Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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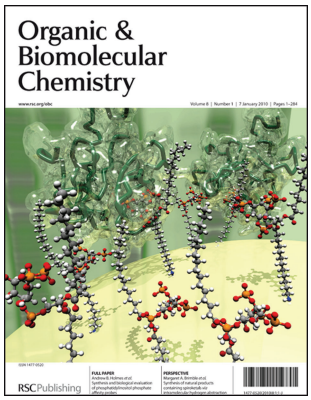
IN THIS ISSUE

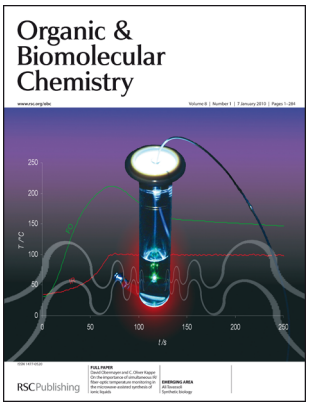
ISSN 1477-0520 CODEN OBCRAK 8(1) 1–284 (2010)



Cover

See Andrew B. Holmes *et al.*, pp. 66–76.
The cover page illustrates a phosphatidylinositol (3,4,5)-trisphosphate analogue bound to an affinity bead interacting with the PH domain of GRP1, representing the pulldown of intracellular signalling proteins from the cytosolic extracts of pig neutrophil and colon cancer cells (Created by Karl Harrison, University of Oxford).

Image reproduced by permission of Andrew B. Holmes from *Org. Biomol. Chem.*, 2010, **8**, 66.



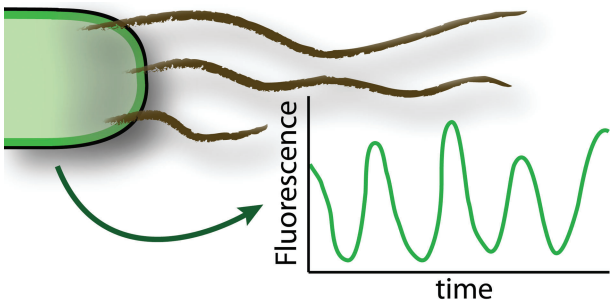
Inside cover

See David Obermayer and C. Oliver Kappe, pp. 114–121.
Seeing is believing: infrared sensors used in most of today's microwave reactors can easily lead to incorrect reaction temperature measurements – internal fiber-optic probes do a much better job.

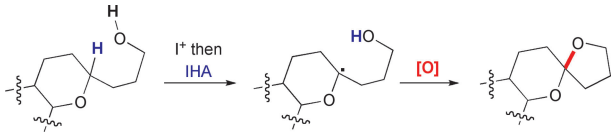
Image reproduced by permission of C. Oliver Kappe from *Org. Biomol. Chem.*, 2010, **8**, 114.

EDITORIAL

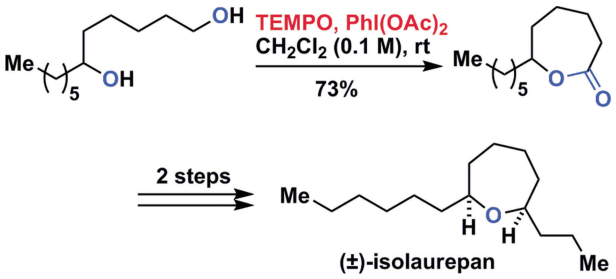
EMERGING AREA

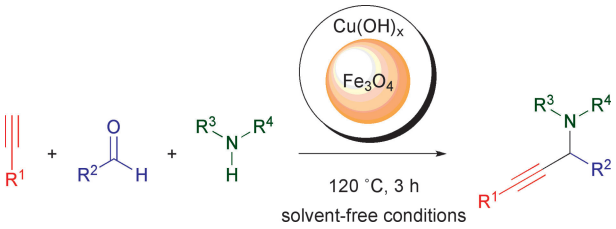


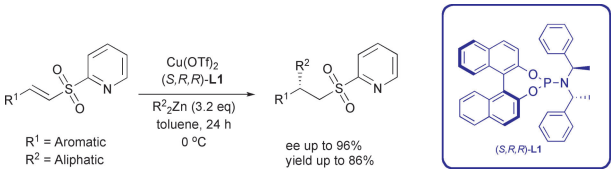
PERSPECTIVE



COMMUNICATIONS







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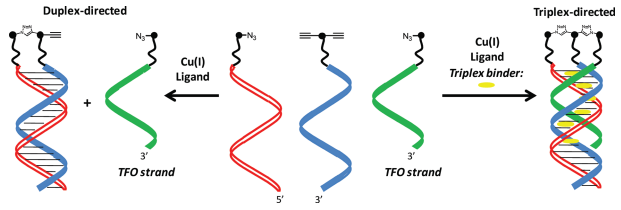
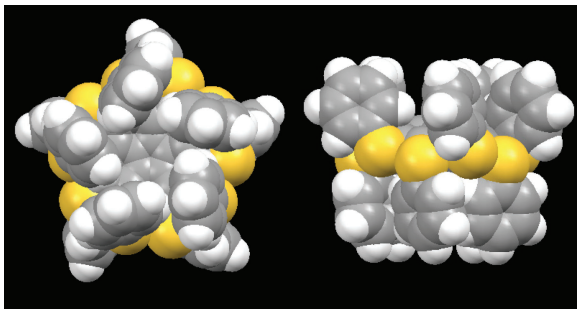


Small molecule induced control in duplex and triplex DNA-directed chemical reactions

Mikkel F. Jacobsen, Jens B. Ravnsbæk and Kurt V. Gothelf*

Triplex DNA binders can effectively control copper-catalysed alkyne–azide click reactions in DNA architecture, such that either duplex or triplex DNA directed reactions of terminally attached azides and alkynes occur, in the absence or presence of triplex DNA binder, respectively.

53

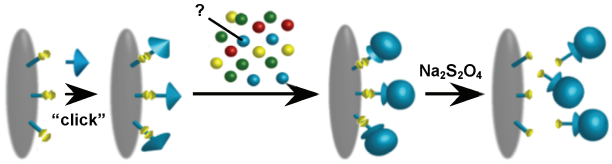


Synthesis, structure and properties of decakis(phenylthio)corannulene

Kim K. Baldridge,* Kenneth I. Hardcastle, T. Jon Seiders and Jay S. Siegel*

Decakis(phenylthio)corannulene adopts a pinwheel conformation with multiple T-shaped (edge-to-face) arene interactions.

56

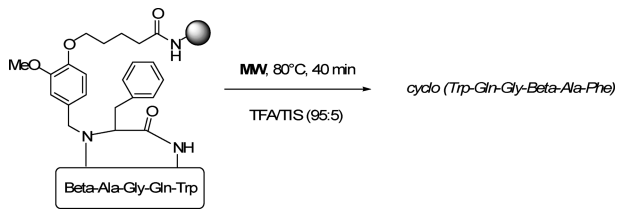


Synthesis and application of a new cleavable linker for "click"-based affinity chromatography

Felicetta Landi, Conny M. Johansson, Dominic J. Campopiano and Alison N. Hulme*

"Click" coupling of a ligand to an azo-functionalised linker allows affinity capture and separation of proteins from a complex mixture (such as fetal bovine serum) and mild release with sodium dithionite.

60

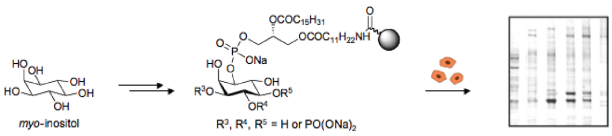


Development of a new microwave-assisted cleavable backbone amide linker (BAL): a comparative study

Stijn Claerhout, Thibault Duchène, Dirk Tourwé and Erik V. Van der Eycken*

A thorough comparative study to demonstrate the properties of a new microwave labile backbone amide linker is presented.

66

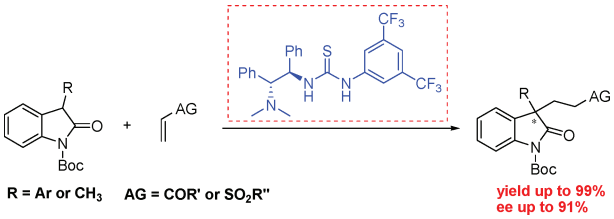


Synthesis and biological evaluation of phosphatidylinositol phosphate affinity probes

S. J. Conway, J. Gardiner,* S. J. A. Grove, M. K. Johns, Z.-Y. Lim, G. F. Painter, D. E. J. E. Robinson,* C. Schieber, J. W. Thuring, L. S.-M. Wong, M.-X. Yin, A. W. Burgess, B. Catimel, P. T. Hawkins, N. T. Ktistakis, L. R. Stephens and A. B. Holmes*

A versatile approach to the synthesis of the complete family of phosphatidylinositol phosphate (PIP) analogues and their use as affinity probes are described.

77



Asymmetric Michael addition reaction of 3-substituted-*N*-Boc oxindoles to activated terminal alkenes catalyzed by a bifunctional tertiary-amine thiourea catalyst

Xin Li, Zhi-Guo Xi, Sanzhong Luo* and Jin-Pei Cheng*

An enantioselective Michael addition reaction of 3-substituted oxindoles to terminal alkenes which realized the construction of an all carbon-substituted quaternary stereocenter has been reported using catalysis by a bifunctional tertiary-amine thiourea organocatalyst.

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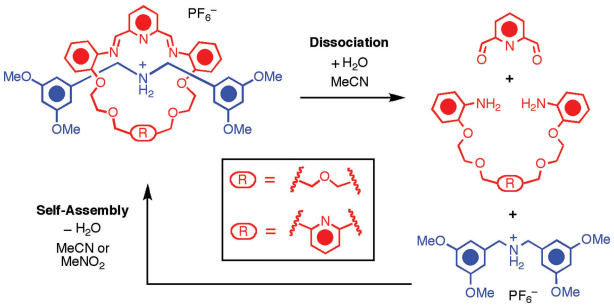

The stability of imine-containing dynamic [2]rotaxanes to hydrolysis

Ken Cham-Fai Leung,* Wing-Yan Wong, Fabio Aricó, Philip C. Haussmann and J. Fraser Stoddart*

The self-assembly as well as the dissociation of two dynamic [2]rotaxanes have been demonstrated. Somewhat surprisingly, the [2]rotaxanes show remarkable relative stabilities in the presence of large amounts of water. In particular, the dissociation rates of the rotaxanes toward hydrolysis have been determined.

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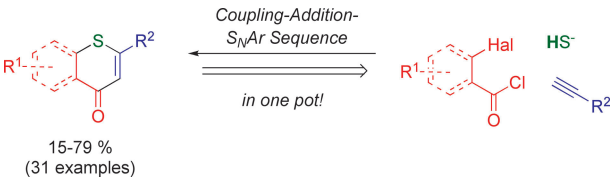
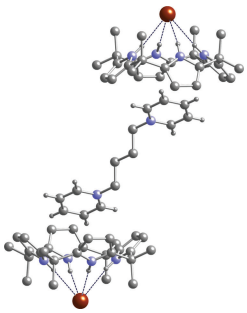
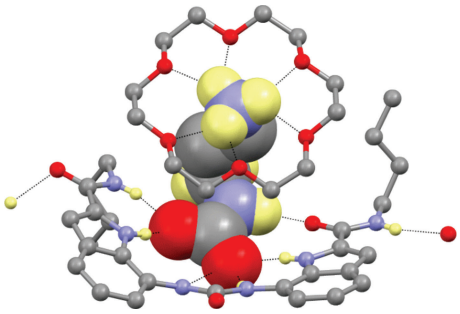


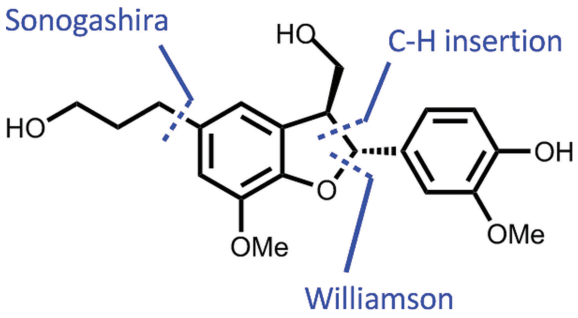
Microwave-assisted three-component coupling-addition-S_NAr (CASNAR) sequences to annelated 4*H*-thiopyran-4-ones

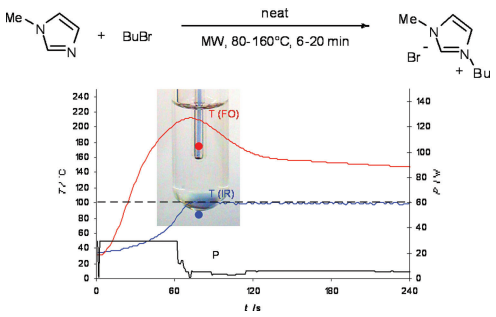
Benjamin Willy, Walter Frank and Thomas J. J. Müller*

Annelated 4*H*-thiopyran-4-ones can be readily synthesized from readily available (het)aroyl chlorides, alkynes and sodium sulfide nonahydrate in good yields by a microwave-assisted consecutive one-pot three-component reaction.









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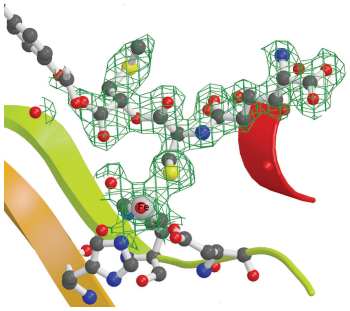

The crystal structure of an LLL-configured depsipeptide substrate analogue bound to isopenicillin N synthase

Wei Ge, Ian J. Clifton, Jeanette E. Stok, Robert M. Adlington, Jack E. Baldwin* and Peter J. Rutledge*

Stereochemistry is all-important to enzyme catalysis, so what will isopenicillin N synthase, a key player in penicillin biosynthesis, make of an LLL-configured depsipeptide substrate analogue when its natural substrate is an LLD-configured tripeptide?

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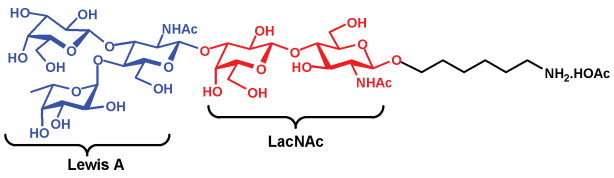

Total synthesis of Le^{A}-LacNAc pentasaccharide as a ligand for *Clostridium difficile* toxin A

Ping Zhang, Kenneth Ng and Chang-Chun Ling*

Le^{A}-LacNAc was found to be a ligand for toxin A released by *Clostridium difficile.* Here we report the efficient synthesis of the pentasaccharide for use to characterize the carbohydrate-binding site of the toxin by X-ray crystallography.

