

Organic & Biomolecular Chemistry

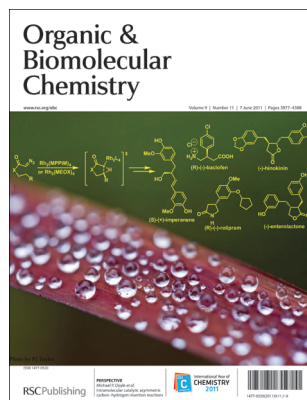
An international journal of synthetic, physical and biomolecular organic chemistry

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IN THIS ISSUE

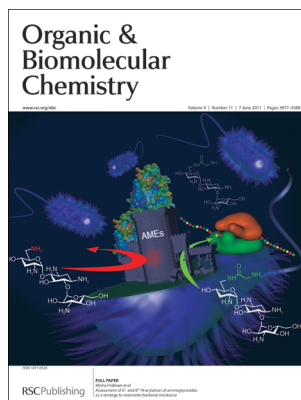
ISSN 1477-0520 CODEN OBCRAK 9(11) 3977–4388 (2011)



Cover

See Michael P. Doyle *et al.*, pp. 4007–4016.

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Inside cover

See Micha Fridman *et al.*, pp. 4057–4063.

Aminoglycoside acetyltransferase AAC(6') belonging to the aminoglycoside-modifying enzymes (AMEs) does not deactivate the 6'-N-glycyl tobramycin which attacks the bacterial ribosome (green arrow). In contrast, the parent aminoglycoside tobramycin cannot pass through bacterial resistance mechanism (red arrow).

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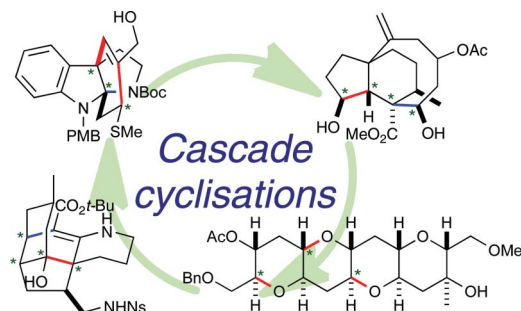
EMERGING AREA

3997

Cascade polycyclisations in natural product synthesis

Edward A. Anderson*

Cascade reactions provide an unparalleled method to synthesise polycyclic ring systems; in this Emerging Area article, a selection of the most recent and impressive examples of applications to natural product synthesis, and future directions for the field, are discussed.



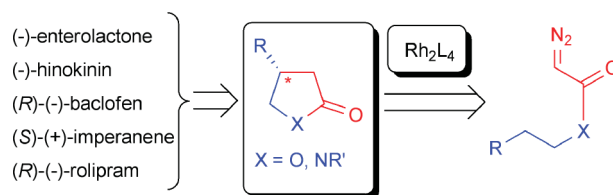
PERSPECTIVE

4007

Intramolecular catalytic asymmetric carbon–hydrogen insertion reactions. Synthetic advantages in total synthesis in comparison with alternative approaches

Michael P. Doyle,* Maxim Ratnikov and Yu Liu

Chiral dirhodium(II) carboxamidates are optimum catalysts for highly stereoselective carbon–hydrogen insertion reactions that produce biologically relevant lactones and lactams, and this methodology is generally superior to alternative processes.



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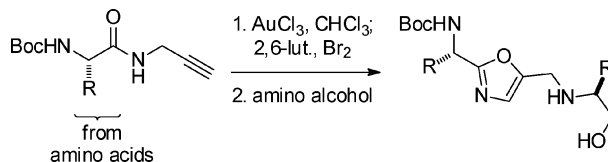
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4017

Gold-catalysed synthesis of amino acid-derived 2,5-disubstituted oxazoles

Christopher L. Paradise, Pooja R. Sarkar, Mina Razzak and Jef K. De Brabander*

We describe a tandem gold(III)-catalysed cycloisomerisation–bromination of propargylic amides, followed by further processing into valuable *bis*-heterocyclic compounds including novel dipeptide mimetics.

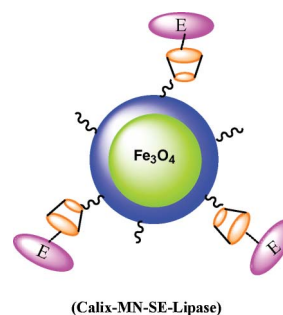


4021

Improvement of catalytic properties of *Candida Rugosa* lipase by sol–gel encapsulation in the presence of magnetic calix[4]arene nanoparticles

Serkan Sayin, Elif Yilmaz and Mustafa Yilmaz

Candida rugosa lipase (CRL) was encapsulated within a chemically inert sol-gel support prepared by polycondensation with tetraethoxysilane and octyltriethoxysilane in the presence of *N*-methylglucamine based calix[4]arene magnetic nanoparticles. The results indicate that the magnetic calix[4]arene based encapsulated lipase showed particularly high conversion and enantioselectivity.

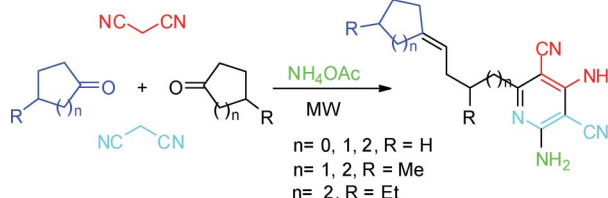


4025

New multicomponent cyclization: domino synthesis of pentasubstituted pyridines under solvent-free conditions

Bo Jiang, Xiang Wang, Feng Shi, Shu-Jiang Tu* and Guigen Li*

New five-component domino reaction for rapid synthesis of highly functionalized pentasubstituted pyridines was established giving up to 87% yield.

