

Organic & Biomolecular Chemistry

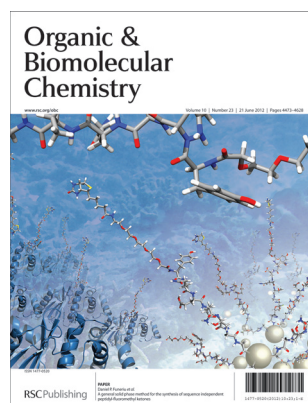
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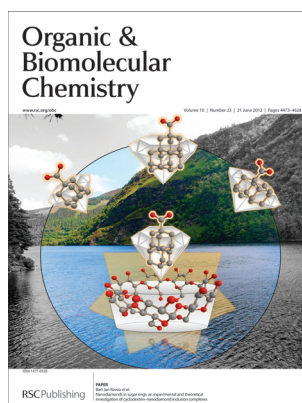
ISSN 1477-0520 CODEN OBCRAK 10(23) 4473–4628 (2012)



Cover

See Daniel P. Funeriu *et al.*, pp. 4516–4523.

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Inside cover

See Bart Jan Ravoo *et al.*, pp. 4524–4530.

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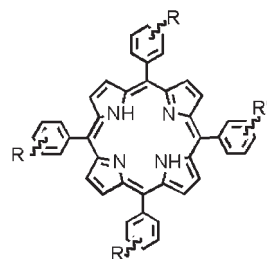
PERSPECTIVE

4485

Tumor targeting in photodynamic therapy. From glycoconjugated photosensitizers to glycodendrimeric one. Concept, design and properties

S  verine Ballut, Ali Makky, Beno  t Chauvin, Jean-Philippe Michel, Athena Kasselouri, Philippe Maillard* and V  ronique Rosilio

In this paper, we discuss the evolution over the last 15 years in the Curie Institute of the concept, the development of the design and some properties of glycoconjugated photosensitizers with the aim to optimize the tumor targeting in photodynamic therapy.



R = R' = α -, *m*- or *p*-O- β -Glycosyl

R' = H, R = α -, *m*- or *p*-O- β -Glycosyl

R' = H, R = *p*-O(CH₂CH₂O)₂- α -Glycosyl

R = H, R' = *p*-CONH-CHR'-CONH-C[CH₂CH₂-CONH-(CH₂CH₂O)_n-sugar]₃

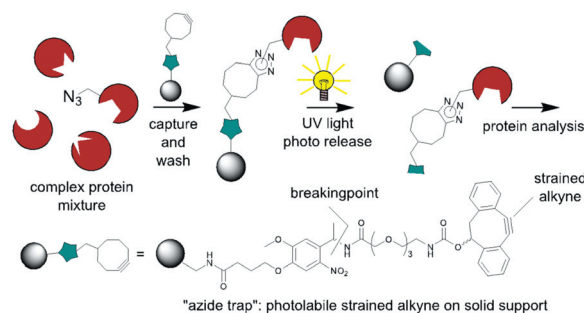
COMMUNICATIONS

4496

Strategy for catch and release of azide-tagged biomolecules utilizing a photolabile strained alkyne construct

Martin Golkowski, Carlo Pergola, Oliver Werz and Thomas Ziegler*

An immobilized photocleavable strained alkyne construct facilitates selective, "reagent-free" and time economic catch and release of azide-tagged molecules.



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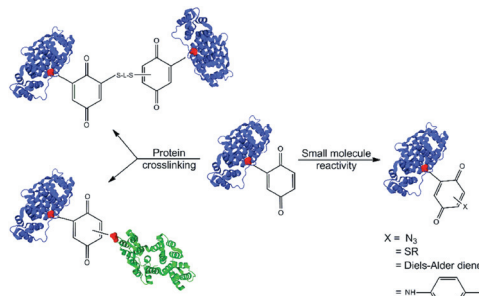
COMMUNICATIONS

4500

Site-specific crosslinking of annexin proteins by 1,4-benzoquinone: a novel crosslinker for the formation of protein dimers and diverse protein conjugates

Peng Yu, Ivona Strug, Tanya R. Cafarella, Barbara A. Seaton and Allen Krantz*

Thiol-specific crosslinking of annexin proteins using 1,4-quinone-based methodology for the coupling of proteins, and novel, diverse conjugate chemistry are described.

