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Organic & Biomolecular Chemistry

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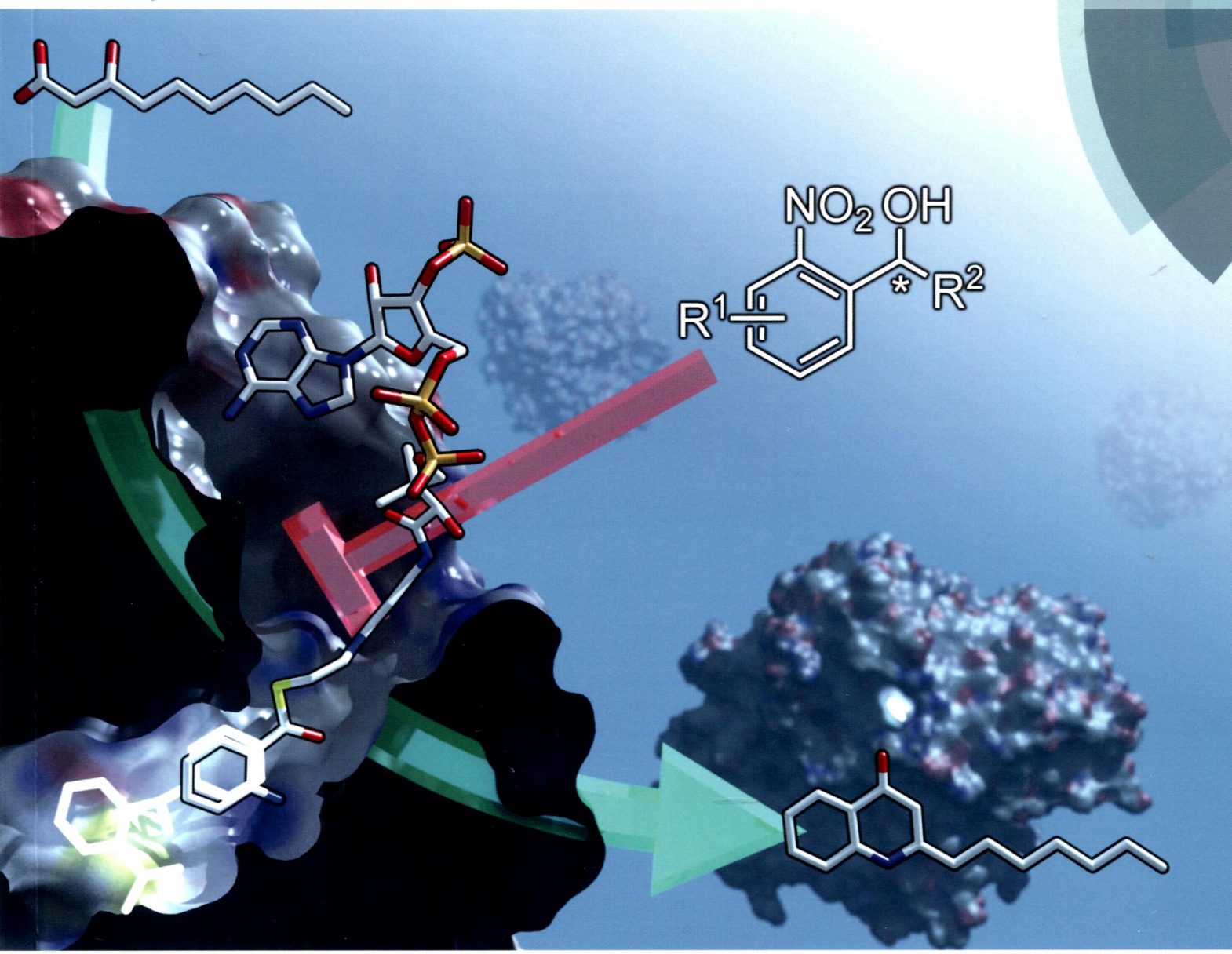

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ROYAL SOCIETY OF CHEMISTRY

PAPER
Martin Empting, Rolf W. Hartmann *et al.*
From *in vitro* to *in cellulo*: structure–activity relationship of (2-nitrophenyl)-methanol derivatives as inhibitors of PqsD in *Pseudomonas aeruginosa*

Organic & Biomolecular Chemistry

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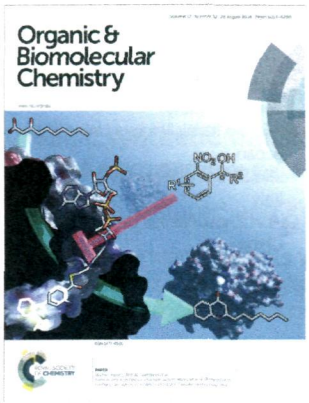

Cover
See Martin Empting, Rolf W. Hartmann *et al.*, pp. 6094–6104.