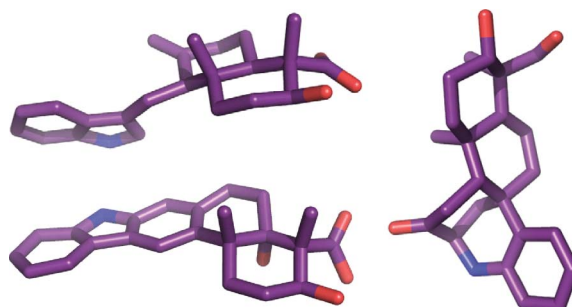


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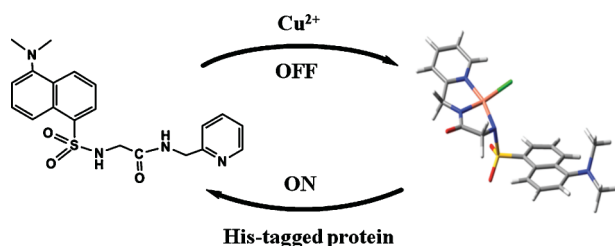
A family of multicyclic indolosesquiterpenes from a bacterial endophyte

Ling Ding, Armin Maier, Heinz-Herbert Fiebig, Wen-Han Lin and Christian Hertweck*

Three multicyclic indolosesquiterpenes, xiamycin B, indosespene, and sespenine, along with the known xiamycin A, share an unusual terpene alkaloid pathway in *Streptomyces* sp. HKI0595, an endophyte of the widespread mangrove tree *Kandelia candel*.



4032

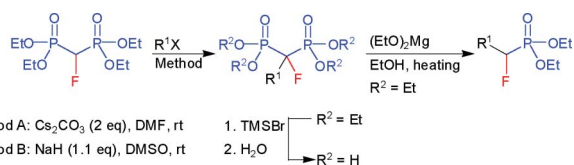


The switch-on luminescence sensing of histidine-rich proteins in solution: a further application of a Cu²⁺ ligand

Bin Wang, Yang Gao, Hong-Wei Li, Zhi-Peng Hu and Yuqing Wu*

A new **1**/Cu²⁺ complex for the detection of His-tagged protein has been developed, based on an improved probe by closely mimicking the structure of a peptide, ATCUN. In aqueous solution, **1**/Cu²⁺ has good selectivity to histidine and cysteine, and further can detect histidine-rich protein by releasing the quenched fluorescence.

4035

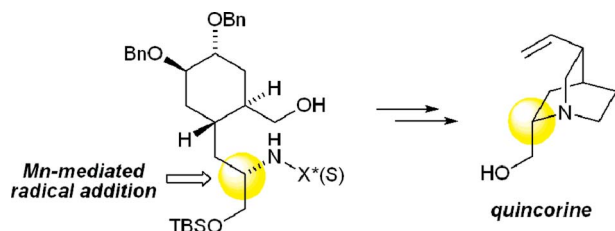


A new route to α -alkyl- α -fluoromethylenebisphosphonates

Petr Beier,* Stanislav Opekar, Mikhail Zibinsky, Inessa Bychinskaya and G. K. Surya Prakash*

Synthesis of α -alkyl- α -fluoromethylenebisphosphonates and corresponding bisphosphonic acids is described by alkylation of tetraethyl fluoromethylenebisphosphonate. Alkoxide-induced carbon-phosphorus bond cleavage of title compounds gave α -fluorophosphonates.

4039



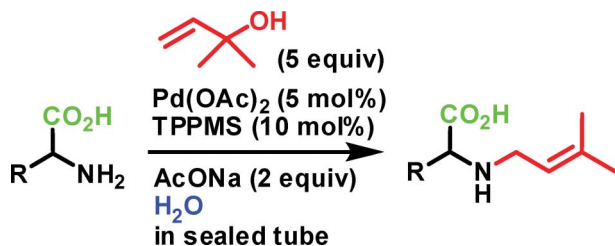
Intermolecular radical addition to *N*-acylhydrazones as a stereocontrol strategy for alkaloid synthesis: formal synthesis of quinine

Gregory K. Friestad,* An Ji, Chandra Sekhar Korapala and Jun Qin

Synthesis of quinine demonstrates the utility of intermolecular radical addition to imino compounds as a stereocontrol strategy in synthesis of complex multifunctional targets.

PAPERS

4044



Palladium-catalyzed mono-*N*-allylation of unprotected amino acids with 1,1-dimethylallyl alcohol in water

Hidemasa Hikawa* and Yuusaku Yokoyama*

Palladium-catalyzed *N*-allylation of unprotected amino acids with 1,1-dimethylallyl alcohol gave mono-*N*-allylated amino acids in good yield.

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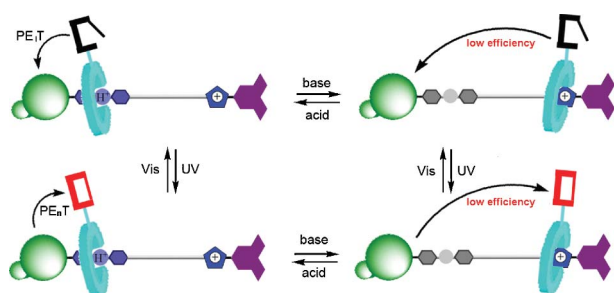
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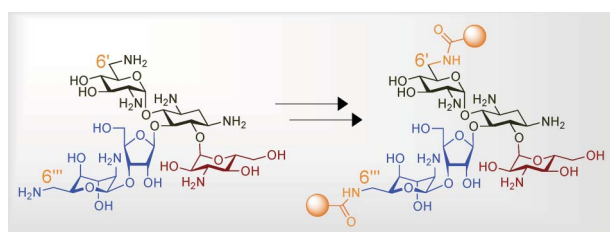


Altering intercomponent interactions in a photochromic multi-state [2]rotaxane

Hui Zhang, Xin-Xin Kou, Qiong Zhang, Da-Hui Qu* and He Tian*

By introducing a dithienylethene photochromic group in a [2]rotaxane, the multi-mode alteration of the intercomponent interactions can be realized on a unimolecular platform.