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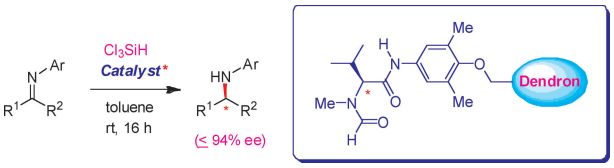

Dendron-anchored organocatalysts: the asymmetric reduction of imines with trichlorosilane, catalysed by an amino acid-derived formamide appended to a dendron

Marek Figlus, Stuart T. Caldwell, Dawid Walas, Gulen Yesilbag, Graeme Cooke,* Pavel Kočovský,* Andrei V. Malkov* and Amitav Sanyal*

Ketimines **1a–f** can be reduced with Cl_3SiH in the presence of the Lewis-basic *N*-methylvaline-derived formamide catalyst (5 mol%) anchored to a soluble dendron (**11c**) with ≤94% ee; this protocol represents a simplification of the isolation procedure and recovery of the catalyst.

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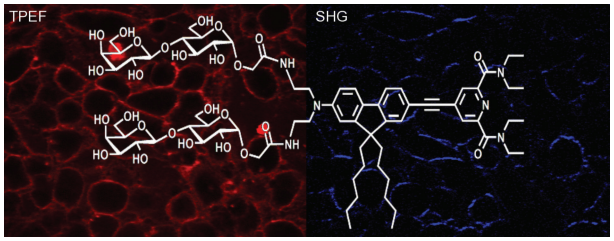

Neutral push-pull chromophores for nonlinear optical imaging of cell membranes

Cyril Barsu, Rouba Cheaib, Stéphane Chambert, Yves Queneau, Olivier Maury, Davy Cottet, Hartmut Wege, Julien Douady, Yann Bretonnière* and Chantal Andraud*

A series of amphiphilic second order nonlinear probes for cell membrane imaging was studied by combined two-photon excited fluorescence (TPEF) and second harmonic generation (SHG) microscopies.

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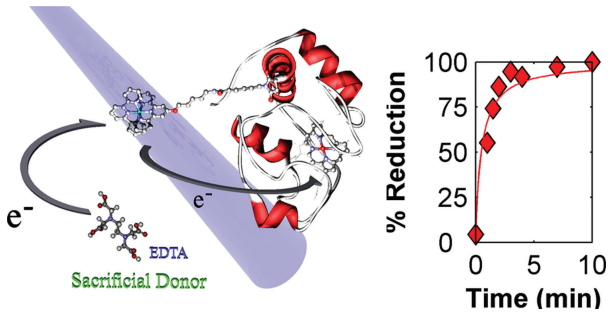

Synthesis and room temperature photo-induced electron transfer in biologically active bis(terpyridine)ruthenium(II)–cytochrome *c* bioconjugates and the effect of solvents on the bioconjugation of cytochrome *c*

Joshua R. Peterson, Trevor A. Smith and Pall Thordarson*

Room temperature photo-induced electron transfer studies of bis(terpyridine)ruthenium(II) cytochrome *c* bioconjugates show that the protein is effectively reduced within 5 min in the presence of 20 mM EDTA.

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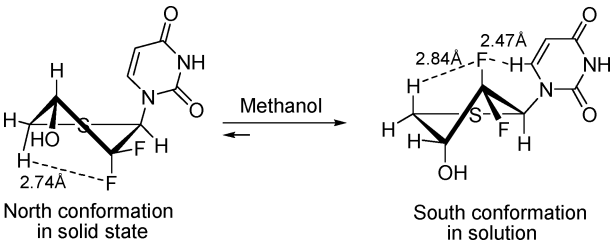

Synthesis and conformational analysis of D-2′-deoxy-2′,2′-difluoro-4′-dihydro-4′-thionucleosides

Feng Zheng, Lin Fu, Renxiao Wang and Feng-Ling Qing*

An efficient synthesis of D-2′-deoxy-2′,2′-difluoro-4′-thionucleosides is described. The conformations of D-2′-deoxy-2′,2′-difluoro-4′-thiouridine were studied by X-ray crystallography, NMR spectroscopy and molecular modeling in an attempt to explore the roles of the two *gem*-difluorine atoms in the conformer preferences of the thionucleosides.

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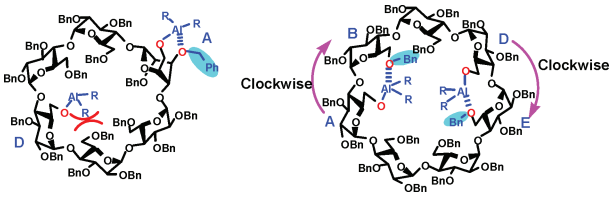

DIBAL-H mediated triple and quadruple debenzylations of perbenzylated cyclodextrins

Girish K. Rawal, Shikha Rani, Sandra Ward and Chang-Chun Ling*

Sequential triple and quadruple debenzylations by diisobutylaluminium hydride were investigated for α-, β- and γ-cyclodextrins. A distinct regioselective debenzylation path was observed for α-CD compared to β- and γ-cyclodextrins.

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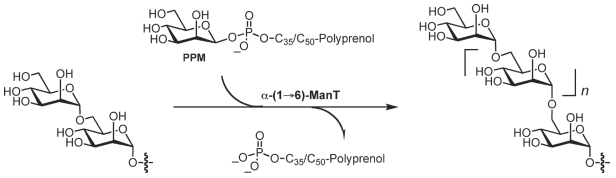


Epimeric and amino disaccharide analogs as probes of an α-(1→6)-mannosyltransferase involved in mycobacterial lipoarabinomannan biosynthesis

Pui Hang Tam and Todd L. Lowary

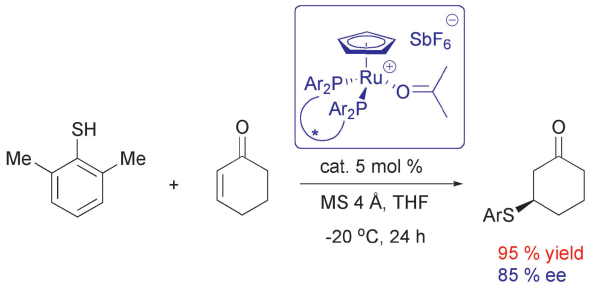
A panel of disaccharide analogs have been synthesized and used to probe a mannosyltransferase involved in lipoarabinomannan biosynthesis in mycobacteria, including the human pathogen *Mycobacterium tuberculosis*.

193

Asymmetric ruthenium-catalyzed 1,4-additions of aryl thiols to enones

Andrei Bădoiu, Gerald Bernardinelli, Céline Besnard and E. Peter Kündig*

Ruthenium half-sandwich Lewis-acids can efficiently catalyze 1,4-additions of aryl thiols to enones with remarkable levels of activity and selectivity, in spite of stereocontrol complexity and potential catalyst inhibition. NMR experiments provide an insight to the intricate equilibria governing the reaction mechanism.



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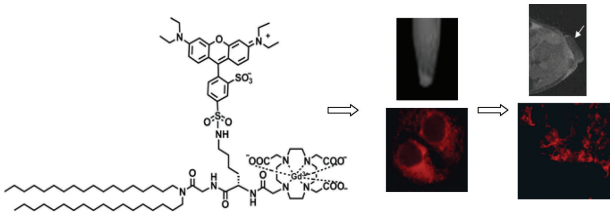
A novel bimodal lipidic contrast agent for cellular labelling and tumour MRI

Nazila Kamaly, Tammy Kalber, Gavin Kenny, Jimmy Bell, Michael Jorgensen* and Andrew Miller*

Gd·DOTA·Rhoda·DSA: a novel bimodal lipidic MRI contrast agent.



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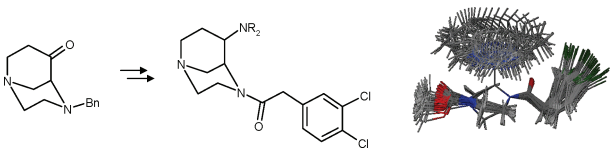
Stereoselective synthesis and structure–affinity relationships of bicyclic κ receptor agonists

Daniel Kracht, Elisabeth Rack, Dirk Schepmann, Roland Fröhlich and Bernhard Wünsch*

The bioactive conformation of flexible κ agonists was approached by the design, synthesis and pharmacological evaluation of conformationally constrained 1,4-diazabicyclo[3.3.1]nonanes. It was shown that *endo*-orientation of the amino group is crucial for high κ receptor affinity.



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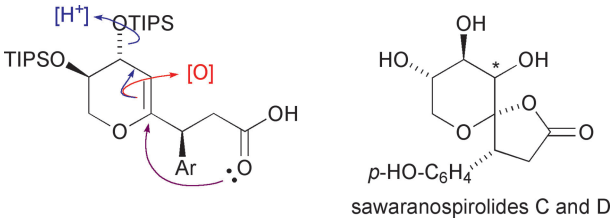
Oxidative spirocyclisation routes towards the sawaranospirolides. Synthesis of *ent*-sawaranospirolides C and D

Jeremy Robertson,* Praful T. Chovatia, Thomas G. Fowler, Jonathan M. Withey and Daniel J. Woollaston

ent-Sawaranospirolides C and D are prepared by the electrophilic spirocyclisation of a 3-(dihydropyran-2-yl)propanoic acid derivative.



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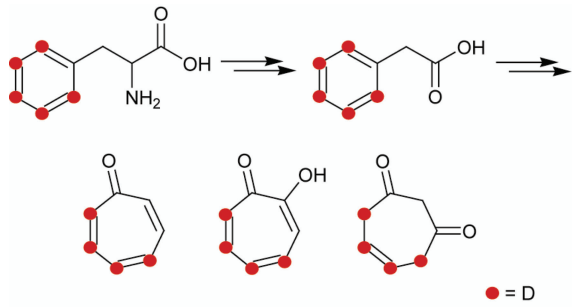
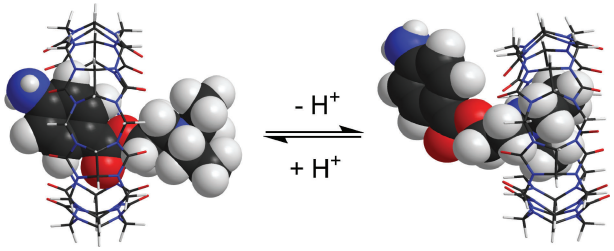


Identification and biosynthesis of tropone derivatives and sulfur volatiles produced by bacteria of the marine *Roseobacter* clade

Verena Thiel, Thorsten Brinkhoff, Jeroen S. Dickschat, Susanne Wickel, Jörg Grunenberg, Irene Wagner-Döbler, Meinhard Simon and Stefan Schulz*

The volatile tropone, its derivatives, and several thioesters are produced by *Phaeobacter gallaeciensis*, a bacterium of the *Roseobacter* clade that dominates many marine bacterial communities.

247



Host–guest complexations of local anaesthetics by cucurbit[7]uril in aqueous solution

Ian W. Wyman and Donal H. Macartney*

The cucurbit[7]uril host molecule binds to procaine, and other local anaesthetic drugs, 2–3 orders of magnitude stronger than β-cyclodextrin in aqueous solution, resulting in increases in the value of pK_1 and enhanced fluorescence.

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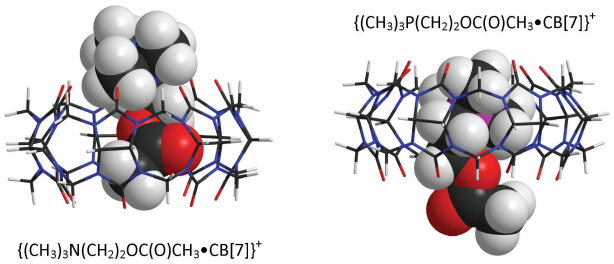

Cucurbit[7]uril host–guest complexes of cholines and phosphonium cholines in aqueous solution

Ian W. Wyman and Donal H. Macartney*

The cucurbit[7]uril host molecule forms host–guest complexes with a series of cholines and phosphonium cholines ($R_3XCH_2CHR'OR''^+$) in aqueous solution, with stability constants and guest positioning that reflects the natures of the peralkylonium head groups (R_3X^+) and substituents (R′ and R″).

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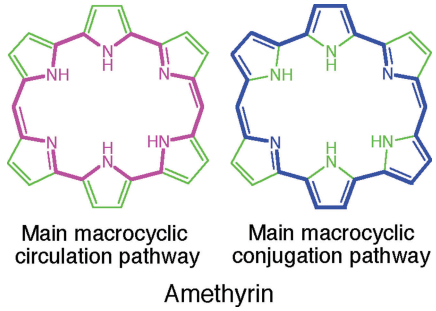


Prediction of the main macrocyclic conjugation pathway for porphyrinoids from the ring current distribution

Jun-ichi Aihara* and Masakazu Makino

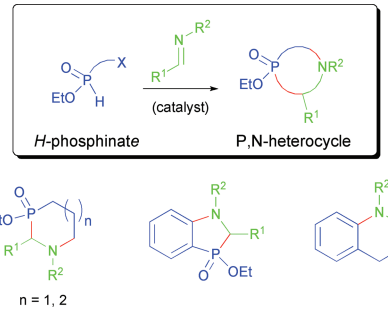
Using our analytical theory of ring-current diamagnetism, main macrocyclic conjugation pathways in porphyrinoids were successfully predicted from the global ring current distributions.

267

Facile P,N-heterocycle synthesis *via* tandem aminomethylation–cyclization of *H*-phosphinate building blocks

Clémence Queffélec and Jean-Luc Montchamp*

Various heterocycles containing phosphorus and nitrogen are easily synthesized from readily available *H*-phosphinate building blocks *via* aminomethylation and *in situ* cyclization through substitution or cross-coupling.



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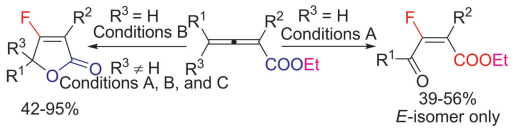
Study on the selectivity in the electrophilic monofluorination of 2,3-allenoates with Selectfluor™: an efficient synthesis of 4-fluoro-2(5*H*)-furanones and 3-fluoro-4-oxo-2(*E*)-alkenoates

Bo Lü, Chunling Fu and Shengming Ma*

4-Fluoro-2(5*H*)-furanones and (*E*)-3-fluoro-4-oxo-2-alkenoates were highly selectively generated from 2,4-disubstituted 2,3-allenoates with Selectfluor™ in moderate to high yields under different reaction conditions. A mechanism has been proposed.



Conditions A: 3.0 equiv Selectfluor, 0.5 equiv H_2O, MeCN, 80 °C. Conditions B: 1.7-2.5 equiv Selectfluor, MeCN/H_2O = 2/1, 80 °C. Conditions C: 1.2 equiv Selectfluor, MeCN or $MeNO_2$, 80 °C.

* Indicates the author for correspondence: see article for details.

Electronic supplementary information (ESI) is available *via* the online article (see http://www.rsc.org/esi for general information about ESI).