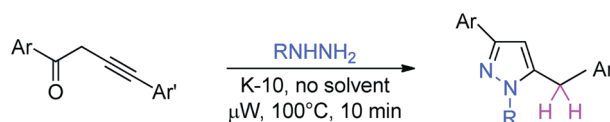


4505

Synthesis of diversely 1,3,5-trisubstituted pyrazoles via 5-*exo-dig* cyclization

Dmitry A. Borkin, Mirela Puscau, Alena Carlson, Agnes Solan, Kraig A. Wheeler, Béla Török* and Roman Dembinski*

Tandem condensation/5-*exo-dig* cyclization reactions of propargyl ketone with hydrazines gives easy access to 1,3,5-unsymmetrically substituted pyrazoles.



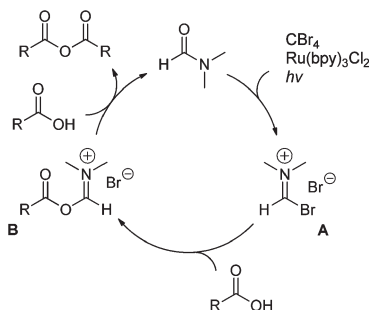
R = H, alkyl, aryl, PhCO; Ar = Ph, Ar' = *p*-MeC₆H₄

4509

Synthesis of symmetric anhydrides using visible light-mediated photoredox catalysis

Marlena D. Konieczynska, Chunhui Dai and Corey R. J. Stephenson*

A new approach to anhydride formation is reported *via* activation of C–O bonds by the Vilsmeier–Haack reagent formed by Ru(bpy)₃Cl₂ and CBr₄ in DMF.



4512

The ligand and base-free Pd-catalyzed oxidative Heck reaction of arylboronic acids and olefins

Peng Sun, Yan Zhu, Hailong Yang, Hong Yan, Linhua Lu, Xiang Zhang and Jincheng Mao*

Highly effective Pd-catalyzed Heck-type oxidative couplings between arylboronic acids and terminal olefins were reported.



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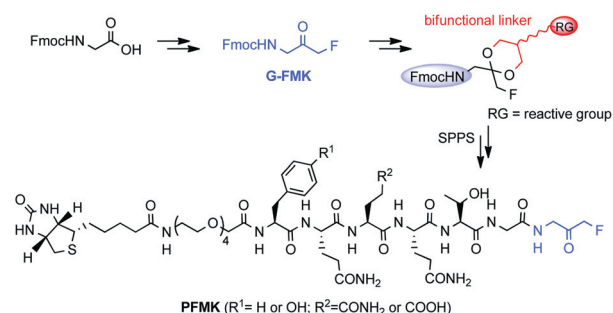
PAPERS

4516

A general solid phase method for the synthesis of sequence independent peptidyl-fluoromethyl ketones

Gheorghe-Doru Roiban, Mihaela Matache, Niculina D. Hădăde* and Daniel P. Funeriu*

A new bifunctional linker for incorporation of fluoromethylketone units at C-terminal of peptide sequences.

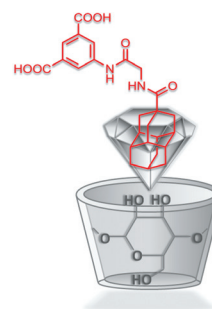


4524

Nanodiamonds in sugar rings: an experimental and theoretical investigation of cyclodextrin–nanodiamond inclusion complexes

Jens Voskuhl, Mark Waller,* Sateesh Bandaru, Boryslav A. Tkachenko, Carlo Fregonese, Birgit Wibbeling, Peter R. Schreiner* and Bart Jan Ravoo*

The carboxylic acid derivatives of diamantanes and triamantanes form exceptionally stable inclusion complexes with cyclodextrins.

