{-1}$.

Regulating tumor glycometabolism and the immune microenvironment by inhibiting lactate dehydrogenase with platinum(IV) complexes

The diagram illustrates the anti-angiogenic effect of Pt(II) complexes. A Pt(II) complex, coordinated by two DCF ligands and two NH₃ ligands, is shown binding to a red blood vessel. This binding leads to 'Anti-angiogenesis'. The diagram also shows 'Macrophages' (M2 and M1) and 'MCTs' (Monocyte Chemoattractant Proteins) involved in the process. A 'Cancer cell' is shown with metabolic pathways involving LDHA, LDHB, Pyruvate, and Lactate.

Accelerating explicit solvent models of heterogeneous catalysts with machine learning interatomic potentials

Efficient Explicit Solvent Models

Solvated Catalyst Interface

ML Potential Accelerated MD & Metadynamics

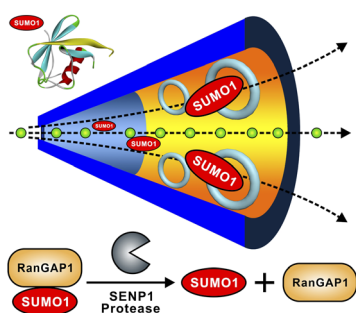
Reaction Free Energy Surface

Via Active Machine Learning

Enantioselective [3+2]-cycloaddition of 2,3-disubstituted cyclobutenones: vicinal quaternary stereocenters construction and skeletal functionalization

The reaction scheme shows the [3+2] cycloaddition of an enamine (R¹-N=C(R²)-CO₂Me) and a maleimide derivative (R³-cyclobutene-1,2-dicarboxylate). The reaction proceeds via a [3+2] cycloaddition to form a bicyclic intermediate, which is then subjected to skeletal functionalization to yield a final product. The final product is a bicyclic system with a maleimide core, substituted with R¹, R², R³, R⁴, R⁵, and R⁶ groups. The reaction is noted to have 29 examples with up to 99% ee.

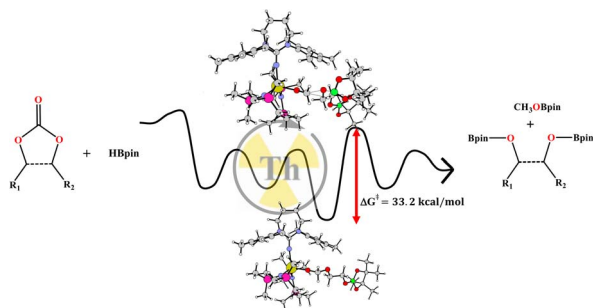
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A highly sensitive nanochannel device for the detection of SUMO1 peptides

Yue Qin, Xiaoyu Zhang, Yanling Song, Bowen Zhong, Lu Liu, Dongdong Wang, Yahui Zhang, Wenqi Lu, Xinjia Zhao, Zhiqi Jia, Minmin Li, Lihua Zhang* and Guangyan Qing*

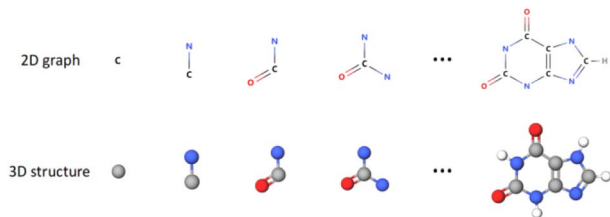
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Catalytic regeneration of metal-hydrides from their corresponding metal-alkoxides via the hydroboration of carbonates to obtain methanol and diols

Hemanta Deka, Ida Ritacco, Natalia Fridman, Lucia Caporaso* and Moris S. Eisen*

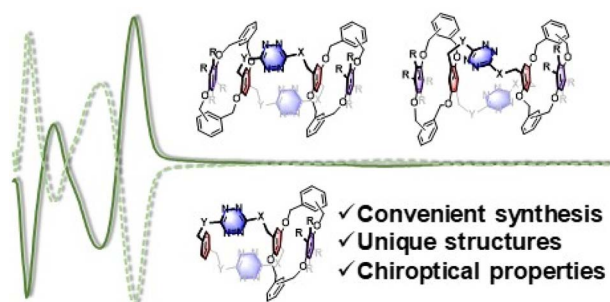
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An equivariant generative framework for molecular graph-structure Co-design

Zaixi Zhang, Qi Liu,* Chee-Kong Lee, Chang-Yu Hsieh and Enhong Chen

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Tetrahomo corona[4]arene-based spirophanes: synthesis, structure, and properties

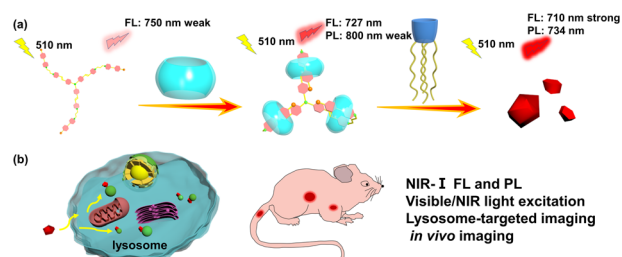
Shen-Yi Guo, Zhuo-Ang Zhang, Shuo Tong,* Qing-Hui Guo, Ruimao Hua and Mei-Xiang Wang*



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Conformationally confined three-armed supramolecular folding for boosting near-infrared biological imaging

Hui-Juan Wang, Meng-Meng Zheng, Wen-Wen Xing, Yong-Xue Li, Yao-Yao Wang, Hongjie Zhu, Ying-Ming Zhang,* Qilin Yu* and Yu Liu*



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The H-NOX protein structure adapts to different mechanisms in sensors interacting with nitric oxide

Byung-Kuk Yoo, Sergei G. Kruglik, Jean-Christophe Lambry, Isabelle Lamarre, C. S. Raman, Pierre Nioche and Michel Negrerie*