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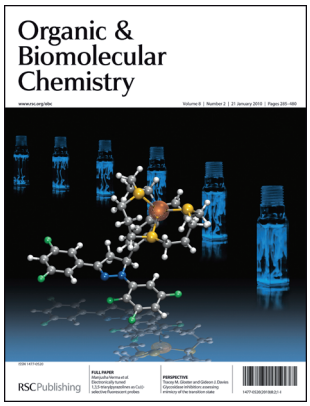


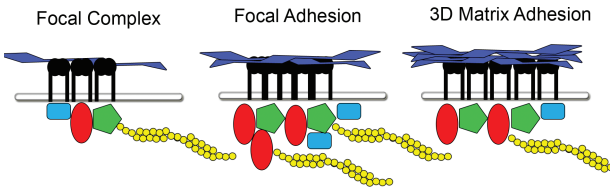
Cover

See Manjusha Verma *et al.*, pp. 363–370.

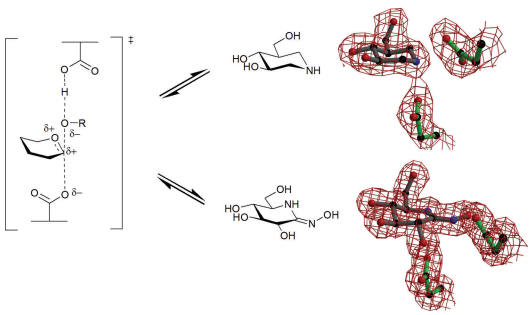
The fluorescence contrast of a Cu(I)-responsive probe was optimized through electronic tuning with varying numbers of fluorine substituents. The cuvettes show the time evolution of fluorescence titrations formed upon addition of the analyte.

Image reproduced by permission of Christoph J. Fahrni from *Organic & Biomolecular Chemistry*, 2010, **8**, 363.

EMERGING AREA



PERSPECTIVE

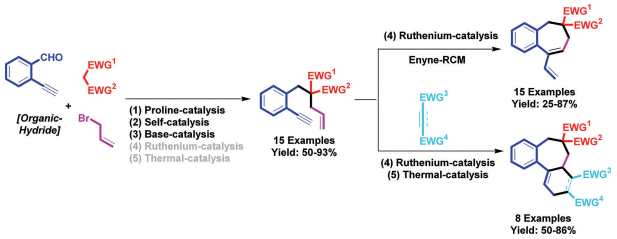


321

Rapid two-step synthesis of drug-like polycyclic substances by sequential multi-catalysis cascade reactions

Dhevalapally B. Ramachary,* Rumpa Mondal and Chintalapudi Venkaiah

An efficient multi-catalysis cascade process for the two-step synthesis of highly substituted drug-like carbocycles was achieved through combinations of cascade TCRA/*C*-allylation/enyne-RCM/Diels–Alder reactions as key steps starting from simple acyclic substrates *via* amino acid-/self-/base-/ruthenium-/thermal-catalysis.

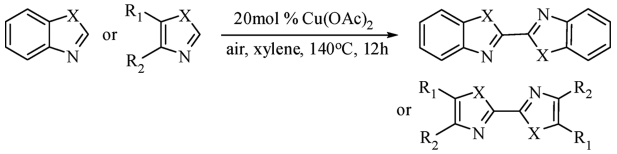


326

An efficient and convenient $Cu(OAc)_2$/air mediated oxidative coupling of azoles *via* C–H activation

Yan Li, Jun Jin, Weixing Qian* and Weiliang Bao*

An efficient and convenient approach to construct C–C bonds at the 2-position of azoles *via* $Cu(OAc)_2$/air mediated oxidative homo- and cross-coupling reaction was reported. The corresponding products were obtained in good to excellent yield.

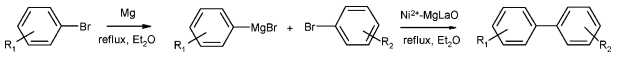


331

Nickel/magnesium–lanthanum mixed oxide catalyst in the Kumada-coupling

Árpád Kiss, Zoltán Hell* and Mária Bálint

A new, heterogeneous, magnesium–lanthanum mixed oxide solid base-supported nickel(II) catalyst was developed. The catalyst was successfully used in the Kumada coupling of aryl halides, especially aryl bromides. The optimal reaction conditions of the coupling were determined.

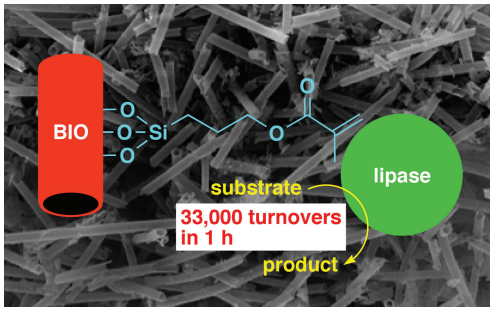


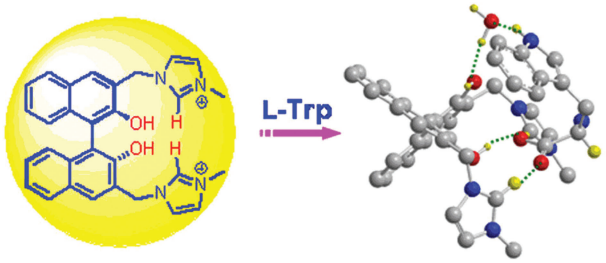
336

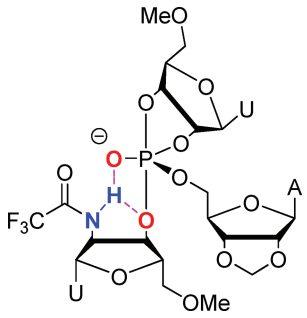
Chemical modification of biogenous iron oxide to create an excellent enzyme scaffold

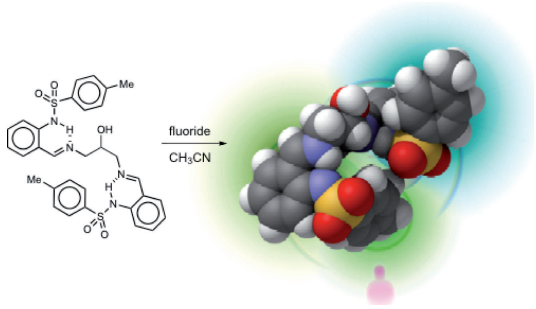
Takashi Sakai,* Yuki Miyazaki, Ai Murakami, Noriko Sakamoto, Tadashi Ema,* Hideki Hashimoto, Mitsuaki Furutani, Makoto Nakanishi, Tatsuo Fujii and Jun Takada*

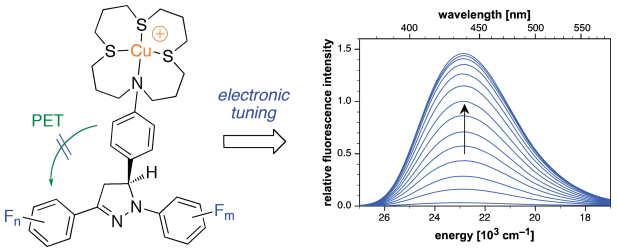
The biogenous iron oxide (BIO) from *Leptothrix ochracea* was transformed to an organic–inorganic hybrid support to prepare an excellent immobilized enzyme showing high catalytic performance.









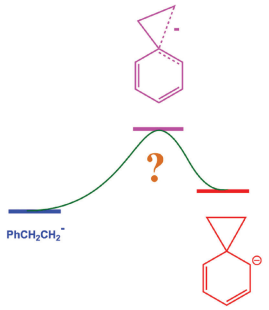


371

Diagnostic fragmentations of adducts formed between carbanions and carbon disulfide in the gas phase. A joint experimental and theoretical study

Micheal J. Maclean, Scott Walker, Tianfang Wang, Peter C. H. Eichinger, Patrick J. Sherman and John H. Bowie*

The structures of selected carbanions have been identified by collisionally activated decomposition reactions of the corresponding adducts with carbon disulfide in a modified LCQ ion trap mass spectrometer.

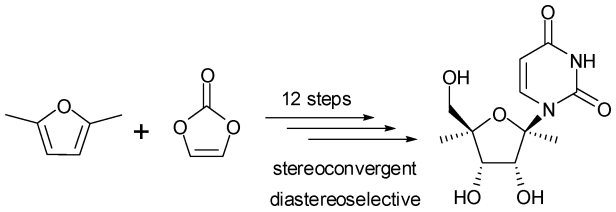


378

Diastereoselective synthesis of (±)-1′,4′-dimethyluridine

Guillaume Sautrey, Damien Bourgeois* and Christian Périgaud

The diastereoselective total synthesis of the title compound is described. It is based on a new methodology involving the stereoconvergent preparation of a suitable sugar ring, followed by a selective Vorbrüggen glycosylation.

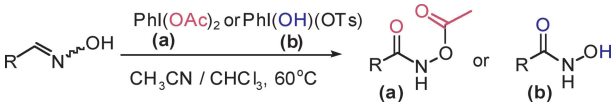


384

Hypervalent iodine(III)-mediated oxidation of aldoximes to *N*-acetoxy or *N*-hydroxy amides

Harisadhan Ghosh and Bhisma K. Patel*

Various aldoximes were converted to either *N*-acetoxy or *N*-hydroxy amides in good yield using the hypervalent iodine(III) reagents (diacetoxyiodo)benzene (DIB) or Koser's reagent [hydroxy(tosyloxy)iodo]benzene (HTIB). A plausible mechanism for this transformation involves the attack of acetate/hydroxy on the intermediate aryl nitrile oxides, which, upon rearrangement, gave the expected *N*-acetoxy or *N*-hydroxy amides.

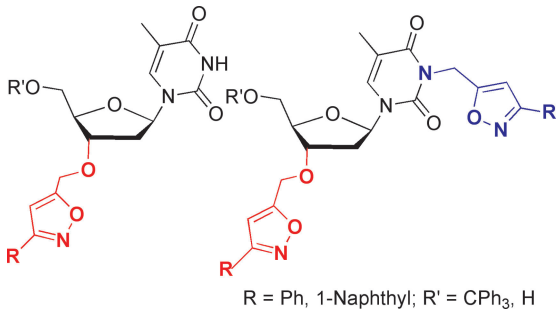


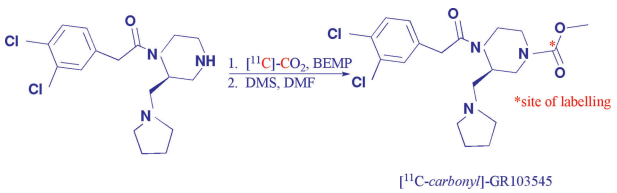
391

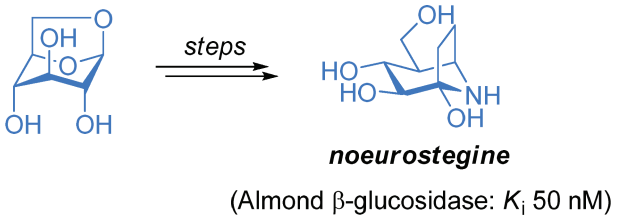
Nucleoside and nucleotide analogues by catalyst free Huisgen nitrile oxide–alkyne 1,3-dipolar cycloaddition

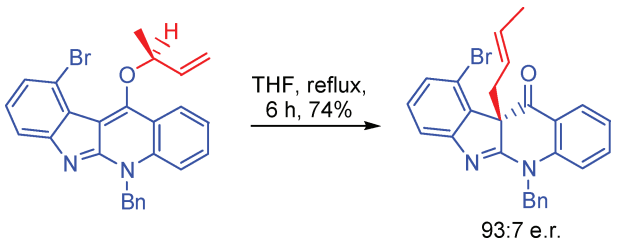
Virginie Algay, Ishwar Singh and Frances Heaney*

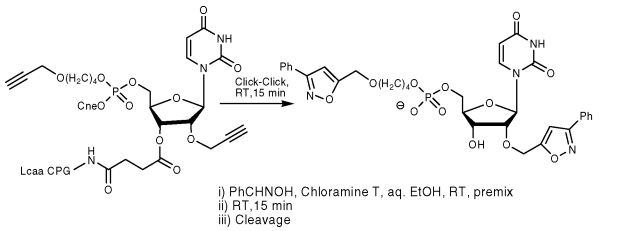
$C^{3'}$-*O*-Isoxazole conjugated, and $C^{3'}$-*O*,N^{3}-bisisoxazole nucleosides and nucleotides are prepared regiospecifically, rapidly and in high yield under atmospheric conditions and in an aqueous environment; the protocol identifies chloramine-T as a practical reagent for *in situ* nitrile oxide formation, and the alkyne partner may be attached to the sugar residue or the nucleobase.

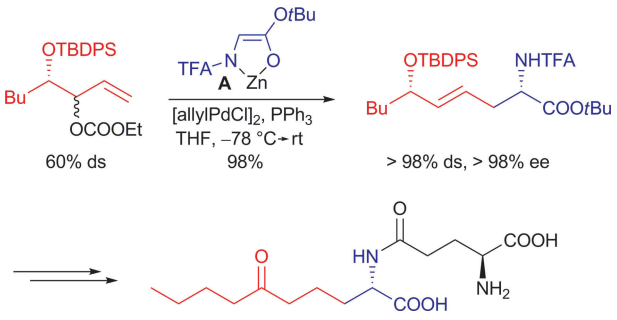


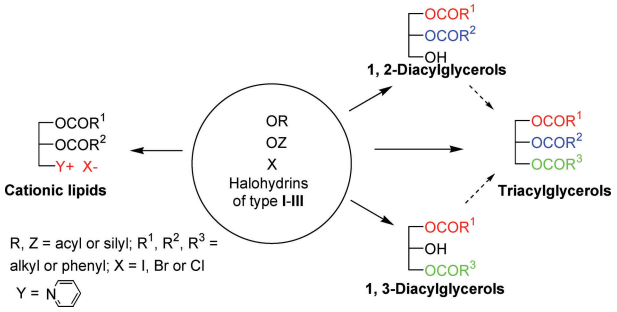












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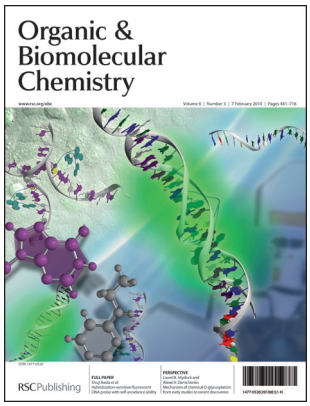
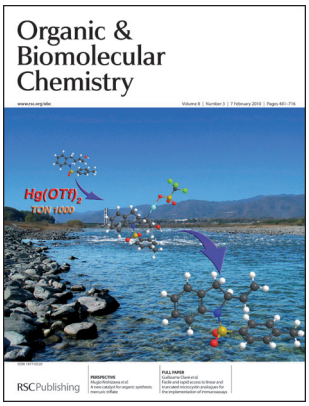


Cover

See Shuji Ikeda *et al.*, pp. 546–551. Inosine (purple)–ethylcytosine (gray) base pair is unstable. The probes containing inosines, ethylcytosines and thiazole orange labels can avoid their self-dimerization (left) and emit hybridization-sensitive fluorescence by hybridization with the target RNA (center).