4057

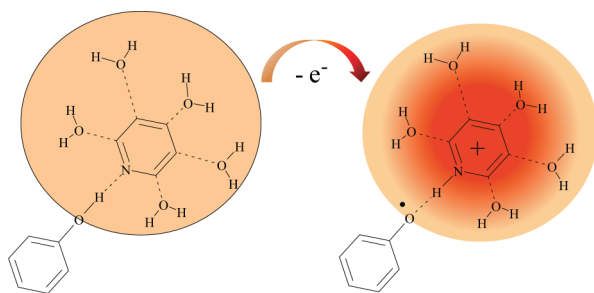


Assessment of 6'- and 6'''-N-acylation of aminoglycosides as a strategy to overcome bacterial resistance

Pazit Shaul, Keith D. Green, Roi Rutenberg, Maria Kramer, Yifat Berkov-Zrihen, Elinor Breiner-Goldstein, Sylvie Garneau-Tsodikova* and Micha Fridman*

As for 1-N-acylation, 6'- and 6'''-N-acylation of clinically used aminoglycosides offer an additional promising direction in the search for new antibiotics capable of overcoming infections by resistant bacteria.

4064

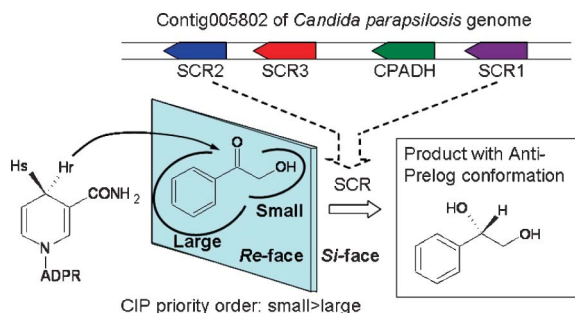


Pyridine as proton acceptor in the concerted proton electron transfer oxidation of phenol

Julien Bonin, Cyrille Costentin, Marc Robert and Jean-Michel Savéant*

In the presence of pyridine, phenol oxidation occurs concertedly with proton transfer, the charge being delocalized over a primary shell of water molecules bound to the pyridinium cation.

4070



Novel anti-Prelog stereospecific carbonyl reductases from *Candida parapsilosis* for asymmetric reduction of prochiral ketones

Yao Nie, Rong Xiao, Yan Xu* and Gaetano T. Montelione*

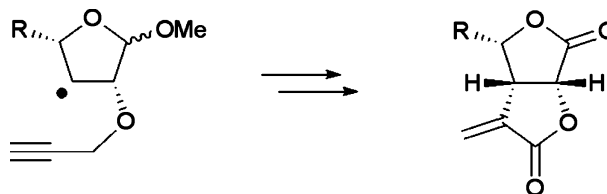
Novel anti-Prelog stereospecific carbonyl reductases discovered by *Candida parapsilosis* genomic mining for asymmetric reduction of prochiral ketones.

4079

Free radical 5-*exo*-dig cyclization as the key step in the synthesis of *bis*-butyrolactone natural products: experimental and theoretical studies

Gangavaram V. M. Sharma,* Devoju Harinada Chary, Nagula Chandramouli, Florian Achraimer, Sateesh Patrudu and Hendrik Zipse*

Radical 5-*exo*-dig cyclization is used as an entry to *bis*-butyrolactone natural products with *L-ara* configuration.

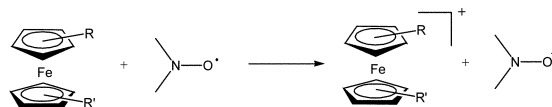


4085

One-electron oxidation of ferrocenes by short-lived *N*-oxyl radicals. The role of structural effects on the intrinsic electron transfer reactivities

Enrico Baciocchi, Massimo Bietti, Claudio D'Alfonso, Osvaldo Lanzalunga,* Andrea Lapi and Michela Salamone

The role of structural effects on the intrinsic ET reactivities of short-lived *N*-oxyl radicals have been examined through a kinetic study of the one electron oxidation reactions of substituted ferrocenes.

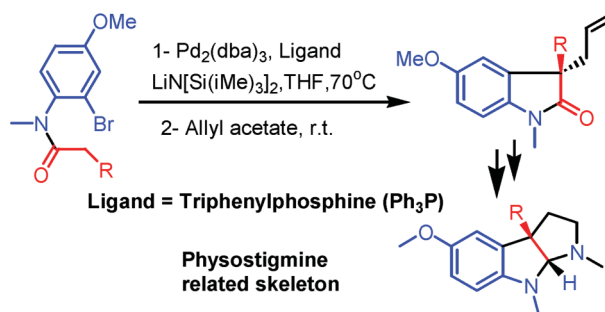


4091

Efficient synthesis of esermethole and its analogues

Yongyun Zhou, Yuanhong Zhao, Xiaoyong Dai, Jianping Liu, Liang Li and Hongbin Zhang*

Based on palladium mediated sequential arylation–allylation of *o*-bromoanilides, a flexible synthetic route towards the synthesis of pyrroloindoline alkaloids was developed.

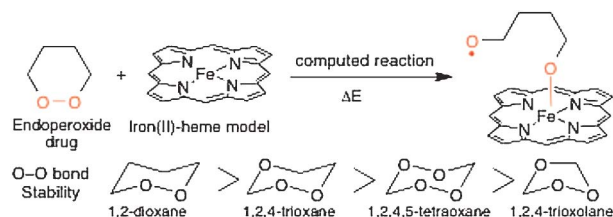


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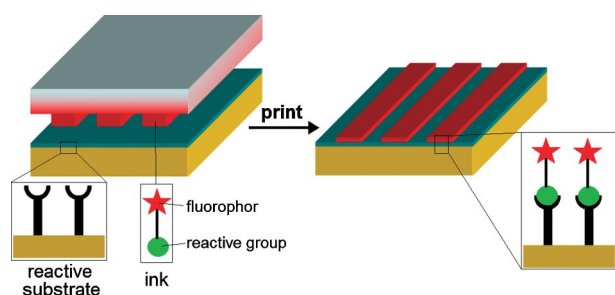
Peroxide bond strength of antimalarial drugs containing an endoperoxide cycle. Relation with biological activity

Israel Fernández* and Anne Robert*

Antimalarial endoperoxides – computed energies of the thermal homolysis of the peroxide: relation with reductive activation by iron(II)-heme, and biological activity.