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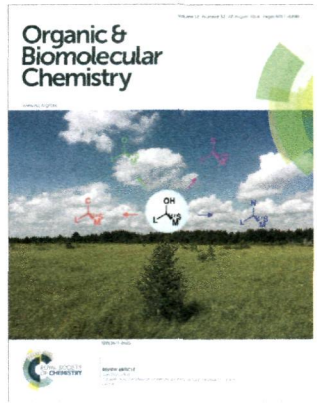

Inside cover
See Jian Zhou *et al.*, pp. 6033–6048.

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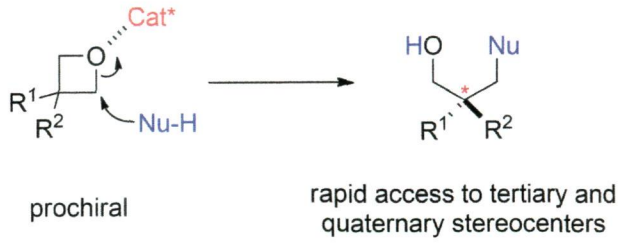
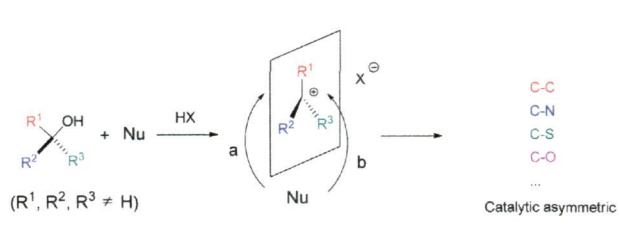
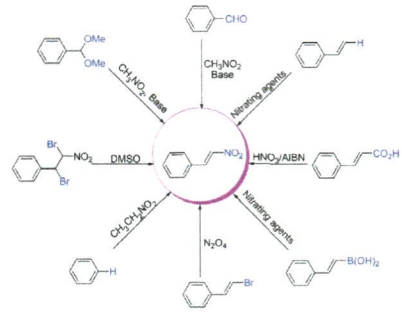
PERSPECTIVE