Image reproduced by permission of Akimitsu Okamoto from *Organic & Biomolecular Chemistry*, 2010, **8**, 546.

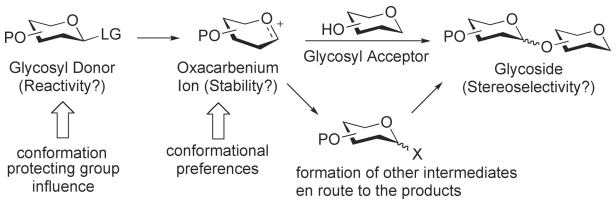


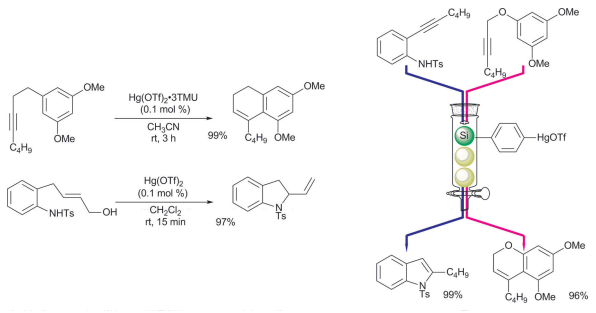
Inside cover

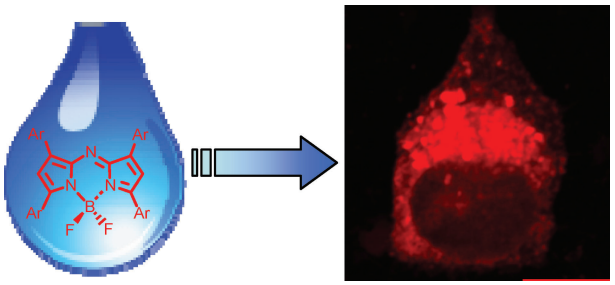
See Mugio Nishizawa *et al.*, pp. 511–521. Rich and clean stream of Yoshino-gawa river, Tokushima, Japan. $Hg(OTf)_2$-catalyzed reaction takes place smoothly in high catalytic turnover under mild conditions.

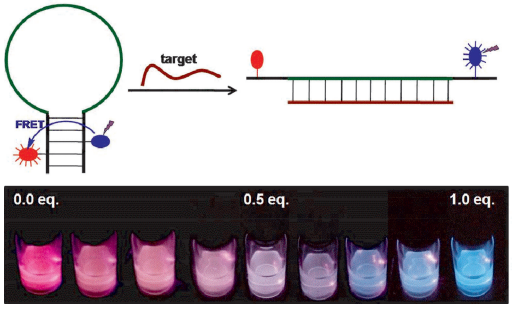
Image reproduced by permission of Mugio Nishizawa from *Organic & Biomolecular Chemistry*, 2010, **8**, 511.

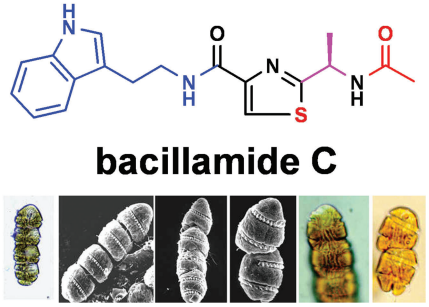
PERSPECTIVES

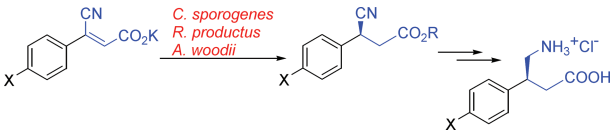


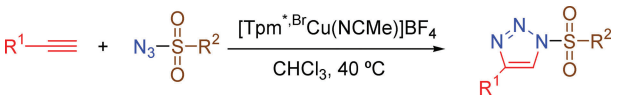


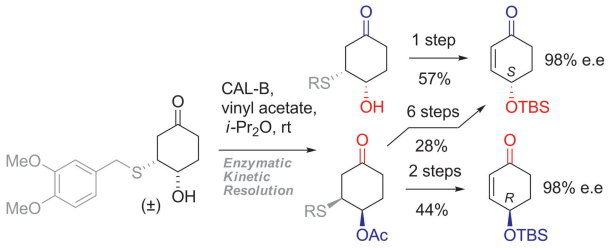


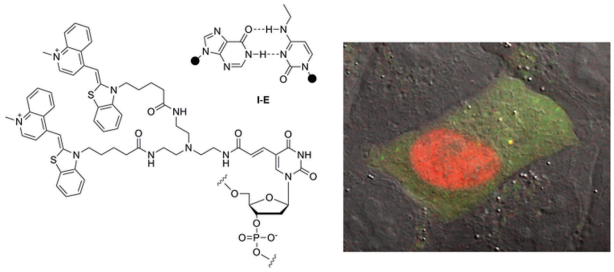


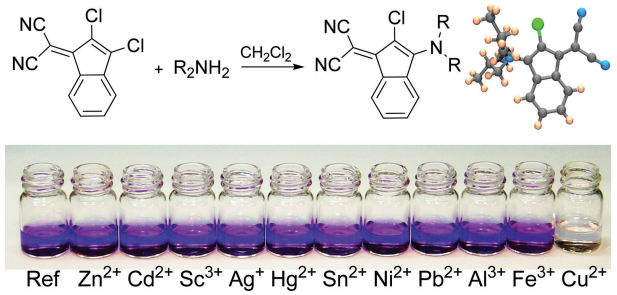










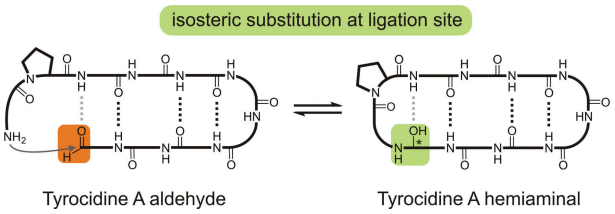


559

The reversible macrocyclization of Tyrocidine A aldehyde: a hemiaminal reminiscent of the tetrahedral intermediate of macrolactamization

Sebastian Enck, Florian Kopp, Mohamed A. Marahiel* and Armin Geyer*

The carboxylate at the native ligation site of Tyrocidine A was isosterically substituted by an aldehyde, which subsequently closes reversibly and stereoselectively to a stable hemiaminal, enabling the NMR spectroscopic analysis of the macrocyclization equilibrium.



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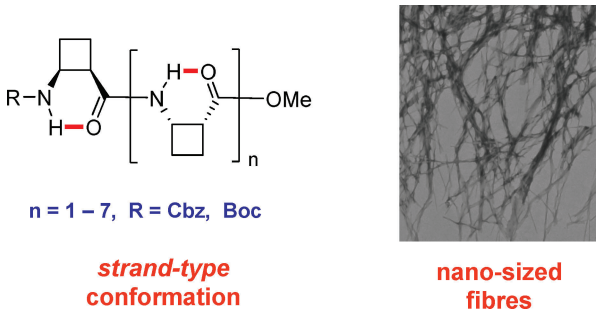
Folding and self-assembling with β-oligomers based on (1*R*,2*S*)-2-aminocyclobutane-1-carboxylic acid

Elisabeth Torres, Esther Gorrea, Kepa K. Burusco, Eric Da Silva, Pau Nolis, Federico Rúa, Stéphanie Boussert, Ismael Díez-Pérez, Samantha Dannenberg, Sandra Izquierdo, Ernest Giralt, Carlos Jaime, Vicenç Branchadell and Rosa M. Ortuño*

All *cis*-cyclobutane β-oligomers show a strand-type preferential conformation in solution. These compounds self-assemble to give nano-sized fibres and some of them also form gels.

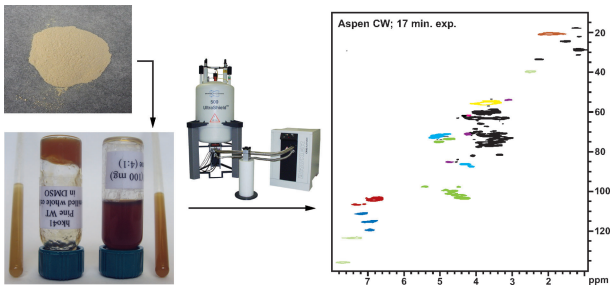


576

Solution-state 2D NMR of ball-milled plant cell wall gels in DMSO-d_6/pyridine-d_5

Hoon Kim* and John Ralph

2D solution-state NMR (HSQC) fingerprinting of entire plant cell wall fractions (*i.e.* without component fractionation) has been improved by using DMSO-d_6/pyridine-d_5 (4 : 1, v/v) gels.



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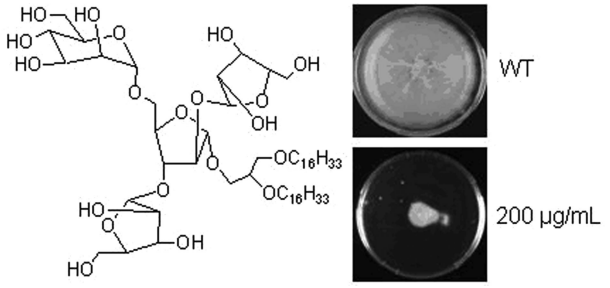
Synthetic arabinomannan glycolipids and their effects on growth and motility of the *Mycobacterium smegmatis*

Kottari Naresh, Binod Kumar Bharati, Prakash Gouda Avaji, Narayanaswamy Jayaraman* and Dipankar Chatterji*

Synthetic arabinomannan glycolipids, relevant to mycobacterial cell-wall components, acted as inhibitors of growth through reduced biofilm formation and impaired motility of bacteria.



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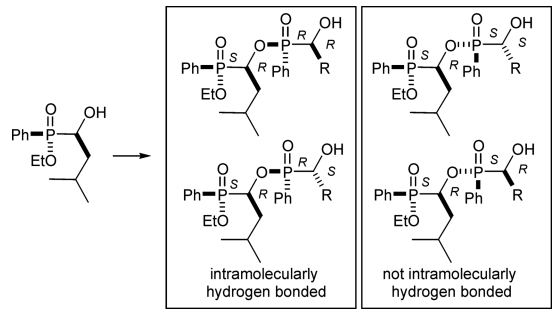

A synthesis of oligomeric α-hydroxy phenylphosphinates and a study of the conformational preferences of the dimers

Kamyar Afarinkia,* Martin Royappa, Ian J. Scowen, Jonathan W. Steed and Hiu-wan Yu

A combination of NMR spectroscopy, X-ray crystallography and computational methods is used to show that the folding patterns of a novel class of oligomers is determined by relative configuration of the carbon and phosphorus stereocenters.

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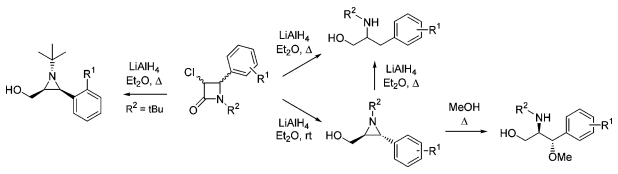
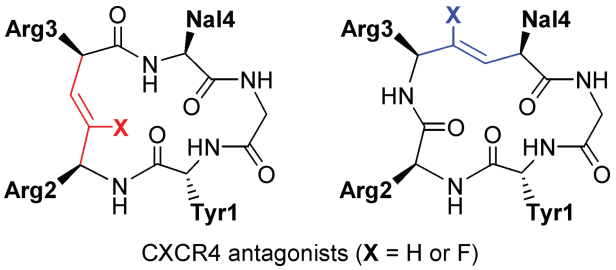


Stereoselective synthesis of *trans*- and *cis*-2-aryl-3-(hydroxymethyl)aziridines through transformation of 4-aryl-3-chloro-β-lactams and study of their ring opening

Matthias D'hooghe, Karen Mollet, Stijn Dekeukeleire and Norbert De Kimpe*

trans- and *cis*-1-Alkyl-4-aryl-3-chloroazetidin-2-ones were transformed into *trans*- and *cis*-2-aryl-3-(hydroxymethyl)aziridines *via* reductive ring contraction.

616

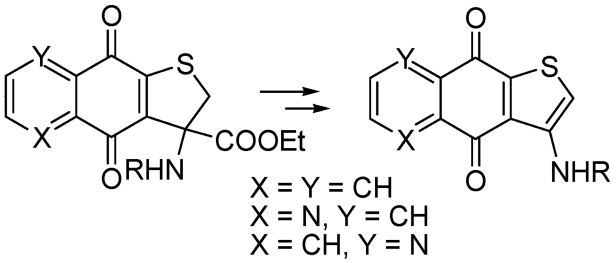


Synthesis and biological evaluation of selective CXCR4 antagonists containing alkene dipeptide isosteres

Tetsuo Narumi, Ryoko Hayashi, Kenji Tomita, Kazuya Kobayashi, Noriko Tanahara, Hiroaki Ohno, Takeshi Naito, Eiichi Kodama, Masao Matsuoka, Shinya Oishi* and Nobutaka Fujii*

A set of cyclic peptide analogues of a selective CXCR4 antagonist FC131 were synthesized and bioevaluated. The CXCR4 antagonism and anti-HIV activity was demonstrated. FC131 and the analogues were shown to selectively inhibit SDF-1 binding to CXCR4.

622



Unprecedented synthesis of a novel amino quinone ring system *via* oxidative decarboxylation of quinone-based α,α-amino esters

Pietro Campiglia, Claudio Aquino, Alessia Bertamino, Nicoletta De Simone, Marina Sala, Sabrina Castellano, Marisabella Santoriello, Paolo Grieco, Ettore Novellino and Isabel M. Gomez-Monterrey*

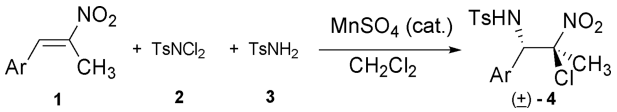
An efficient synthesis of new quinone derivatives through an α,α-amino ester oxidative decarboxylation provides access to new building blocks for the development of potential antitumoral agents.

628

New catalytic system for aminohalogenation of β-methyl-β-nitrostyrenes to give opposite regiochemistry

San-Jun Zhi, Hao Sun, Guangqian Zhang, Guigen Li* and Yi Pan*

A new combination of catalyst and co-additive was found for the aminohalogenation of β-methyl-β-nitrostyrenes with 4-$TsNCl_2$ by using $MnSO_4$ as the catalyst. A mechanism involving the formation of chloronium intermediate was proposed.