4108

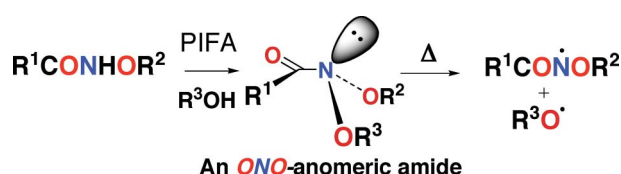


Click chemistry by microcontact printing on self-assembled monolayers: A structure–reactivity study by fluorescence microscopy

Jan Mehlich and Bart Jan Ravoo*

Surface-confined 1,3-dipolar cycloadditions, Diels–Alder cycloadditions and thiol-ene/yne reactions can be induced by microcontact printing of fluorescent inks on reactive self-assembled monolayers.

4116

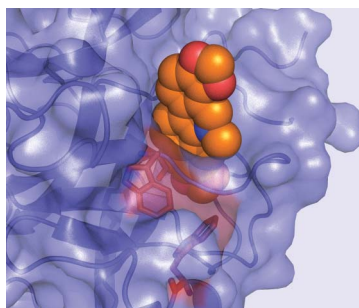


Synthesis and thermal decomposition of *N,N*-dialkoxamides

Katherine M. Digianantonio, Stephen A. Glover,*
Jennifer P. Johns and Adam A. Rosser

N,N-Dialkoxamides — unusual anomeric amides. A new PIFA mediated synthesis and studies of their radical homolysis under thermal conditions.

4127

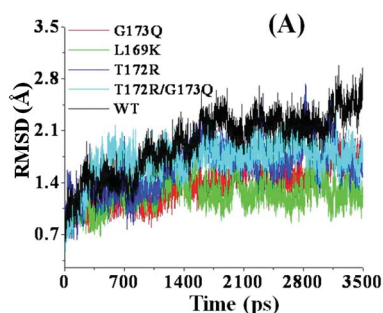


Binding of alkaloids into the S1 specificity pocket of α -chymotrypsin: Evidence from induced circular dichroism spectra

Ferenc Zsila,* Judit Kámán, Borbála Bogányi and
Dávid Józsvai

Binding of planar aromatic molecules into the S1 specificity pocket of α -chymotrypsin can be detected by measuring induced circular dichroism signals.

4138



Computational design of a thermostable mutant of cocaine esterase *via* molecular dynamics simulations

Xiaoqin Huang, Daquan Gao and Chang-Guo Zhan*

High-temperature molecular dynamics simulations have led to discovery of a thermostable mutant of cocaine esterase.

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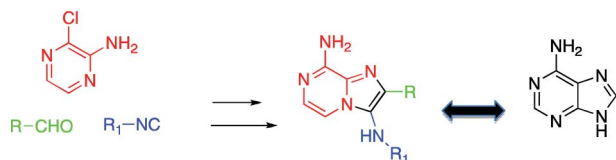
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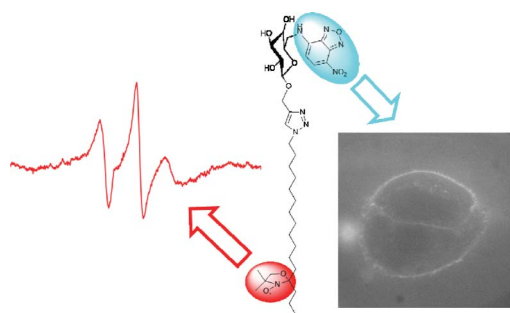


Groebke multicomponent reaction and subsequent nucleophilic aromatic substitution for a convenient synthesis of 3,8-diaminoimidazo[1,2-*a*]pyrazines as potential kinase inhibitors

Margherita Guasconi, Xiaoyun Lu, Alberto Massarotti, Antonio Caldarelli, Elisa Ciraolo, Gian Cesare Tron, Emilio Hirsch, Giovanni Sorba and Tracey Pirali*

In a program aimed at discovering novel protein kinase inhibitors, a convenient synthesis of 3,8-diaminoimidazo[1,2-*a*]pyrazines has been developed exploiting the isocyanide-based multicomponent Groebke reaction.

4150

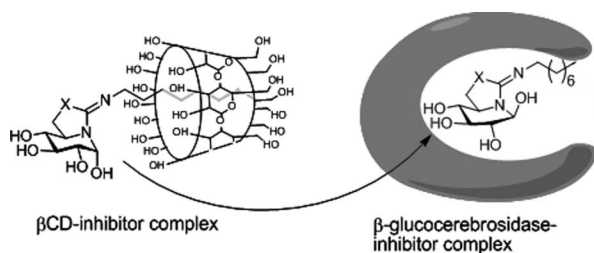


Nitroxide–fluorophore double probes: a potential tool for studying membrane heterogeneity by ESR and fluorescence

Stane Pajk,* Maja Garvas, Janez Štrancar and Slavko Pečar

New nitroxide–fluorophore double probes that enable investigation of lipid dynamics and visualization by fluorescence microscopy.

4160

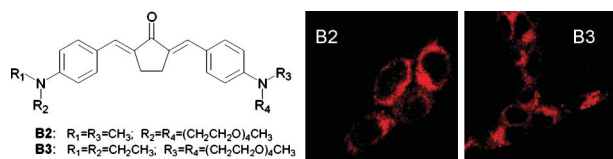


Cyclodextrin-mediated crystallization of acid β -glucosidase in complex with amphiphilic bicyclic nojirimycin analogues

Boris Brumshtein, Matilde Aguilar-Moncayo, Juan M. Benito, José M. García Fernandez, Israel Silman, Yoseph Shaaltiel, David Aviezer, Joel L. Sussman, Anthony H. Futerman and Carmen Ortiz Mellet*

Cyclodextrin-based host–guest chemistry has been exploited to facilitate co-crystallization of recombinant human acid β -glucosidase with amphiphilic bicyclic nojirimycin analogues of the sp^2 -iminosugar type.

4168



Polyethylene glycol-functionalized benzylidene cyclopentanone dyes for two-photon excited photodynamic therapy

Yuxia Zhao, Weijia Wang, Feipeng Wu,* Yang Zhou, Naiyan Huang, Ying Gu, Qianli Zou and Wei Yang

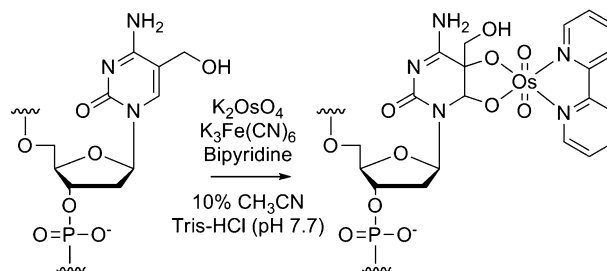
Water-soluble benzylidene cyclopentanone dyes show strong photodynamic activity under one- and two-photon excitation in *in vitro* cell experiments.