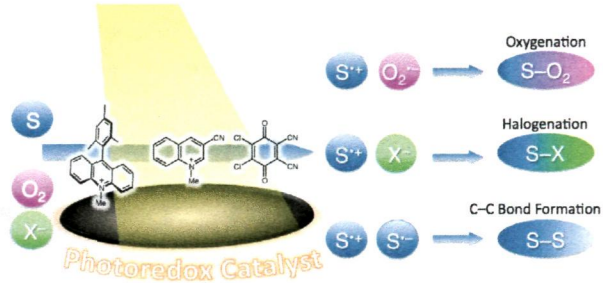


REVIEWS

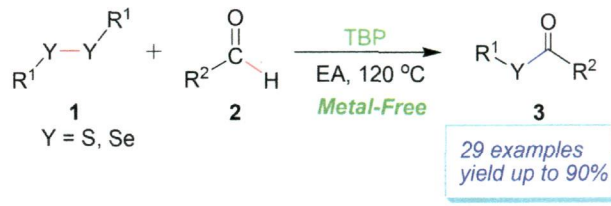


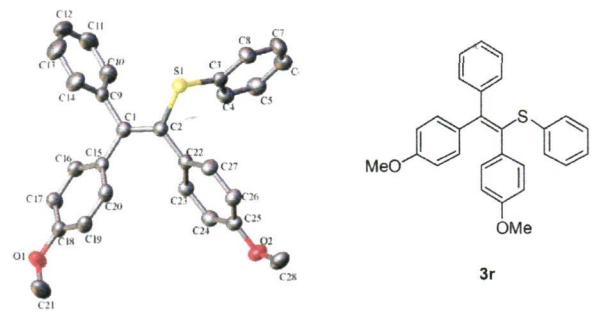
REVIEWS

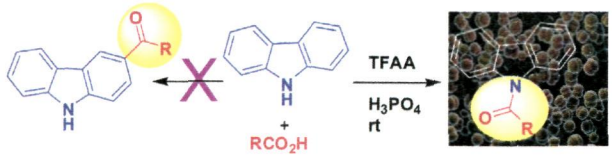




COMMUNICATIONS



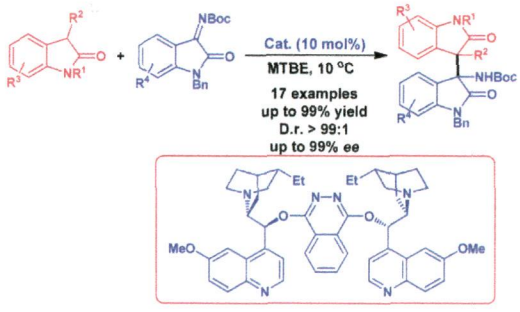




$TFAA/H_3PO_4$ mediated unprecedented N-acylation of carbazoles leading to small molecules possessing anti-proliferative activities against cancer cells

Sunder Kumar Kolli, Bagineni Prasad, P. Vijaya Babu, Mohd Ashraf Ashfaq, Nasreen Z. Ehtesham, R. Ramesh Raju* and Manojit Pal*

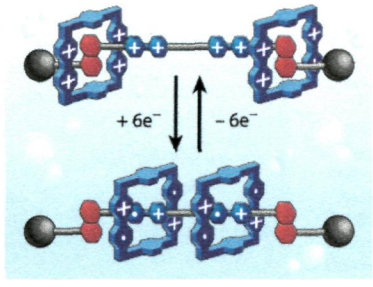
$TFAA/H_3PO_4$-mediated unusual N-acylation of carbazoles afforded potential anti-proliferative agents.



Highly enantioselective synthesis of bisoxindoles with two vicinal quaternary stereocenters *via* Lewis base mediated addition of oxindoles to isatin-derived ketimines

Zhongkai Tang, Yan Shi, Haibin Mao, Xuebin Zhu, Weipeng Li, Yixiang Cheng, Wen-Hua Zheng* and Chengjian Zhu*

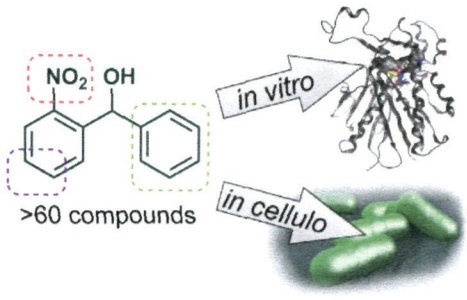
A highly efficient method provides access to the bisoxindole structure moiety with two vicinal quaternary stereogenic centers (>99 : 1 dr, >99% ee).



Relative contractile motion of the rings in a switchable palindromic [3]rotaxane in aqueous solution driven by radical-pairing interactions

Leah S. Witus, Karel J. Hartlieb, Yuping Wang, Aleksandrs Prokofjevs, Marco Frasconi, Jonathan C. Barnes, Edward J. Dale, Albert C. Fahrenbach and J. Fraser Stoddart*

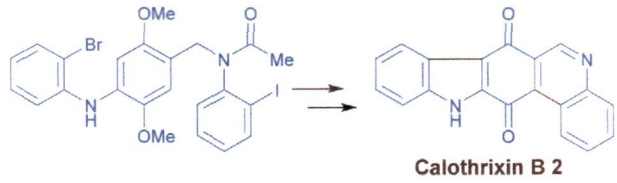
This communication describes a mechanically interlocked molecule (MIM), capable of switchable and reversible linear molecular motion.