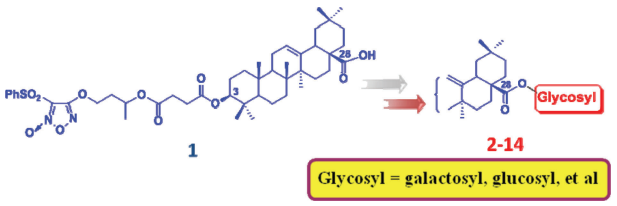


632

Synthesis and *anti*-human hepatocellular carcinoma activity of new nitric oxide-releasing glycosyl derivatives of oleanolic acid

Zhangjian Huang, Yihua Zhang,* Li Zhao, Yongwang Jing, Yisheng Lai, Luyong Zhang,* Qinglong Guo, Shengtao Yuan, Jianjun Zhang, Li Chen, Sixun Peng and Jide Tian

A series of NO-releasing glycosyl derivatives (**2–14**) of oleanolic acid were synthesized, and **3** exhibited better solubility and strong cytotoxicity against human HCC than the active compound **1**.

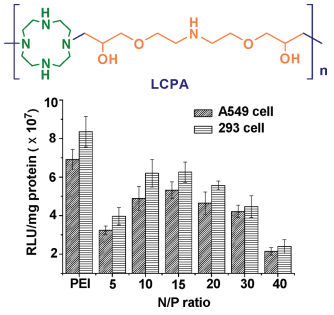


640

Linear cyclen-based polyamine as a novel and efficient reagent in gene delivery

Yong-Zhe Xiang, Zhi-Hua Feng, Ji Zhang,* Yi-Le Liao, Chuan-Jiang Yu, Wen-Jing Yi, Wen Zhu* and Xiao-Qi Yu*

Novel linear cyclen-based polyamine (LCPA) could act as an effective non-viral gene vector towards both A549 and 293 cell lines.

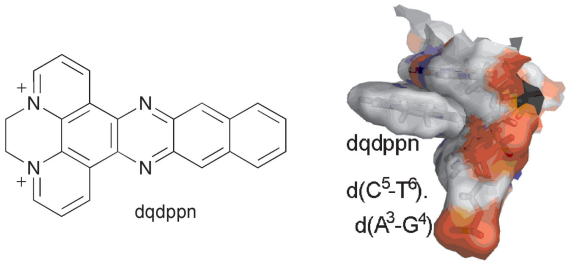


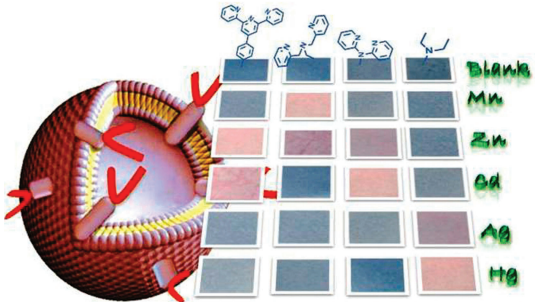
648

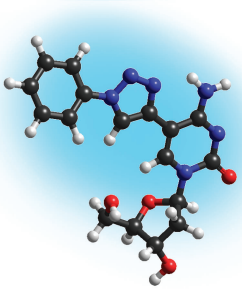
Structural analysis of the binding of the diquaternary pyridophenazine derivative dqdppn to B-DNA oligonucleotides

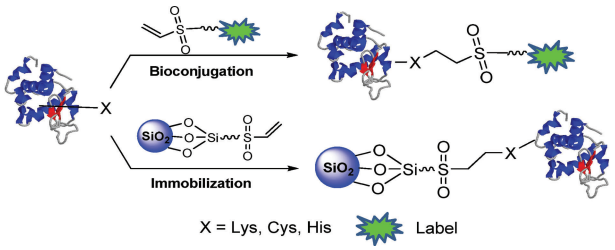
Philip Waywell, James A. Thomas* and Mike P. Williamson*

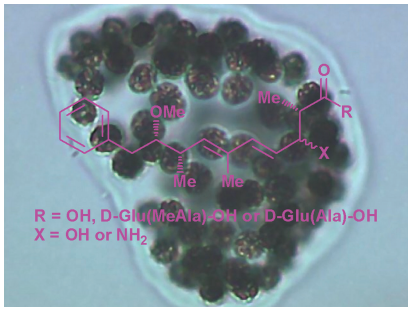
The interaction of dqdppn with several hexa- and octanucleotide duplexes has been studied. The NMR-derived structural model of two of the binding complexes demonstrates that dqdppn intercalates from the major groove in an unusual 'side-on' geometry, rather than threading through the helix.









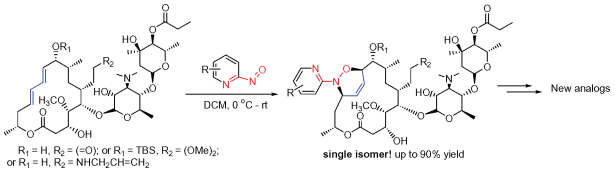


691

Preparation and biological evaluation of novel leucomycin analogs derived from nitroso Diels–Alder reactions

Baiyuan Yang, Tina Zöllner, Peter Gebhardt, Ute Möllmann and Marvin J. Miller*

Novel macrolide analogs were synthesized using nitroso Diels–Alder reactions of leucomycin A7 and subsequent chemical modifications. Hetero cycloaddition reactions proceeded in a highly regio- and stereoselective fashion. Most analogs retained antibiotic profiles similar to leucomycin A7, and, in contrast to leucomycin itself, several exhibited moderate antiproliferative and cytotoxic activity.

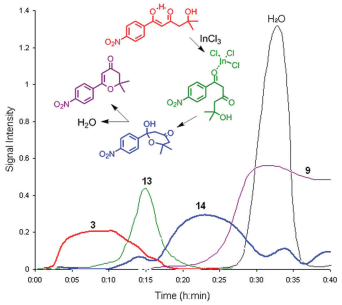


698

Highly efficient indium(III)-mediated cyclisation of 5-hydroxy-1,3-diketones to 2,3-dihydro-4*H*-pyran-4-ones; mechanistic insights from *in situ* Fourier transform infrared spectroscopy

P. C. Andrews,* W. J. Gee, P. C. Junk and H. Krautscheid

Cyclisation of δ-hydroxy-β-diketones to 2,3-dihydro-4*H*-pyran-4-ones occurs efficiently in the presence of a catalytic amount of anhydrous $InCl_3$ and a dehydrating agent, with *in situ* FTIR studies indicating a reaction mechanism sensitive to both temperature and reagent concentration.

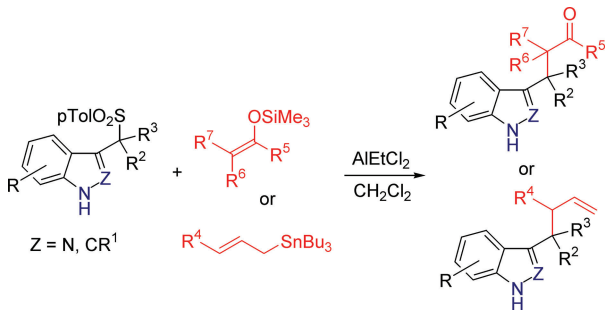


706

Reaction of carbon nucleophiles with alkylideneindazolium and alkylideneindolium ions generated from their 3-(1-arylsulfonylalkyl) indazole and indole precursors

Laura Marsili, Alessandro Palmieri and Marino Petrini*

Nucleophilic substitution of *p*-toluenesulfinate anion on sulfonyl indazoles and sulfonyl indoles is carried out *via* the corresponding iminium ion generated by reaction with $AlEtCl_2$.



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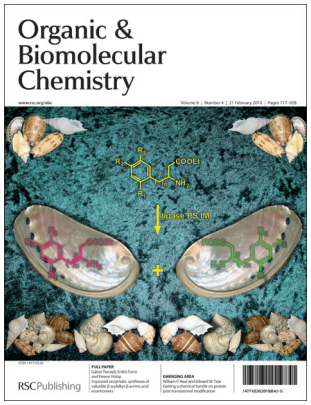

Cover

See Ferenc Fülöp *et al.*, pp. 793–799.
The enantioselective *Burkholderia cepacia*-catalysed hydrolyses of biologically relevant β-arylalkyl-substituted β-amino esters were performed with high enantiomeric excesses and in good yields.

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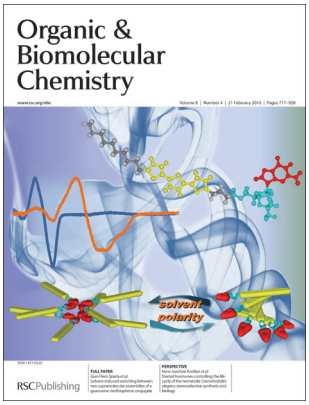
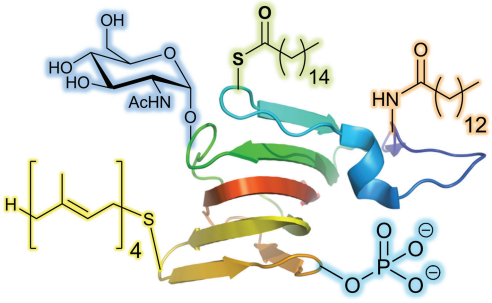


Inside cover

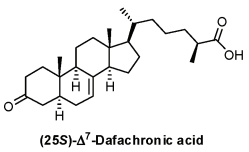
See Gian Piero Spada *et al.*, pp. 774–781.
Guanine or terthienyl: which one leads the self-assembly of the guanosine–terthiophene conjugate? Upon increasing solvent polarity, the supramolecular aggregate directed by guanine stacking is reversibly converted into a terthienyl stacked architecture.

Image reproduced by permission of Gian Piero Spada *et al.* from *Org. Biomol. Chem.*, 2010, **8**, 774.

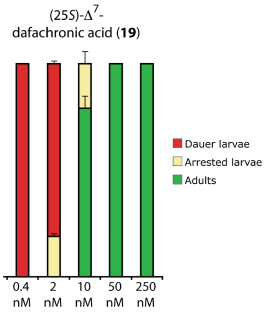
EMERGING AREA



PERSPECTIVE



(25*S*)-Δ^7-Dafachronic acid

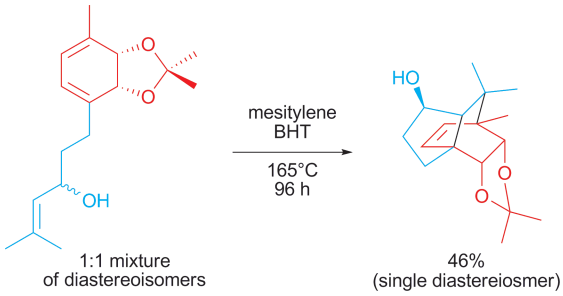


751

Chemoenzymatic and enantiodivergent routes to 1,2-ring-fused bicyclo[2.2.2]octane and related tricyclic frameworks

Kerrie A. B. Austin, Jon D. Elsworth, Martin G. Banwell* and Anthony C. Willis

The chemoenzymatically derived triene undergoes a facially-selective IMDA reaction to give an adduct incorporating the carbocyclic framework of the sesquiterpene (–)-khusiol.

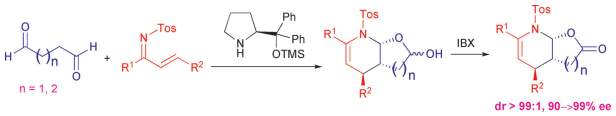


755

Enantioselective construction of lactone[2,3-*b*]piperidine skeletons *via* organocatalytic tandem reactions

Zhao-Quan He, Bo Han, Rui Li,* Li Wu and Ying-Chun Chen*

A highly enantioselective construction of δ- and γ-lactone[2,3-*b*]piperidine skeletons was accomplished by tandem aza-Diels–Alder reaction–hemiacetal formation–oxidation from *N*-Tos-1-aza-1,3-butadienes and aliphatic dialdehydes.

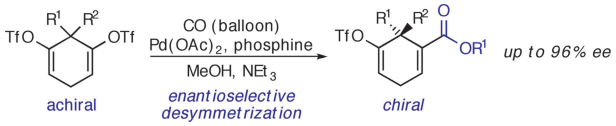


758

Enantioselective desymmetrizing palladium catalyzed carbonylation reactions: the catalytic asymmetric synthesis of quaternary carbon center containing 1,3-dienes

Simon J. Byrne, Anthony J. Fletcher, Paul Hebeisen and Michael C. Willis*

A desymmetrization protocol has been used to develop a palladium catalyzed enantioselective carbonylation process. Achiral cyclic bis-alkenyltriflates are converted to their corresponding monoester derivatives with selectivities of up to 96% ee.

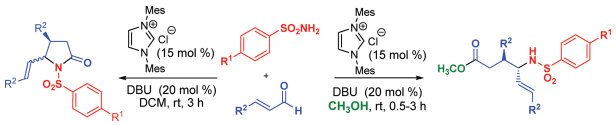


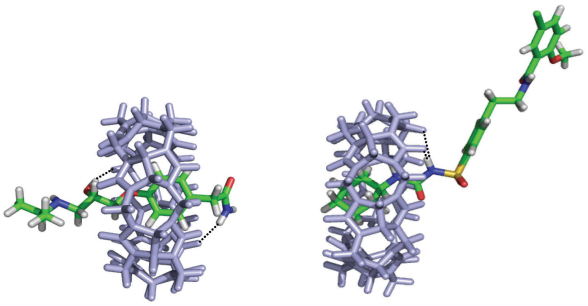
761

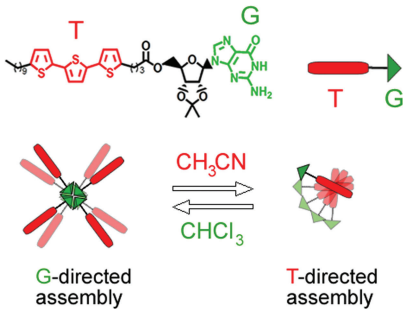
A novel pseudo four component reaction involving homoenolate for the synthesis of γ-aminobutyric acid (GABA) derivatives

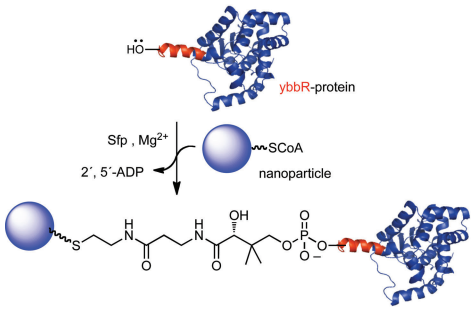
Vijay Nair,* Vimal Varghese, Beneesh P. Babu, C. R. Sinu and Eringathodi Suresh

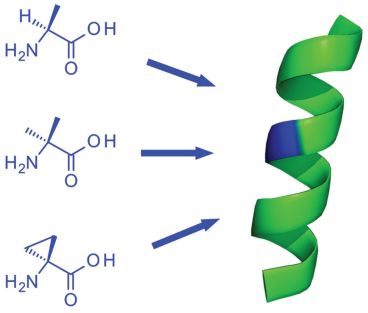
Homoenolate generated from α,β-unsaturated aldehydes by NHC catalysis underwent facile addition to conjugated sulfonimines and subsequent methanolysis to afford protected GABA derivatives stereoselectively and in high yields, thus constituting a novel pseudo four component reaction.