4176

Facile synthesis of hydroxymethylcytosine-containing oligonucleotides and their reactivity upon osmium oxidation

Kaori Sugizaki, Shuji Ikeda, Hiroyuki Yanagisawa and Akimitsu Okamoto*

The osmium oxidation of a 5-hydroxymethylcytosine-containing DNA provided a 5-hydroxymethylcytosine glycol–dioxidoosmium–bipyridine ternary complex in the DNA.

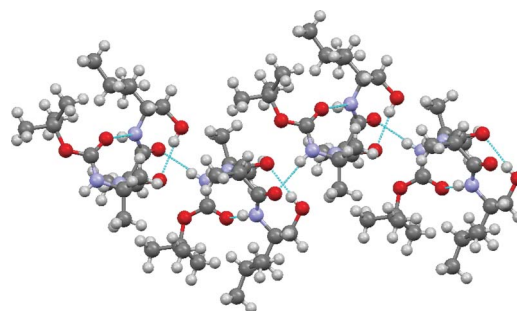


4182

A facile synthesis and crystallographic analysis of *N*-protected β -amino alcohols and short peptaibols

Sandip V. Jadhav, Anupam Bandyopadhyay, Sushil N. Benke, Sachitanand M. Mali and Hosahudya N. Gopi*

A facile method for the synthesis of *N*-protected β -amino alcohols and peptaibols using *N*-hydroxysuccinimide active esters is described, and their conformations in crystals studied.

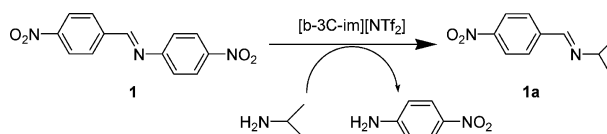


4188

Transimination reactions in [b-3C-im][NTf₂] ionic liquid

Chao-Wen Chen, Ming-Chung Tseng, San-Kai Hsiao, Wen-Hao Chen and Yen-Ho Chu*

Compared to conventional molecular solvents, the ionic liquid [b-3C-im][NTf₂] was found to promote transimination reactions with up to ~100-fold rate enhancement.

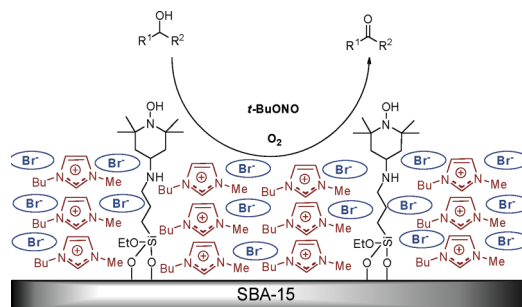


4194

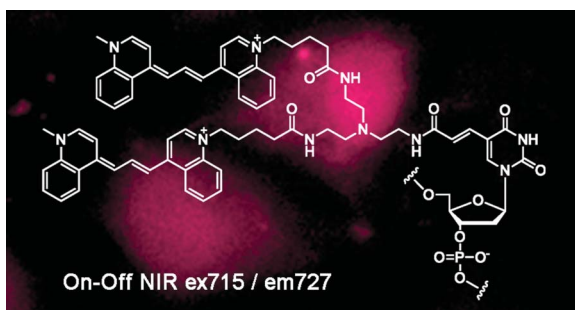
SBA-15-functionalized TEMPO confined ionic liquid: an efficient catalyst system for transition-metal-free aerobic oxidation of alcohols with improved selectivity

Babak Karimi* and Ebrahim Badreh

A novel SBA-15-functionalized TEMPO confined ionic liquid [BMIm]Br was found to be a highly efficient and recyclable catalyst system for the transition-metal-free aerobic oxidation of a wide range of structurally diverse alcohols.



4199

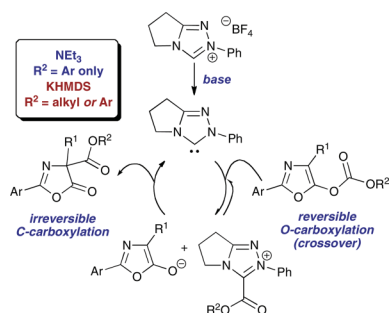


Hybridization-sensitive fluorescence control in the near-infrared wavelength range

Shuji Ikeda, Hiroyuki Yanagisawa, Akiko Nakamura, Dan Ohtan Wang, Mizue Yuki and Akimitsu Okamoto*

A series of near-infrared fluorescent probes were designed based on the concept of emission control caused by interdy excitonic interaction.

4205

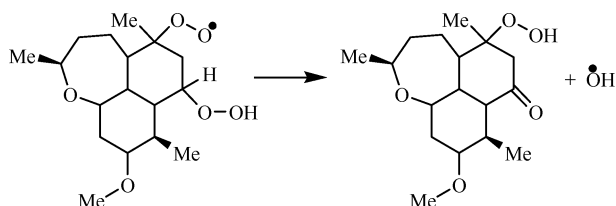


Organic base effects in NHC promoted O- to C-carboxyl transfer; chemoselectivity profiles, mechanistic studies and domino catalysis

Craig D. Campbell, Christopher J. Collett, Jennifer E. Thomson, Alexandra M. Z. Slawin and Andrew D. Smith*

The O- to C-carboxyl transfer of oxazolyl carbonates promoted by triazolinylienes, generated *in situ* with NEt₃, shows a different rate and chemoselectivity profile to the same reaction using KHMDS; the mechanism of these pathways has been probed through crossover studies.