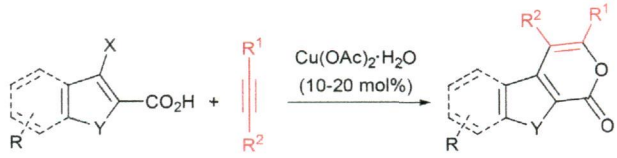


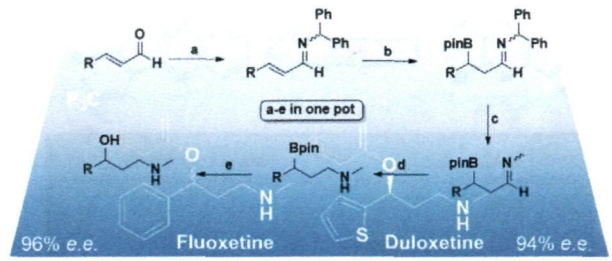
From *in vitro* to *in cellulo*: structure–activity relationship of (2-nitrophenyl)methanol derivatives as inhibitors of PqsD in *Pseudomonas aeruginosa*

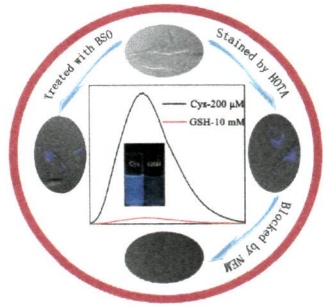
Michael P. Storz, Giuseppe Allegretta, Benjamin Kirsch, Martin Empting* and Rolf W. Hartmann*

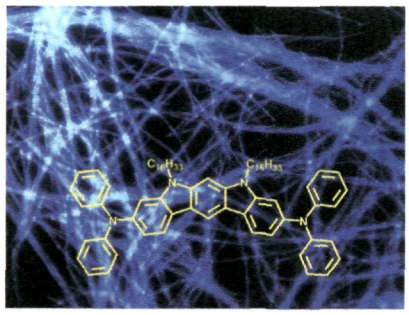
More than 60 derivatives of (2-nitrophenyl)methanol were synthesized and evaluated regarding their potency to inhibit PqsD. *In vitro* and *in cellulo* structure–activity relationships were derived.







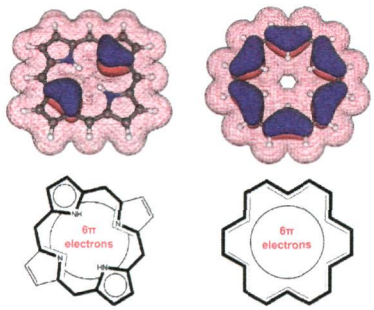




Balanced π–π interactions directing the self-assembly of indolocarbazole-based low molecular mass organogelators

Peng Gong, Pengchong Xue, Chong Qian, Zhenqi Zhang and Ran Lu*

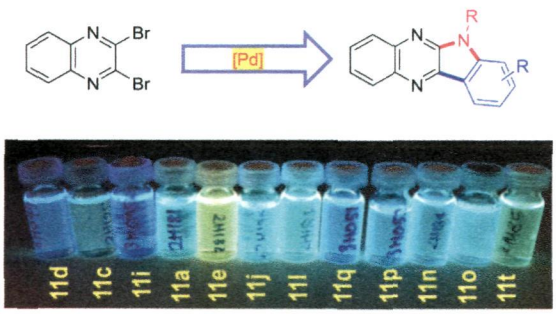
New indolocarbazole-based organogelators emitting strong blue light have been synthesized.



Deciphering aromaticity in porphyrinoids *via* adaptive natural density partitioning

Alexander S. Ivanov and Alexander I. Boldyrev*

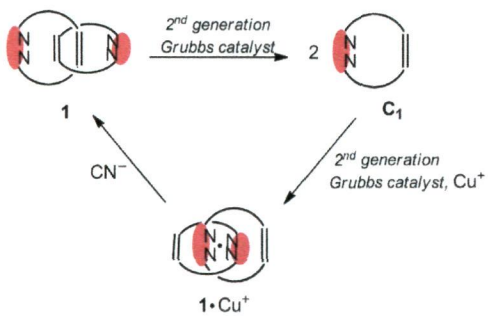
Aromaticity in porphyrins is described by the adaptive natural density partitioning analysis.



Palladium catalyzed synthesis and physical properties of indolo[2,3-*b*]quinoxalines

Tran Quang Hung, Do Huy Hoang, Ngo Ngoc Thang, Tuan Thanh Dang,* Khurshid Ayub, Alexander Villinger, Aleksej Friedrich, Stefan Lochbrunner, Gerd-Uwe Flechsig and Peter Langer*

A series of indolo[2,3-*b*]quinoxaline derivatives were efficiently synthesized from 2,3-dibromoquinoxaline by two pathways.