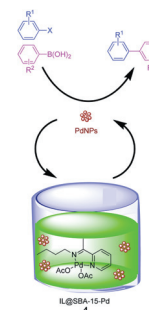


4531

SBA-15-functionalized palladium complex partially confined with ionic liquid: an efficient and reusable catalyst system for aqueous-phase Suzuki reaction

Babak Karimi* and Asghar Zamani

A novel SBA-15 functionalized palladium complex partially confined with 1-butyl-3-methylimidazolium hexafluorophosphate ionic liquid was found to be a very efficient and reusable catalyst in the Suzuki–Miyaura coupling reaction of aryl halides under aqueous conditions.

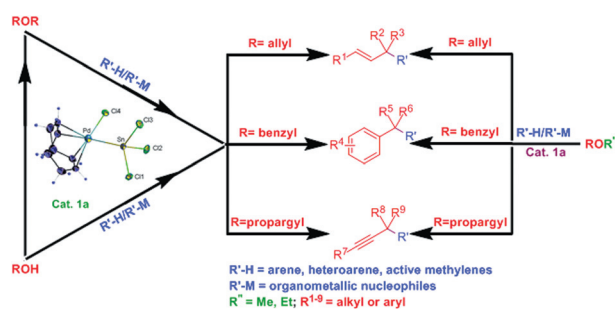


4537

First example of a heterobimetallic ‘Pd–Sn’ catalyst for direct activation of alcohol: efficient allylation, benzylation and propargylation of arenes, heteroarenes, active methylenes and allyl-Si nucleophiles

Debjit Das, Sanjay Pratihar, Ujjal Kanti Roy, Dipakranjan Mal* and Sujit Roy*

Arenes, heteroarenes, 1,3-dicarbonyls and organosilicon nucleophiles undergo highly efficient alkylation with allylic, propargylic and benzylic alcohols in the presence of a new ‘Pd–Sn’ bimetallic catalyst.



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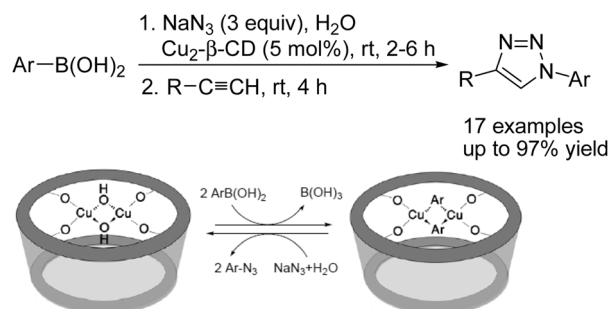
PAPERS

4543

One-pot synthesis of 1,2,3-triazoles from boronic acids in water using Cu(II)- β -cyclodextrin complex as a nanocatalyst

Babak Kaboudin,* Yaghoub Abedi and Tsutomu Yokomatsu

The Cu₂- β -CD catalyzed one-pot *in situ* azidation of arylboronic acids for the synthesis of 1,2,3-triazoles by click cyclization in water is reported.

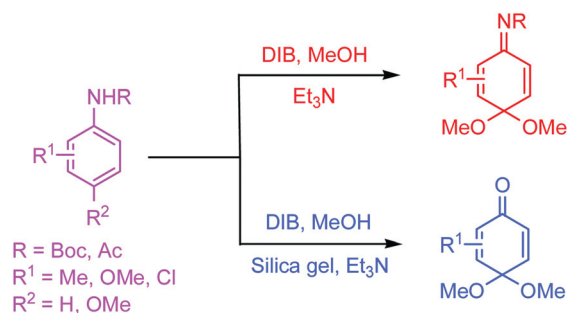


4549

Hypervalent iodine mediated synthesis of carbamate protected *p*-quinone monoimide ketals and *p*-benzoquinone monoketals

Naganjaneyulu Bodipati and Rama Krishna Peddinti*

A practical synthesis of *p*-quinone monoimide ketals and *p*-quinone monoketals are obtained from single starting materials, *viz.* 4-methoxyanilides, under different conditions. The double oxidation on simple anilides provided *p*-quinone monoimide ketals.