4219

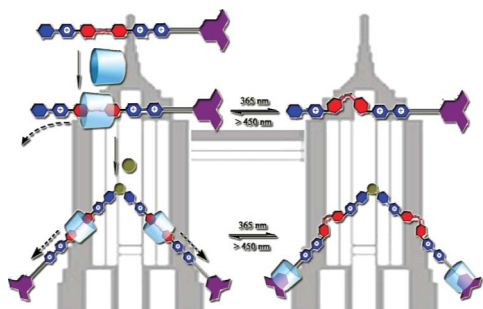


An important role of intramolecular free radical reactions in antimalarial activity of artemisinin and its analogs

Evgeny Denisov*

A new mechanism of free radical reactions of artemisinin and its analogs is proposed, where the initiation of hydroxy radicals plays a key role in the antimalarial effect.

4226

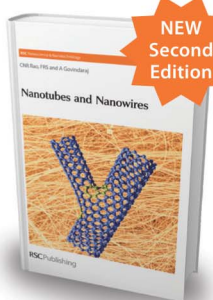


Coordination-assembly for quantitative construction of bis-branched molecular shuttles

Liangliang Zhu, Meiqun Lu, Dahui Qu, Qiaochun Wang and He Tian*

Coordination-assembly was employed to construct bis-branched molecular shuttles, and transformation of ring shuttling direction was observed in these complexes.

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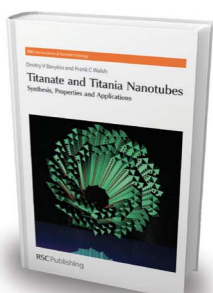
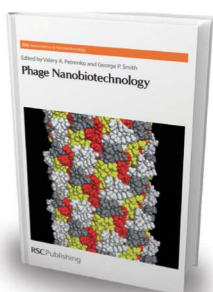
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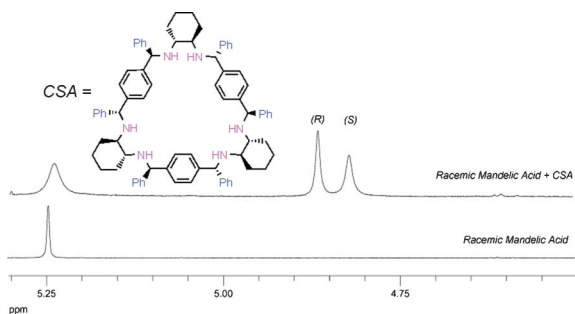
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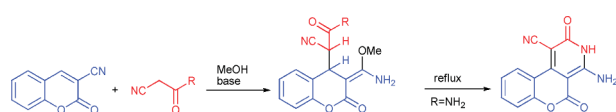


C-hexaphenyl-substituted trianglamine as a chiral solvating agent for carboxylic acids

Andrea Gualandi,* Stefano Grilli, Diego Savoia, Marcin Kwit and Jacek Gawroński*

Chiral hexaphenyl-substituted macrocycles containing twelve stereocenters have been tested as chiral solvating agents (CSAs) for α -substituted carboxylic acids, with excellent results. The conformations of the free and protonated macrocycles were inferred by spectroscopic and computational studies.

4242

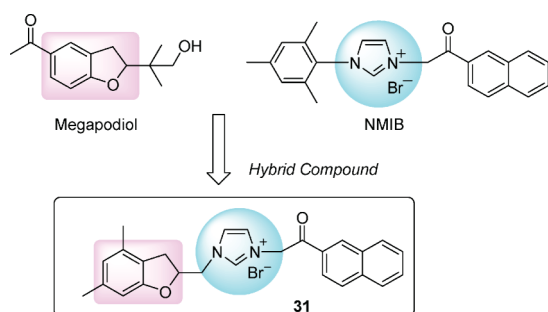


Synthesis of novel chromene scaffolds for adenosine receptors

Marta Costa, Filipe Areias, Marian Castro, Jose Brea, María I. Loza and Fernanda Proença*

A one-pot procedure was developed for the synthesis of novel chromene derivatives from 2-oxo-2*H*-chromene-3-carbonitriles and cyanoacetamides. These new scaffolds proved to be active at adenosine receptors and 4 hits were identified in this study with affinities in the submicromolar range.

4250

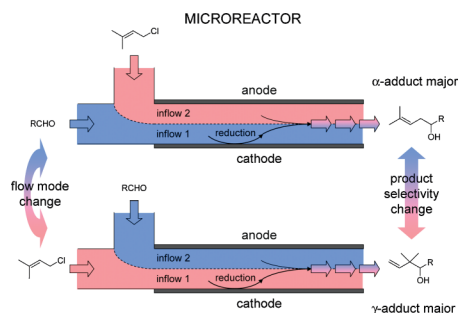


Design, synthesis and cytotoxic activities of novel hybrid compounds between dihydrobenzofuran and imidazole

Wen Chen, Xiao-Dong Yang, Yan Li, Li-Juan Yang, Xue-Quan Wang, Gao-Lan Zhang and Hong-Bin Zhang*

A series of novel hybrid compounds between dihydrobenzofuran and imidazole were synthesized and their antitumor structure–activity relationship studies were reported.

4256



Product selectivity control induced by using liquid–liquid parallel laminar flow in a microreactor

Fumihito Amemiya, Hideyuki Matsumoto, Keishi Fuse, Tsuneo Kashiwagi, Chiaki Kuroda, Toshio Fuchigami and Mahito Atohe*

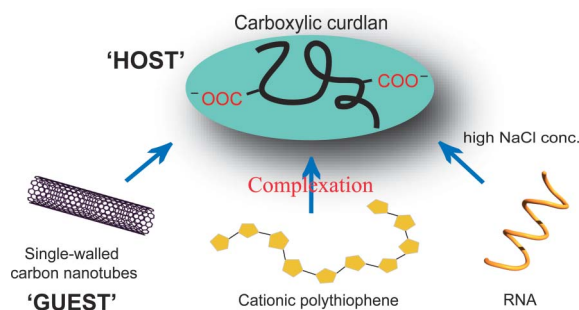
The product selectivity of cathodic cross-coupling reaction can be controlled by using liquid–liquid parallel laminar formed in an electrochemical microreactor.