Copper(I)-induced amplification of a [2]catenane in a virtual dynamic library of macrocyclic alkenes

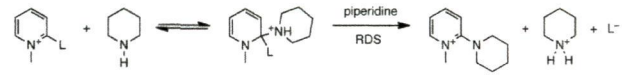
José Augusto Berrocal, Marko M. L. Nieuwenhuizen, Luigi Mandolini, E. W. Meijer and Stefano Di Stefano*

The interlocked virtual component **1** of a well-behaved dynamic library of cyclic olefins is resuscitated by means of the template effect.

Reactivity in the nucleophilic aromatic substitution reactions of pyridinium ions

Jeannette T. Bowler, Freeman M. Wong, Scott Gronert,* James R. Keeffe* and Weiming Wu*

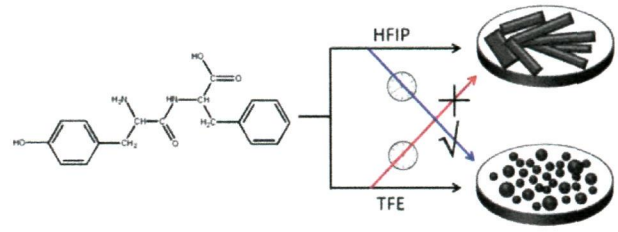
The nucleophilic aromatic substitution reactions of piperidine with *N*-methylpyridinium ions in methanol occur *via* rate determining preassociation of a second piperidine molecule with the addition intermediate followed by barrier-free deprotonation. Loss of leaving group is concurrent with deprotonation for Cl, Br, and I (E2), but subsequent to deprotonation, although rapid, for CN and F ($E1cB_{IRR}$).



1,1,1,3,3,3-Hexafluoro-2-propanol and 2,2,2-trifluoroethanol solvents induce self-assembly with different surface morphology in an aromatic dipeptide

Samala Murali Mohan Reddy, Ganesh Shanmugam* and Asit Baran Mandal*

1,1,1,3,3,3-Hexafluoro-2-propanol and 2,2,2-trifluoroethanol solvents, which are known to disaggregate self-assembled peptides, induce the self-assembly of aromatic dipeptides to give structures with different surface morphologies.



Synthetic and mechanistic aspects of the regioselective base-mediated reaction of perfluoroalkyl- and perfluoroarylsilanes with heterocyclic *N*-oxides

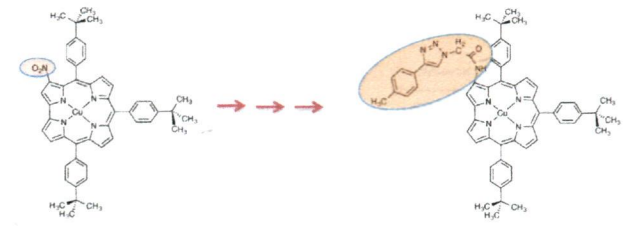
David E. Stephens, Gabriel Chavez, Martin Valdes, Monica Dovalina, Hadi D. Arman and Oleg V. Larionov*

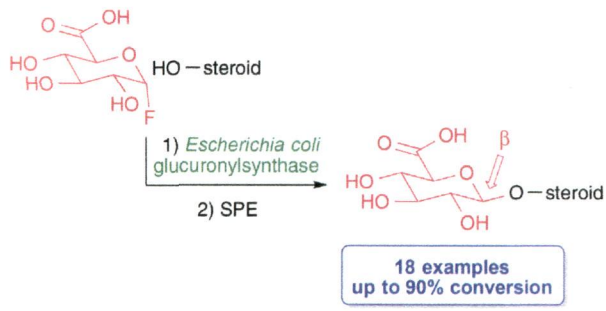
Novel and efficient method of direct perfluoroalkylation of azine *N*-oxides has been developed and interesting mechanistic details have been provided.

3-NO_2-5,10,15-triarylcorrolato-Cu as a versatile platform for synthesis of novel 3-functionalized corrole derivatives

M. Stefanelli, M. Mancini, M. Raggio, S. Nardis,* F. R. Fronczek, G. T. McCandless, K. M. Smith and R. Paolesse

By way of a β-acylated copper corrolate, a novel corrole derivative bearing an alkyl azide group on the peripheral positions was obtained and successfully exploited in click chemistry reactions.