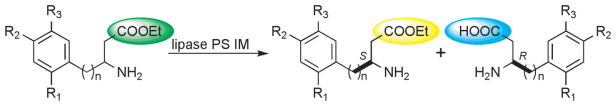


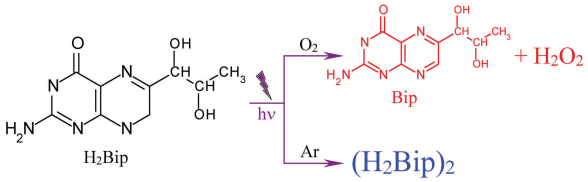


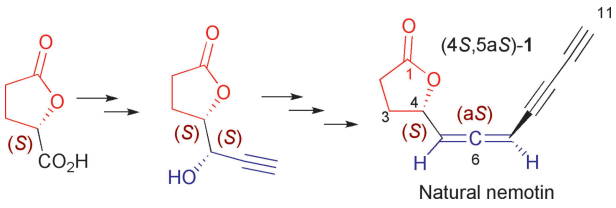


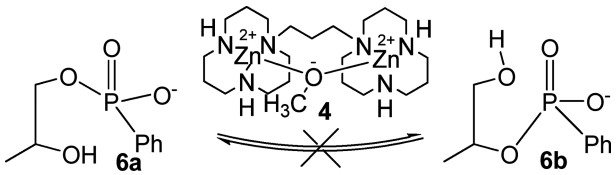


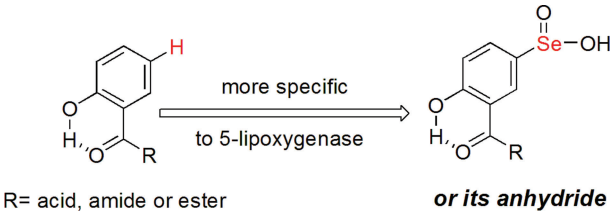








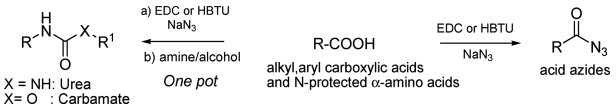




5-Selenization of salicylic acid derivatives yielded isoform-specific 5-lipoxygenase inhibitors

Sun-Chol Yu, Hartmut Kuhn,* Constantin-Gabriel Daniliuc, Igor Ivanov, Peter G. Jones and Wolf-Walther du Mont*

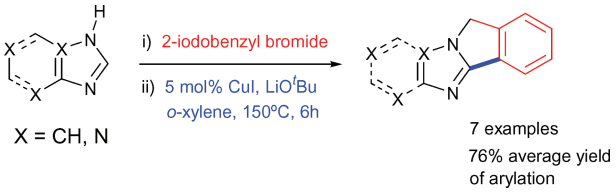
5-Seleninic acids or anhydrides of salicylic acid amides or esters are promising inhibitors more selective to recombinant human 5-lipoxygenase than to rabbit reticulocyte 12/15-lipoxygenase.



New and simple synthesis of acid azides, ureas and carbamates from carboxylic acids: application of peptide coupling agents EDC and HBTU

Vommina V. Sureshbabu,* H. S. Lalithamba, N. Narendra and H. P. Hemantha

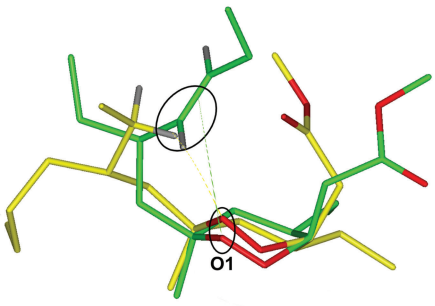
Acid azides have been efficiently prepared from carboxylic acids using peptide coupling agents EDC or HBTU; and the reaction has been extended to the one pot synthesis of ureas and carbamates from carboxylic acids



Ligand-free copper(I)-catalysed intramolecular direct C–H functionalization of azoles

Nekane Barbero, Raul SanMartin* and Esther Domínguez*

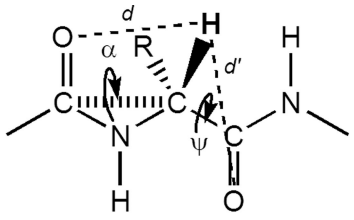
The first examples of copper-catalysed intramolecular direct C-arylation of azaheterocycles for the synthesis of complex heterofused compounds is presented, featuring an unprecedented arylation *via* C–H activation of 9*H*-purine and 4-azabenzimidazole.



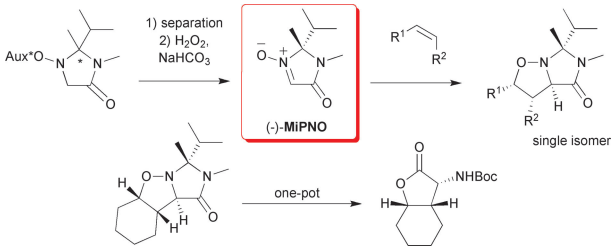
Insight into the mechanism of action of plakortins, simple 1,2-dioxane antimalarials

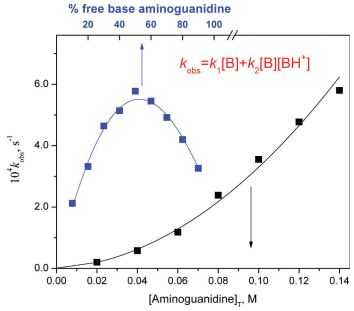
Orazio Taglialatela-Scafati, Ernesto Fattorusso, Adriana Romano, Fernando Scala, Vincenzo Barone, Paola Cimino, Emiliano Stendardo, Bruno Catalanotti, Marco Persico and Caterina Fattorusso*

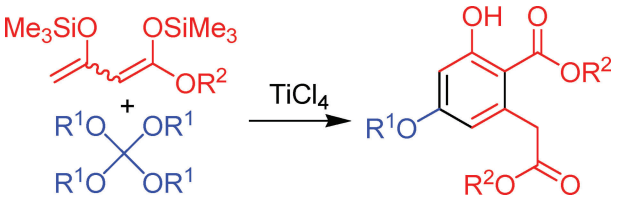
Computational calculations and chemical reactions give insight into the mechanism of the antimalarial action of plakortin and dihydroplakortin, simple 1,2-dioxanes isolated from a marine sponge.



$$\delta = 2.87 + \sigma_R + 1.32\cos^2\frac{(\alpha - 25)}{d} + 0.75\cos^2\frac{(\psi - 10)/2}{d'}$$







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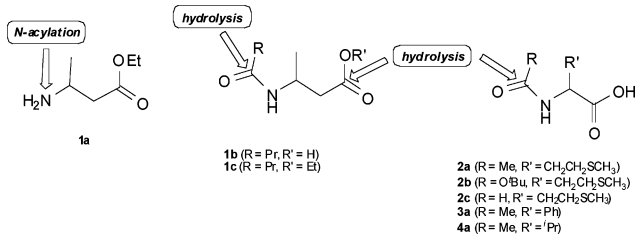

Formation and hydrolysis of amide bonds by lipase A from *Candida antarctica*; exceptional features

Arto Liljeblad,* Pauli Kallio, Marita Vainio, Jarmo Niemi and Liisa T. Kanerva

Exceptional lipase: the ability of lipase A from *Candida antarctica* (CAL-A) to form and hydrolyze amide bonds was studied with **1a–c**, **2a–c**, **3a** and **4a**. The possible role of enzyme contaminants in the reactions was studied by fractionation and sequence-based identification of the commercial CAL-A preparation Cat#ICR-112 (Codexis).

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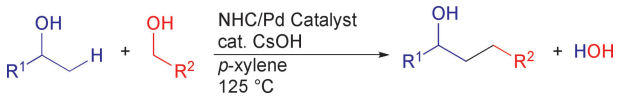
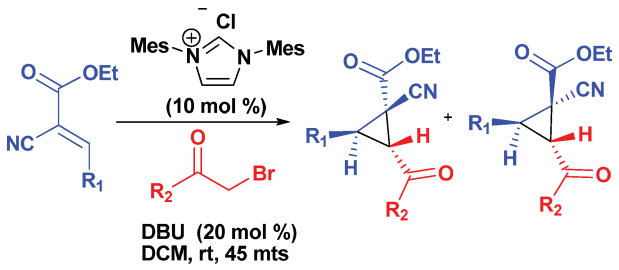


Cross-coupling reaction of alcohols for carbon–carbon bond formation using pincer-type NHC/palladium catalysts

Osamu Kose and Susumu Saito*

A cross-coupling reaction of different alcohols was achieved using a pincer-type NHC/PdBr complex as the catalyst precursor, and the reaction, under either Ar or H_2 gas, displayed a broad substrate scope with respect to both primary and secondary alcohol components, with high product alcohol selectivity.

901

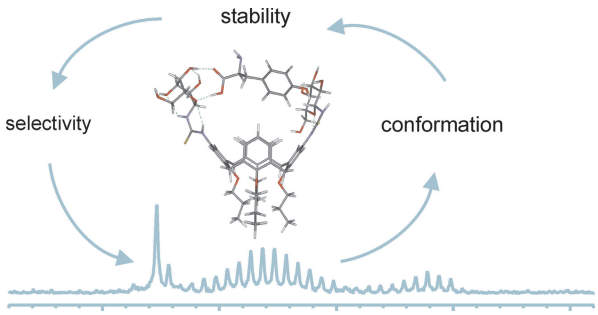


Nucleophilic heterocyclic carbene as a novel catalyst for cyclopropanation of cyano acrylates

Anabha E. Raveendran, Rony Rajan Paul, Eringathodi Suresh and Vijay Nair*

Nucleophilic heterocyclic carbenes (NHCs) have been used or the first time as catalysts in the cyclopropanation of ethyl cyanocinnamates with phenacyl bromide by Michael-initiated ring-closure (MIRC).

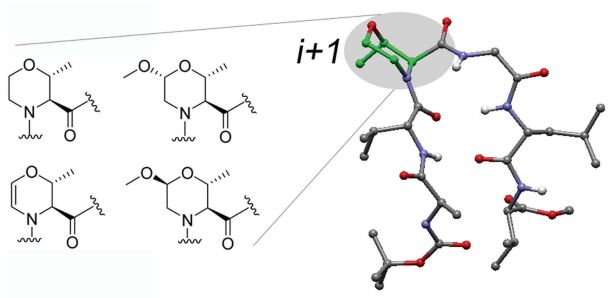
906



Glucosylthioureidocalix[4]arenes: Synthesis, conformations and gas phase recognition of amino acids

Mika Torvinen, Raisa Neitola, Francesco Sansone, Laura Baldini, Rocco Ungaro, Alessandro Casnati,* Pirjo Vainiotalo* and Elina Kalenius*

Conformational properties of glucosylcalixarenes and their selective complexation with amino acids have been clarified in solution and gas-phase.



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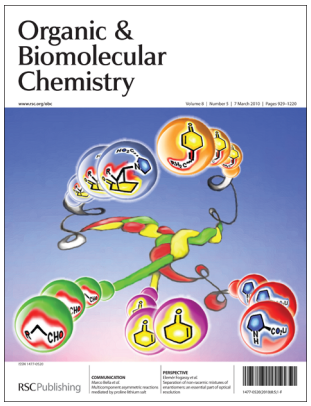
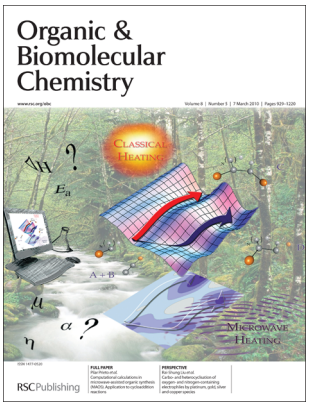
ISSN 1477-0520 CODEN OBCRAK 8(5) 929–1220 (2010)



Cover

See Marco Bella *et al.*, pp. 980–983.
Bicyclic adducts bearing five stereocenters and novel fragrances are produced by the multicomponent reaction between proline lithium salt, aliphatic aldehydes and 2-cyclohexen-1-one. Authors thank Miss Susy Piovesana for designing this cover.

Image reproduced by permission of Polyssena Renzi, Jacob Overgaard and Marco Bella from *Org. Biomol. Chem.*, 2010, **8**, 980.

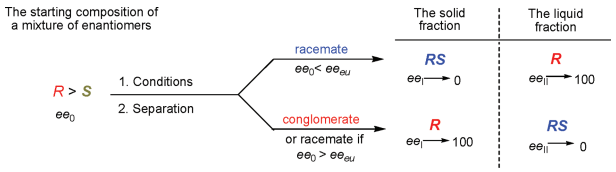


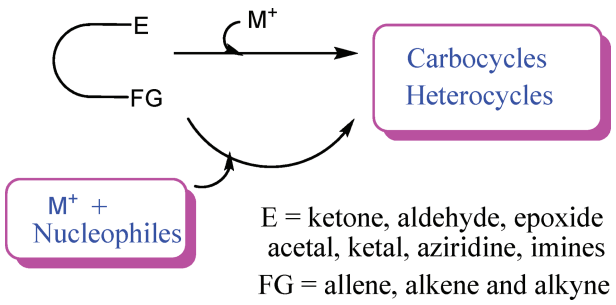
Inside cover

See Pilar Prieto *et al.*, pp. 1000–1009.
The occurrence of thermal and non-thermal effects of microwave irradiation in some reactions could be studied using computational calculations.

Image reproduced by permission of A. de Cózar, M. C. Millán, C. Cebrián, P. Prieto, A. Díaz-Ortiz, A. de la Hoz and F. P. Cossío from *Org. Biomol. Chem.*, 2010, **8**, 1000.

PERSPECTIVES



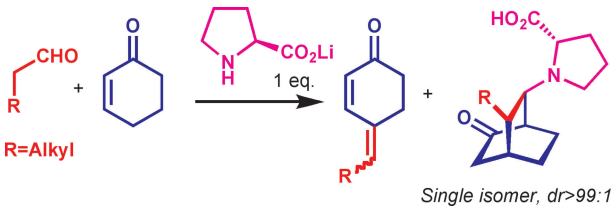


980

Multicomponent asymmetric reactions mediated by proline lithium salt

Polyssena Renzi, Jacob Overgaard and Marco Bella*

Bicyclic adducts bearing five sterocenters and novel fragrances are produced by the multicomponent reaction between proline lithium salt, aliphatic aldehydes and 2-cyclohexen-1-one.