4266

A pH-responsive carboxylic β -1,3-glucan polysaccharide for complexation with polymeric guests

Le Thi Ngoc Lien, Tomohiro Shiraki, Arnab Dawn, Youichi Tsuchiya, Daisuke Tokunaga, Shun-ichi Tamaru,* Naoya Enomoto, Junichi Hojo and Seiji Shinkai*

A β -1,3-glucan polysaccharide bearing dissociable COOH groups behaves as a host for SWNTs, RNA and conjugated polymers, resulting in supramolecular complexes.

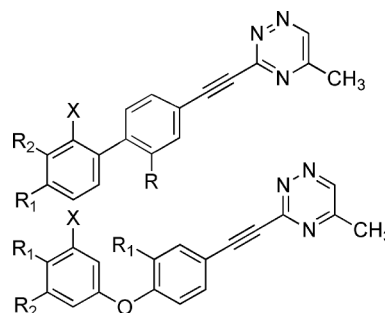


4276

Synthesis and evaluation of 1,2,4-methyltriazines as mGluR5 antagonists

Jeremy P. Olson, Moses G. Gichinga, Elizabeth Butala, Hernan A. Navarro, Brian P. Gilmour and F. Ivy Carroll*

We report the synthesis of 11 new mGluR5 antagonists based on 1,2,4-methyltriazine. The most potent analogue **5f** has an IC₅₀ of 28.2 nM at mGluR5.

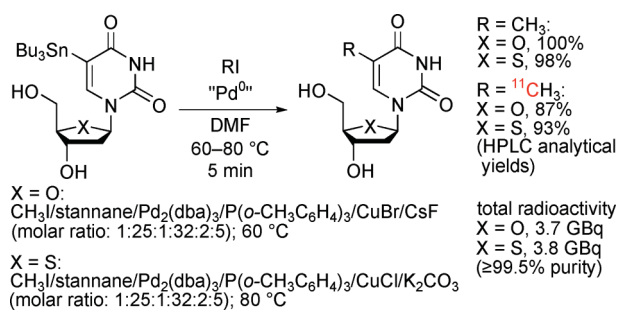


4287

Highly efficient syntheses of [methyl-¹¹C]thymidine and its analogue 4'-[methyl-¹¹C]thiothymidine as nucleoside PET probes for cancer cell proliferation by Pd⁰-mediated rapid C-[¹¹C]methylation

Hiroko Koyama, Siqin, Zhouen Zhang, Kengo Sumi, Yuma Hatta, Hiroko Nagata, Hisashi Doi and Masaaki Suzuki*

[Methyl-¹¹C]thymidine and 4'-[methyl-¹¹C]thiothymidine as nucleoside PET probes for cancer cell proliferation have been synthesized efficiently based on the Pd⁰-mediated rapid cross-coupling using [¹¹C]CH₃I and tributylstannyl precursors.

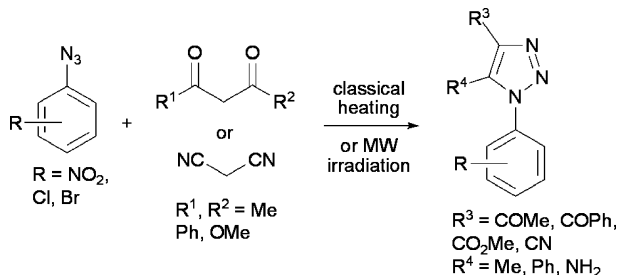


4295

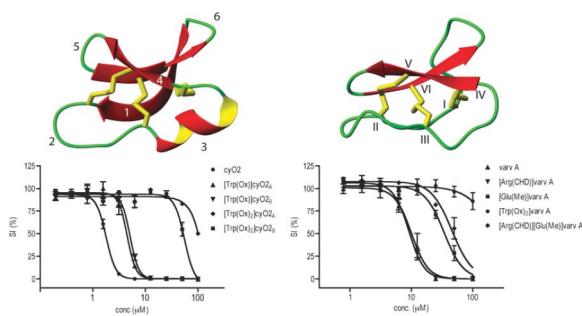
A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes

Sarah Zeghada, Ghenia Bentabed-Ababsa,* Aïcha Derdour, Safer Abdelmounim, Luis R. Domingo,* José A. Sáez, Thierry Roisnel, Ekhliss Nassar and Florence Mongin*

Cycloadditions between aryl azides and activated alkenes *e.g.* coming from β -dicarbonyl compounds were performed; their mechanism and regioselectivity were theoretically studied using DFT methods at the B3LYP/6-31G* level.



4306

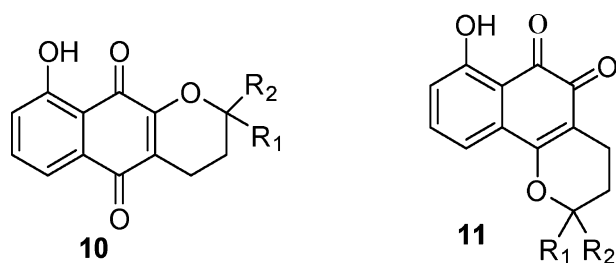


Cytotoxic potency of small macrocyclic knot proteins: Structure–activity and mechanistic studies of native and chemically modified cyclotides

Robert Burman, Anders Herrmann, Rossetti Tran, Jan-Erik Kivelä, Andrei Lomize, Joachim Gullbo and Ulf Göransson*

Investigations on the cytotoxic effects of cyclic disulfide rich mini-proteins—cyclotides—show the importance of a correct distribution of charged and hydrophobic residues for maintaining the ultimate degree of potency.

4315

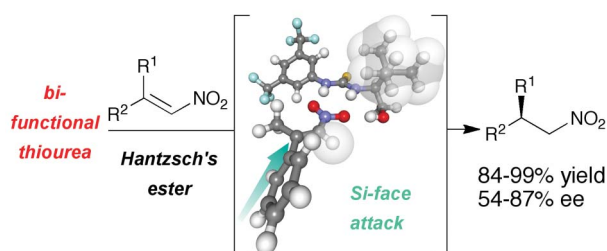


Synthesis of new 9-hydroxy- α - and 7-hydroxy- β -pyran naphthoquinones and cytotoxicity against cancer cell lines

David R. da Rocha,* Ana C. G. de Souza, Jackson A. L. C. Resende, Wilson C. Santos, Evelyne A. dos Santos, Cláudia Pessoa, Manoel O. de Moraes, Leticia V. Costa-Lotufo, Raquel C. Montenegro and Vitor F. Ferreira*

A synthetic route to 9-hydroxy- α - and 7-hydroxy- β -pyran naphthoquinones and its cytotoxicity against cancer lines were studied.