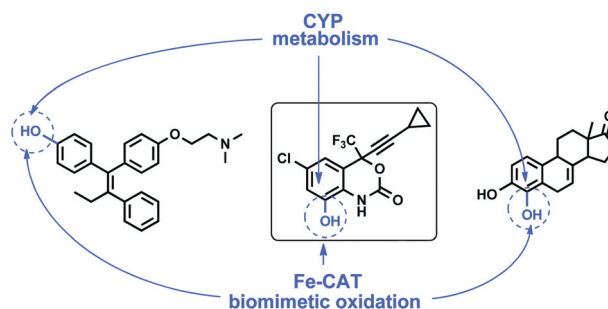


4554

Biomimetic oxidation of aromatic xenobiotics: synthesis of the phenolic metabolites from the anti-HIV drug efavirenz

Riccardo Wanke,* David A. Novais, Shrika G. Harjivan, M. Matilde Marques and Alexandra M. M. Antunes*

We report the oxidation of efavirenz, equilin and tamoxifen by a bio-inspired Fe-complex, yielding the phenolic metabolites of these xenobiotics.

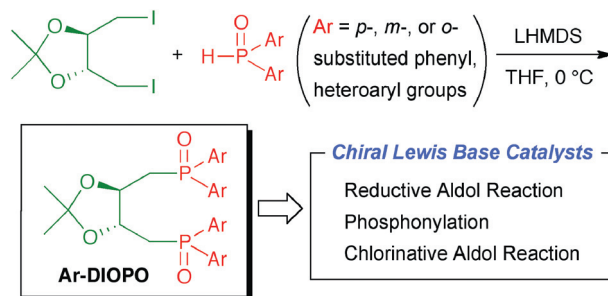


4562

Synthesis of aryl group-modified DIOP dioxides (Ar-DIOPs) and their application as modular Lewis base catalysts

Yusuke Ohmaru, Norimasa Sato, Makoto Mizutani, Shunsuke Kotani, Masaharu Sugiura* and Makoto Nakajima*

Aryl group-modified DIOP dioxides (Ar-DIOPs) are readily available and serve as effective modular chiral Lewis base catalysts.





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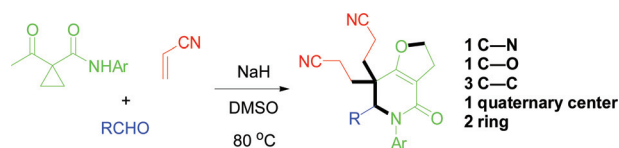
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4571

Multi-component anion relay cascade of 1-acetylcyclopropanecarboxamides, aldehydes and acrylonitrile: access to biscyanoethylated furo[3,2-*c*]pyridinones

Shaoxia Lin, Ying Wei, Fushun Liang,* Baozhong Zhao, Yanling Liu and Pengjun Liu*

A highly efficient multi-component anion relay cascade reaction provides strategically novel and atom-economic access to biologically important biscyanoethylated furo[3,2-*c*]pyridinones.

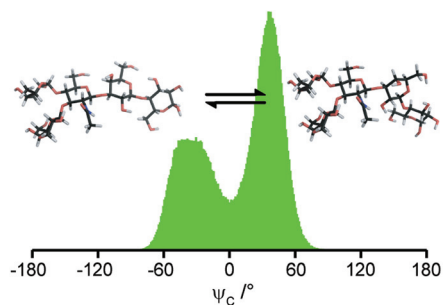


4577

Conformational flexibility of the pentasaccharide LNF-2 deduced from NMR spectroscopy and molecular dynamics simulations

Elin Säwén, Florian Hinterholzinger, Clas Landersjö and Göran Widmalm*

The bioactive LNF-2 pentasaccharide, with its Lewis A epitope, may have a prearranged three-dimensional structure for binding to protein receptors.