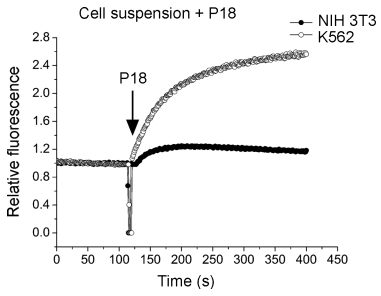


984

Anticancer mechanism of peptide P18 in human leukemia K562 cells

Chengkang Tang, Ximing Shao, Binbin Sun, Wenli Huang, Feng Qiu, Yongzhu Chen, Ying-kang Shi, Er-yong Zhang, Chen Wang and Xiaojun Zhao*

Studies on the anticancer mechanism of peptide P18 in human leukemia K562 cells revealed that P18 causes the K562 cell death by depolarizing plasma membrane potential and enhancing membrane permeability, rather than activating the classical apoptosis pathway.

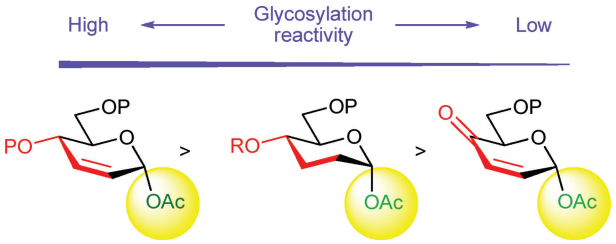


988

Chemoselective glycosylations using 2,3-unsaturated-4-keto glycosyl donors

Shunichi Kusumi, Sainan Wang, Tatsuya Watanabe, Kaname Sasaki, Daisuke Takahashi and Kazunobu Toshima*

Chemoselective glycosylations were effectively performed using 2,3-unsaturated glycosyl and 2,3-dideoxy glycosyl acetates as armed glycosyl donors, and 2,3-unsaturated-4-keto glycosyl acetates as disarmed glycosyl donors.

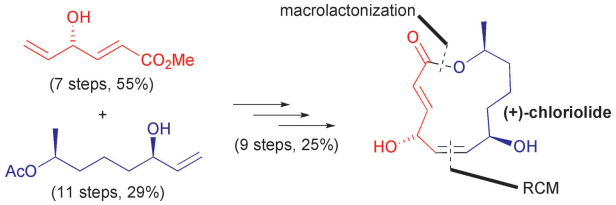


991

Total synthesis of (+)-chloriolide

Timm T. Haug and Stefan F. Kirsch*

The first total synthesis of (+)-chloriolide, a 12-membered macrolide from *Chloridium virescens* (var. *chlamydosporum*), was accomplished in a longest linear sequence of 20 steps from commercial materials in 7% overall yield.

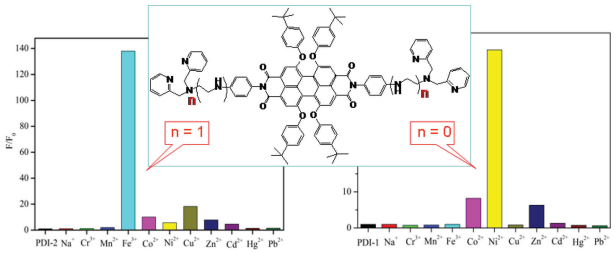


1017

Nickel(II) and iron(III) selective off-on-type fluorescence probes based on perylene tetracarboxylic diimide

Haixia Wang, Delou Wang, Qi Wang, Xiyou Li* and Christoph A. Schalley*

Two novel fluorescent probes based on perylene tetracarboxylic diimde (PDI) with turn-on output have been prepared. Because of the different linkers between the receptor and the fluorophore, the selectivity of the probes is significantly altered.

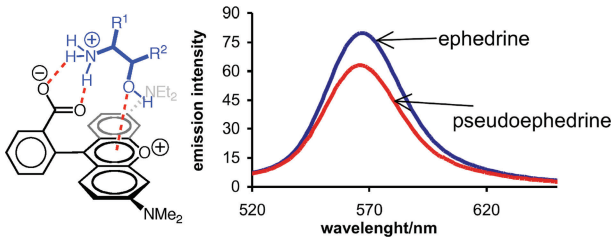


1027

A fluorescent diastereoselective molecular sensor for 1,2-aminoalcohols based on the rhodamine B lactone–zwitterion equilibrium

Clifton J. Stephenson and Ken D. Shimizu*

Rhodamine dye was shown to be able to differentiate and measure the diastereoselectivity of 1,2-aminoalcohols by monitoring the fluorescence of the zwitterionic form.

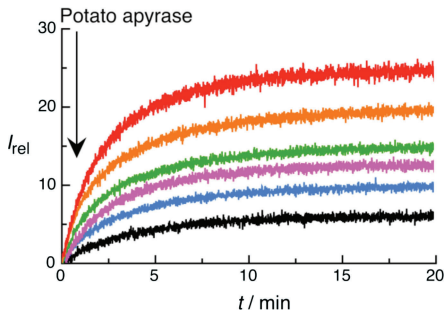


1033

Implementation of anion-receptor macrocycles in supramolecular tandem assays for enzymes involving nucleotides as substrates, products, and cofactors

Mara Florea and Werner M. Nau*

Anion-receptor macrocycles, in combination with fluorescent dyes, can be exploited for the kinetic monitoring of the activity of nucleotide triphosphate-dependent enzymes such as apyrases.

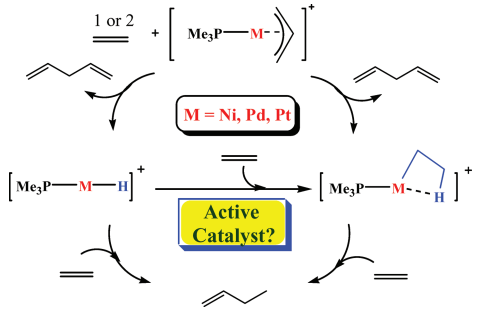


1040

Ni-, Pd-, or Pt-catalyzed ethylene dimerization: a mechanistic description of the catalytic cycle and the active species

Dipankar Roy and Raghavan B. Sunoj*

Mechanistic insights on ethylene dimerization by using $[M(\eta_3\text{-allyl})(PMe_3)]^+$, where M = Ni(II), Pd(II), and Pt(II), are presented. The computed DFT energies have been employed to propose the likely nature of the 'active catalyst' in the catalytic cycle.

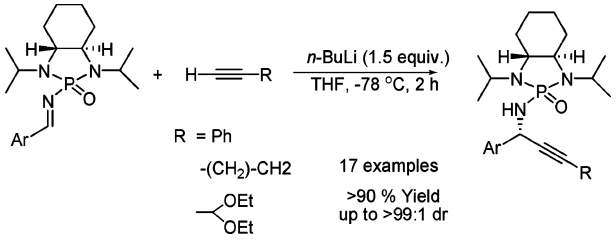


1091

Chiral *N*-phosphonyl imine chemistry: an efficient asymmetric synthesis of chiral *N*-phosphonyl propargylamines

Parminder Kaur, Gaurav Shakya, Hao Sun, Yi Pan* and Guigen Li*

Chiral *N*-phosphonylimines were reacted with lithium acetylides to give substituted chiral propargylamines. The types of bases for generating acetylides and solvents are crucial for effectiveness of this asymmetric reaction. Seventeen examples were studied to give excellent yields (>90%) and diastereoselectivities (>96 : 4 to >99 : 1).

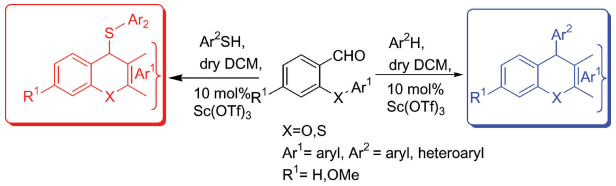


1097

Scandium triflate-catalyzed one-pot domino approach towards general and efficient syntheses of unsymmetrical 9-substituted xanthene derivatives

Ritesh Singh and Gautam Panda*

A general and efficient one-pot cascade/tandem approach to synthesize unsymmetrical 9-aryl/heteroaryl xanthenes as well as 9-(thioaryl) xanthenes has been developed under extremely mild reaction conditions using 10 mol% $Sc(OTf)_3$ as a catalyst.

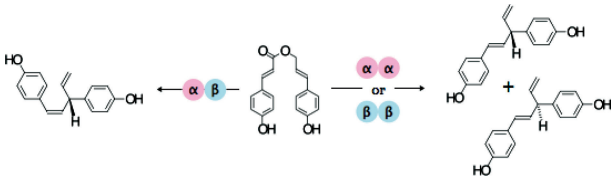


1106

Subunit composition of hinokiresinol synthase controls enantiomeric selectivity in hinokiresinol formation

Masaomi Yamamura, Shiro Suzuki, Takefumi Hattori and Toshiaki Umezawa*

Subunit composition of hinokiresinol synthase can control not only *cis*/*trans* isomerism but also enantioselectivity in hinokiresinol formation

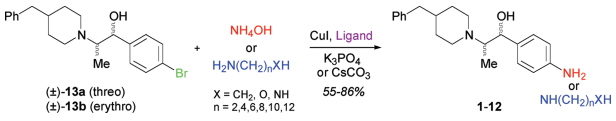


1111

Copper-catalyzed amination of (bromophenyl)ethanolamine for a concise synthesis of aniline-containing analogues of NMDA NR2B antagonist ifenprodil

Cédric Bouteiller, Javier Becerril-Ortega, Patrice Marchand, Olivier Nicole, Louisa Barré, Alain Buisson and Cécile Perrio*

Anilines **1–12** were prepared by copper-catalyzed amination of bromoarenes **13** using CuI and *N*,*N*-diethylsalicylamide, 2,4-pentadione or 2-acetylcyclohexanone as catalytic systems, and were evaluated as NR2B antagonists.

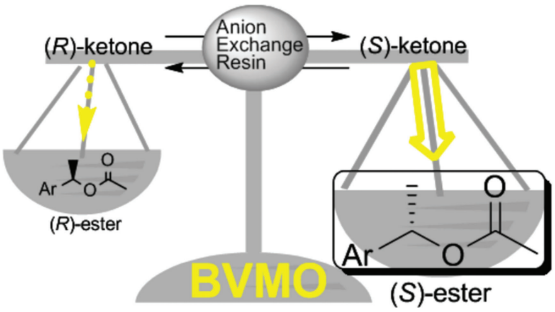


1121

BVMO-catalysed dynamic kinetic resolution of racemic benzyl ketones in the presence of anion exchange resins

Cristina Rodríguez, Gonzalo de Gonzalo, Ana Rioz-Martínez, Daniel E. Torres Pazmiño, Marco W. Fraaije and Vicente Gotor*

Dynamic kinetic resolutions of different benzyl ketones were performed by combining the selective Baeyer–Villiger oxidation catalysed by HAPMO with anion exchange racemisation in order to obtain the corresponding (*S*)-benzyl esters with high yields and optical purities.

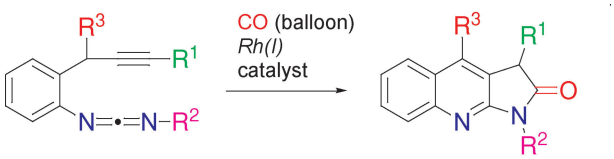


1126

A facile synthesis of pyrrolo[2,3-*b*]quinolines *via* a Rh(I)-catalyzed carbodiimide-Pauson–Khand-type reaction

Takao Saito,* Naoki Furukawa and Takashi Otani

A Rh(I)-catalyzed Pauson–Khand-type [2 + 2 + 1] cocyclization of *N*-[2-(2-alkyn-1-yl)phenyl]carbodiimides provides a new, straightforward synthetic method for pyrrolo[2,3-*b*]quinolin-2-ones.



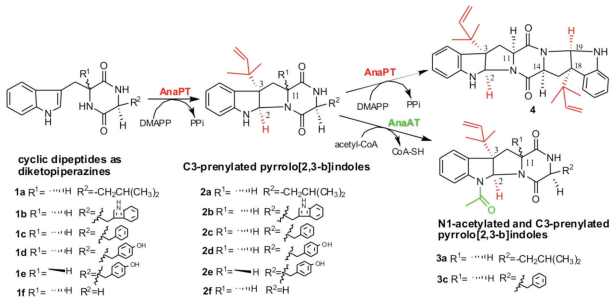
R^1 = Pent, Me, *t*-Bu, Ph, or TBS, R^2 = Pr, Bn, Cy, or Ph, R^3 = H or Me

1133

Reconstruction of pyrrolo[2,3-b]indoles carrying an α-configured reverse C3-dimethylallyl moiety by using recombinant enzymes

Wen-Bing Yin, Xiu-Lan Xie, Marco Matuschek and Shu-Ming Li*

Nine reversely C3-prenylated pyrrolo[2,3-b]indoles were successfully prepared by using recombinant AnaPT and AnaAT. An α-configurated fused ring between the indoline and the diketopiperazine rings was introduced.

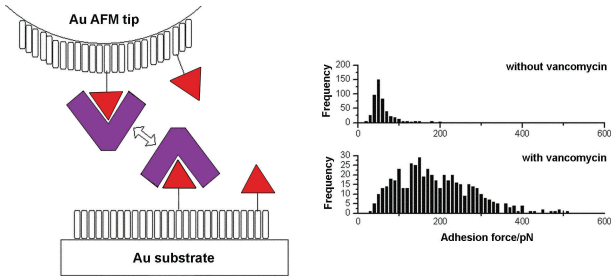


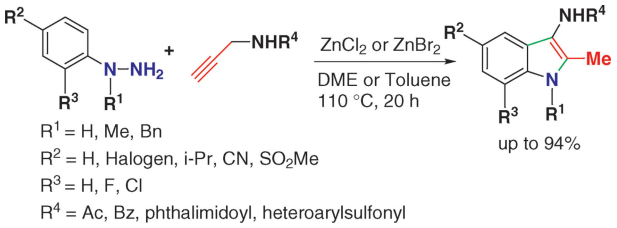
1142

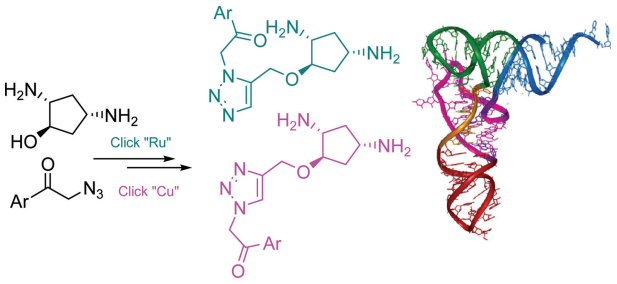
Vancomycin dimer formation between analogues of bacterial peptidoglycan surfaces probed by force spectroscopy

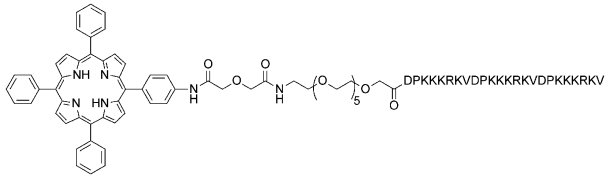
Matthew Batchelor,* Dejian Zhou, Matthew A. Cooper, Chris Abell and Trevor Rayment

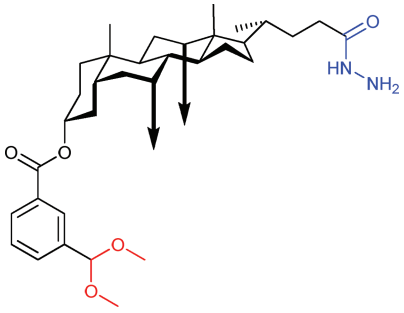
Force spectroscopy was used to investigate the rupture of interfacial vancomycin dimer complexes formed between pairs of vancomycin molecules when bound to model bacterial cell-wall surfaces.