4323

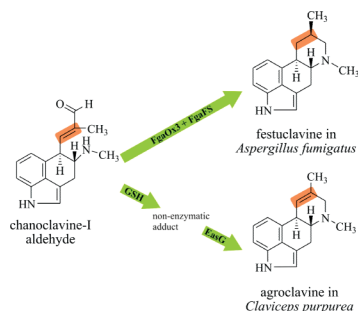


Readily available hydrogen bond catalysts for the asymmetric transfer hydrogenation of nitroolefins

Jakob F. Schneider, Markus B. Lauber, Vanessa Muhr, Domenic Kratzer and Jan Paradies*

Easily available thiourea catalysts for the asymmetric transfer hydrogenation have been developed.

4328



New insights into ergot alkaloid biosynthesis in *Claviceps purpurea*: An agroclavine synthase EasG catalyses, via a non-enzymatic adduct with reduced glutathione, the conversion of chanoclavine-I aldehyde to agroclavine

Marco Matuschek, Christiane Wallwey, Xiulan Xie and Shu-Ming Li*

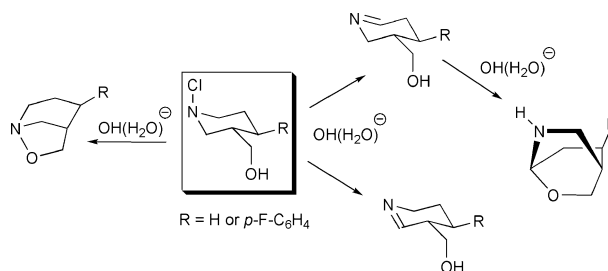
The conversion of chanoclavine-I aldehyde to agroclavine was catalysed by EasG of *C. purpurea* in the presence of NADPH, via a non-enzymatic adduct with reduced glutathione (GSH).

4336

Base-catalyzed reactions of environmentally relevant *N*-chloro-piperidines. A quantum-chemical study

Davor Šakić, Hendrik Zipse and Valerije Vrčec*

Electronic structure methods have been applied to calculate the gas and aqueous phase reaction energies for base-induced rearrangements of three *N*-chloro-piperidines.

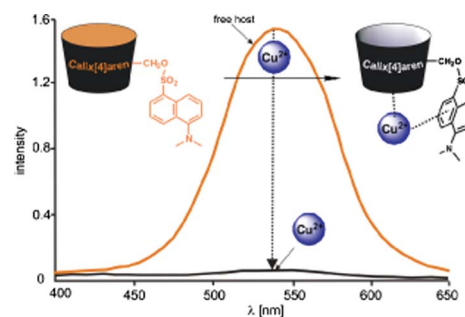


4347

Bridge-substituted calix[4]arenes: syntheses, conformations and application

Conrad Fischer, Tobias Gruber, Wilhelm Seichter and Edwin Weber*

Synthesis and influence on the conformational behaviour both in solid state and solution of calixarenes bearing different laterally attached functional groups are reported, including an example of their potential as a fluorescent chemosensor for the selective detection of Cu²⁺.

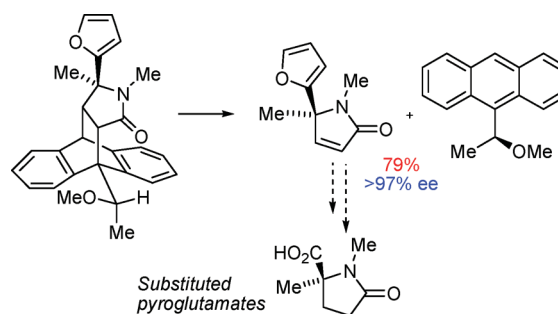


4353

Synthesis of quaternary stereogenic centres *via* stereoselective intermolecular Friedel–Crafts reactions

Jennifer C. Ball, Robert Gleave and Simon Jones*

Highly stereoselective Friedel–Crafts reactions have been performed using a chiral anthracene template to control the selectivity of the reaction and demonstrated to be of use for the construction of pyrrolidinones bearing quaternary stereogenic centres.

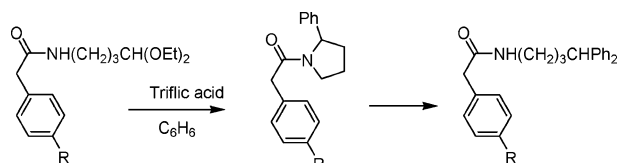


4361

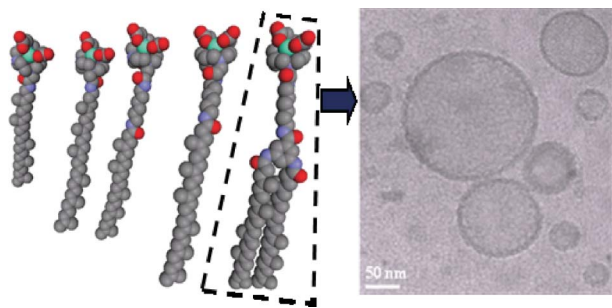
Triflic acid-mediated phenylation of *N*-acylaminoalkyl diethylacetals and *N*-acyl-2-phenyl cyclic amides

Frank D. King* and Stephen Caddick

The reaction of *N*-acylaminoalkyl diethylacetals and *N*-acyl-2-phenyl cyclic amides with triflic acid in benzene gave *N*-acylamino-diphenylalkyls.



4367



Synthesis and physicochemical characterization of new squalenoyl amphiphilic gadolinium complexes as nanoparticle contrast agents

Mohammad Othman, Didier Desmaële, Patrick Couvreur, Luce Vander Elst, Sophie Laurent, Robert N. Muller, Claudie Bourgaux, Estelle Morvan, Thierry Pouget, Sinda Lepêtre-Mouelhi, Philippe Durand and Ruxandra Gref*

Novel amphiphilic squalene–Gd³⁺ complexes spontaneously self-organise as micelles or liposomes and have potential as contrast agents.

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