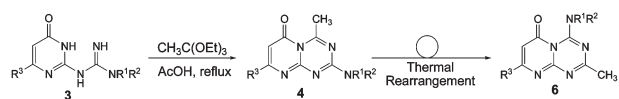


4586

Regioselective synthesis of pyrimido[1,2-*a*][1,3,5]triazin-6-ones *via* reaction of 1-(6-oxo-1,6-dihydropyrimidin-2-yl)guanidines with triethylorthoacetate: observation of an unexpected rearrangement

Nikhil Sachdeva, Anton V. Dolzhenko and Wai Keung Chui*

An unexpected rearrangement was observed in the regioselective synthesis of pyrimido[1,2-*a*][1,3,5]triazin-6-ones *via* the reaction of 1-(6-oxo-1,6-dihydropyrimidin-2-yl)guanidines with triethylorthoacetate.

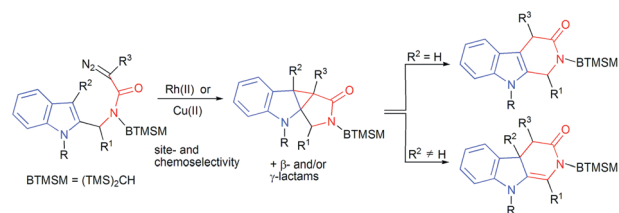


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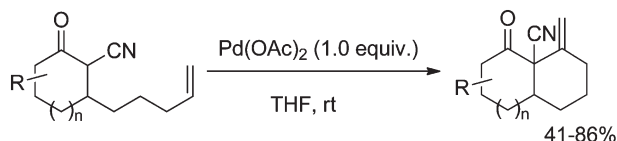
Conformational, steric and electronic effects on the site- and chemoselectivity of the metal-catalyzed reaction of *N*-bis(trimethylsilyl)methyl, *N*-(2-indolyl)methyl α -diazoamides

Bao Zhang and Andrew G. H. Wee*

Good to excellent site- and chemoselectivity are realized in the metal-catalyzed reaction of *N*-bis(trimethylsilyl)methyl, *N*-(indolyl)methyl α -diazoamides, which leads to tetracyclic products that can undergo rearrangement to give β -carboline derivatives.



4609

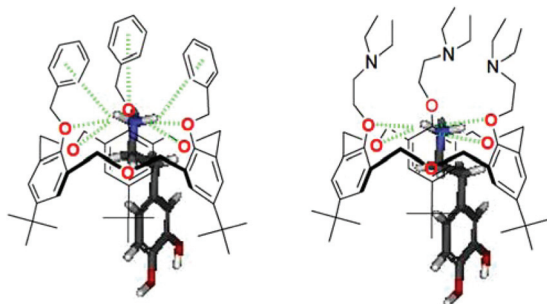


Palladium(II) acetate mediated oxidative cyclization of ω -unsaturated α -cyano ketones for facile construction of methylenecyclohexane ring system

Min-Tsang Hsieh,* Kak-Shan Shia, Hsing-Jang Liu and Sheng-Chu Kuo*

A highly efficient annulative approach has been developed through a convenient 1,4-addition of 4-pentenylmagnesium bromide to 2-cyano-2-cycloalkenones followed by a Pd(II)-mediated oxidative cyclization of the resulting ω -unsaturated α -cyano ketones as a key operative sequence.

4618



Hexahomotrioxacalix[3]arene derivatives as ionophores for molecular recognition of dopamine, serotonin and phenylethylamine

Xin-Long Ni, Shofiur Rahman, Shi Wang, Cheng-Cheng Jin, Xi Zeng, David L. Hughes, Carl Redshaw and Takehiko Yamato*

Hexahomotrioxacalix[3]arene derivatives act as receptors for molecular recognition of dopamine, serotonin and phenylethylamine through hydrophobic effect and intermolecular hydrogen bonding.

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