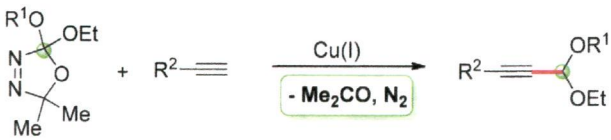




The *Escherichia coli* glucuronylsynthase promoted synthesis of steroid glucuronides: improved practicality and broader scope

Paul Ma, Nicholas Kanizaj, Shu-Ann Chan, David L. Ollis and Malcolm D. McLeod*

Steroid glucuronides can be quickly and conveniently prepared on the milligram scale using the *E. coli* glucuronylsynthase enzyme followed by purification with solid-phase extraction.



CuI-catalyzed cross-coupling of terminal alkynes with dialkoxycarbenes: a general method for the synthesis of unsymmetrical propargylic acetals

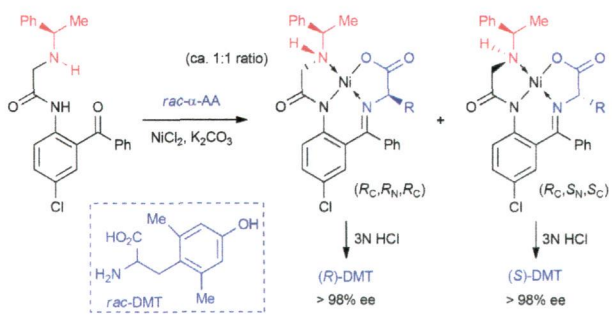
Tiebo Xiao, Ping Zhang, Yang Xie, Jun Wang and Lei Zhou*

A general source of dialkoxycarbenes, 2,2-dialkoxy-5,5-dimethyl-Δ^3-1,3,4-oxadiazolines, have been successfully employed as coupling partners in CuI-catalyzed cross-coupling reactions with terminal alkynes, which afforded various unsymmetrical propargylic acetals in good yields.

One-pot pseudo three-component reaction of nitroketene-*N,S*-acetals and aldehydes for synthesis of highly functionalized hexa-substituted 1,4-dihydropyridines

H. Surya Prakash Rao* and A. Parthiban

Pseudo three-component condensation of aliphatic/aromatic/α,β-unsaturated aldehydes and nitroketene-*N,S*-acetals to afford diversely functionalized hexa-substituted 1,4-dihydropyridines under 2-aminopyridine catalysis was achieved.



Design and synthesis of (*S*)- and (*R*)-α-(phenyl) ethylamine-derived NH-type ligands and their application for the chemical resolution of α-amino acids

Ryosuke Takeda, Akie Kawamura, Aki Kawashima, Hiroki Moriwaki, Tatsunori Sato, José Luis Aceña* and Vadim A. Soloshonok*

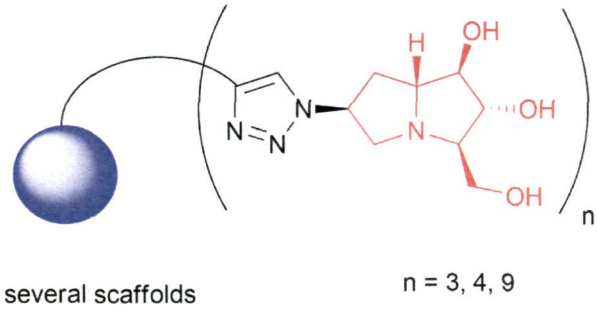
A chiral ligand reacts with racemic amino acids to produce easily separable Ni(II) complexes which can be disassembled to afford both enantiomers of target amino acids.

6250

6-Azido hyacinthacine A_2 gives a straightforward access to the first multivalent pyrrolizidine architectures

Giampiero D'Adamio, Camilla Parmeggiani, Andrea Goti,* Antonio J. Moreno-Vargas, Elena Moreno-Clavijo, Inmaculada Robina and Francesca Cardona*

The synthesis of the first multivalent pyrrolizidine iminosugars is reported, with up to 9 bioactive molecules on the same scaffold.



6267

Synthesis, and the antioxidant, neuroprotective and P-glycoprotein induction activity of 4-arylquinoline-2-carboxylates

Jaideep B. Bharate, Abubakar Wani, Sadhana Sharma, Shahi Imam Reja, Manoj Kumar, Ram A. Vishwakarma,* Ajay Kumar* and Sandip B. Bharate*

An efficient synthesis of 4-arylquinoline-2-carboxylates and their antioxidant, neuroprotective and P-glycoprotein induction activity have been described.