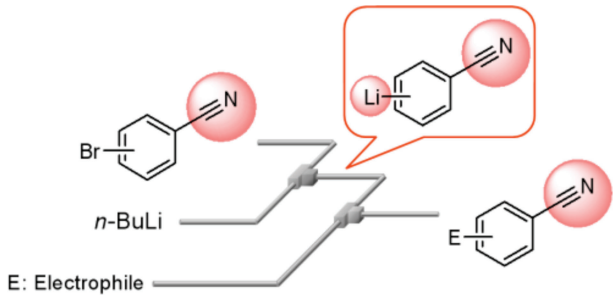


1212

Generation and reaction of cyano-substituted aryllithium compounds using microreactors

Aiichiro Nagaki, Heejin Kim, Hirotsugu Usutani, Chika Matsuo and Jun-ichi Yoshida*

An effective method for the generation and reaction of aryllithium compounds bearing a cyano group has been developed using microflow systems.



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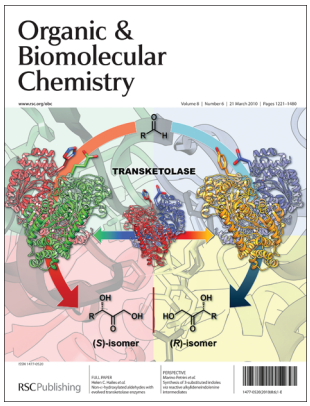

Cover
See Helen C. Hailes *et al.*, pp. 1301–1309.
Single-point active site transketolase mutants enhanced and reversed the stereoselectivity of the wild-type enzyme in the conversion of linear and cyclic aliphatic aldehydes to α,α′-dihydroxyketones.

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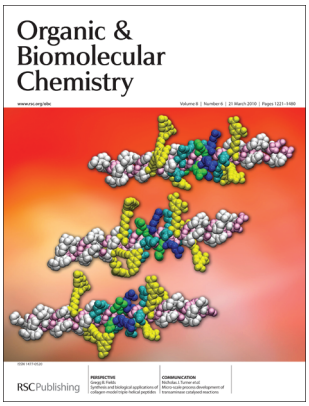

Inside cover
See Gregg B. Fields, pp. 1237–1258.
Dr Fields' research interests are in the use of chemical approaches to better understand how protein three-dimensional structures influence cellular and enzymatic behaviours.

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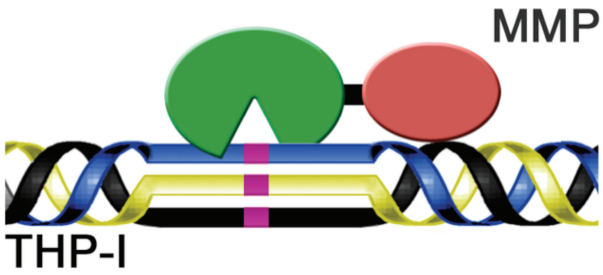
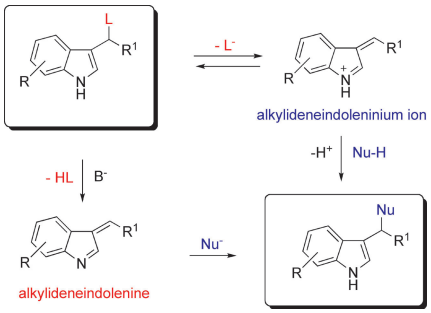
PERSPECTIVES



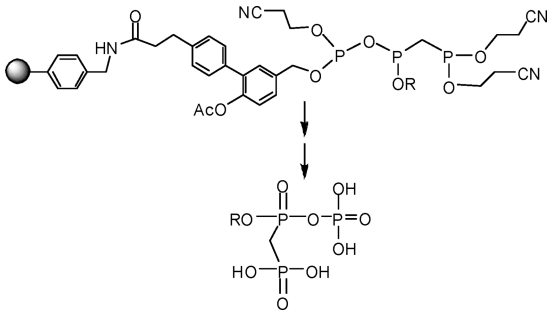


1271

Synthesis of nucleoside 5′-*O*-α,β-methylene-β-triphosphates and evaluation of their potency towards inhibition of HIV-1 reverse transcriptase

Y. Ahmadibeni, C. Dash, M. J. Hanley, S. F. J. Le Grice, H. K. Agarwal and K. Parang*

Herein, we report the solid-phase synthesis of 5′-*O*-nucleoside β-triphosphates containing an α,β-methylene triphosphate bridge by using a novel solid-phase phosphitylating reagent. Cytidine 5′-*O*-α,β-methylene-β-triphosphate inhibited RNase H activity of HIV-1 reverse transcriptase with a K_i value of 225 μM.

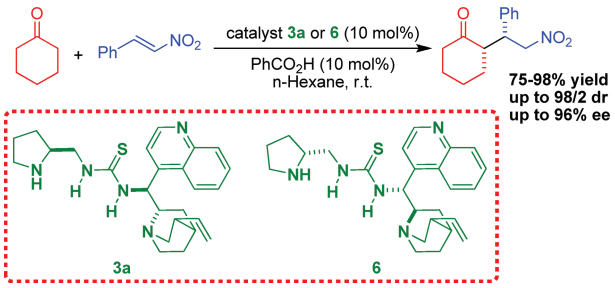


1275

Novel thiourea-amine bifunctional catalysts for asymmetric conjugate addition of ketones/aldehydes to nitroalkenes: rational structural combination for high catalytic efficiency

Jia-Rong Chen,* Yi-Ju Cao, You-Quan Zou, Fen Tan, Liang Fu, Xiao-Yu Zhu and Wen-Jing Xiao*

A series of thiourea-amine bifunctional catalysts have been developed by a rational combination of prolines with cinchona alkaloids, which are found to be highly efficient catalysts for the conjugate addition of ketones/aldehydes to a wide range of nitroalkenes.

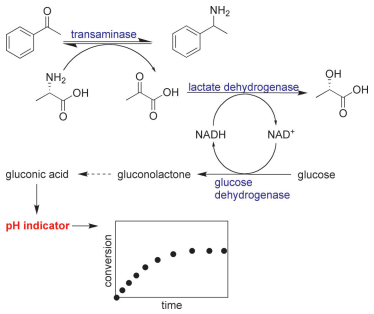


1280

Micro-scale process development of transaminase catalysed reactions

Matthew D. Truppo* and Nicholas J. Turner*

A micro-scale, pH indicator based, colorimetric assay has been developed for the process development of transaminase catalysed reactions. Enzyme activity and stability as a function of multiple reaction parameters have been determined at 100 μL scale.

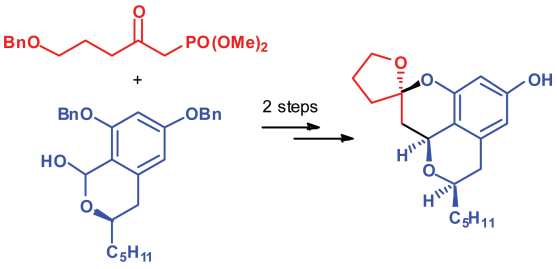


1284

A flexible asymmetric synthesis of the tetracyclic core of berkelic acid using a Horner–Wadsworth–Emmons/oxa-Michael cascade

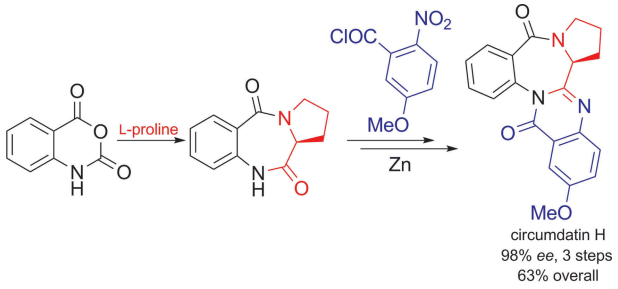
Zoe E. Wilson and Margaret A. Brimble*

The one-pot Horner–Wadsworth–Emmons/oxa-Michael cascade followed by spiroketalisation affords the tetracyclic benzannulated spiroketal core of berkelic acid, an extremophile natural product with selective activity against ovarian cancer.



COMMUNICATIONS

1287

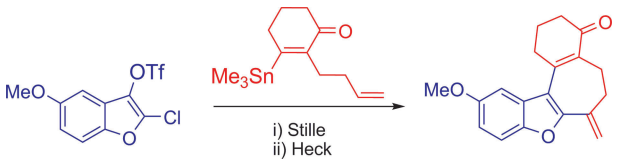


A concise synthesis of enantiopure circumdatins E, H and J

Paul E. Zhichkin,* Xiaomin Jin, Honglu Zhang, Lisa H. Peterson, Catherine Ramirez, Tara M. Snyder and Hilde S. Burton

Enantiopure circumdatins E, H and J were prepared in 3 steps from isatoic anhydrides, L-proline and 2-nitrobenzoic acids.

1290

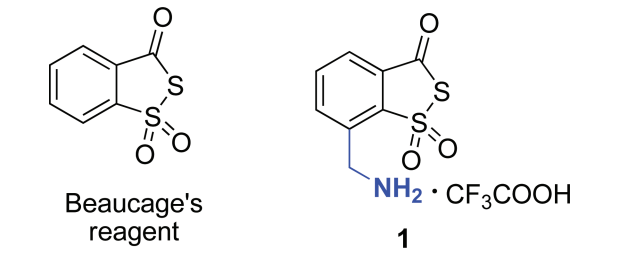


An efficient synthesis of (±)-frondosin B using a Stille–Heck reaction sequence

Kye-Simeon Masters and Bernard L. Flynn*

An efficient synthesis of (±)-frondosin B (34% overall yield) has been developed based on the application of a Stille–Heck reaction sequence of 2-chloro-5-methoxybenzo[*b*]furan-3-yl triflate and 2-(3-butenyl)-3-(trimethylstannyl)cyclohex-2-enone.

1293



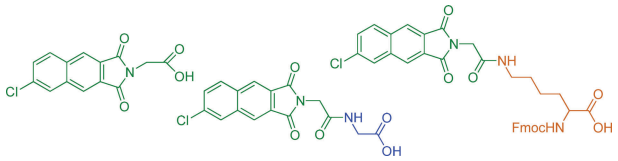
Thiol-dependent DNA cleavage by aminomethylated Beaucage's reagent

Jiahui Zheng, Xiaoqian Liu, Qing Yuan, Yoon-Joo Shin, Daekyu Sun and Yixin Lu*

Aminomethylated Beaucage's reagent **1** was found to be more potent than Beaucage's reagent in causing DNA cleavage. This study demonstrated the importance of the amino functionality in enhancing DNA-cleaving activities, and such findings may facilitate development of novel sulfur-containing DNA-cleaving molecules in cancer therapy.

PAPERS

1296

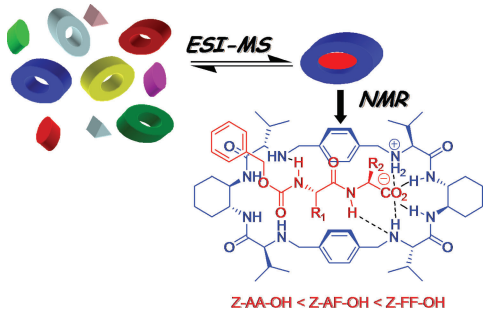


Synthesis and fluorescence of the new environment-sensitive fluorophore 6-chloro-2,3-naphthalimide derivative

Alan R. Katritzky,* Sevil Ozcan and Ekaterina Todadze

Convenient and efficient synthesis of a novel environmentally sensitive chlorine substituted naphthalimide-based fluorophore which can be utilized for the labeling of amino acids is described.

1329

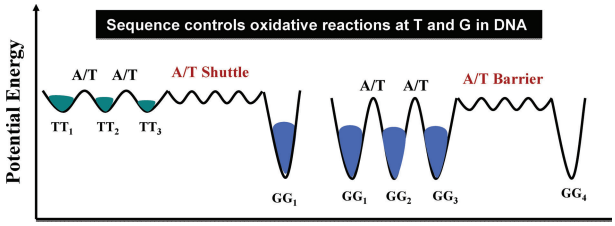


Molecular recognition of *N*-protected dipeptides by pseudopeptidic macrocycles: a comparative study of the supramolecular complexes by ESI-MS and NMR

Ignacio Alfonso,* Michael Bolte, Miriam Bru, M. Isabel Burguete, Santiago V. Luis* and Cristian Vicent

Different experiments based on ESI-MS (competition and CID) and NMR (titration, NOESY and DOSY) were used to study the molecular recognition of N-protected amino acids and dipeptides by pseudopeptidic macrocycles.

1340

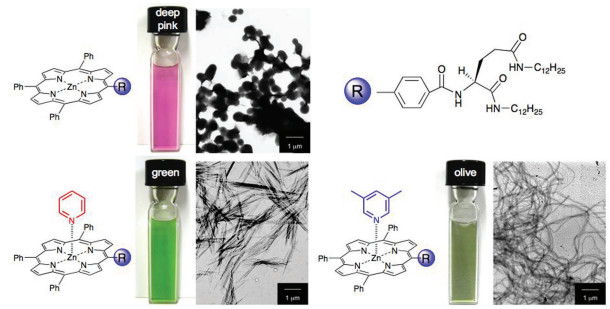


One-electron oxidation of DNA: thymine *versus* guanine reactivity

Sriram Kanvah and Gary B. Schuster*

One-electron oxidation of DNA leads to reaction at guanine because it is the nucleobase with lowest *E*ox. In the absence of guanine, reaction occurs primarily at TT steps. We find that remote guanines "protect" thymines.

1344

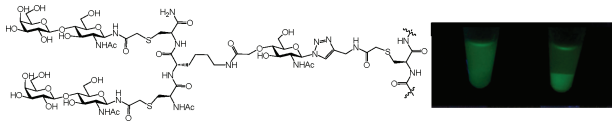


Versatile chiroptics of peptide-induced assemblies of metalloporphyrins

Hirokuni Jintoku, Takashi Sagawa, Tsuyoshi Sawada, Makoto Takafuji and Hirotaka Ihara*

Zinc porphyrin functionalized with L-glutamide has been newly synthesized and its unique responses such as ligand-specific induction of secondary chirality thorough the aggregation morphology change are reported.

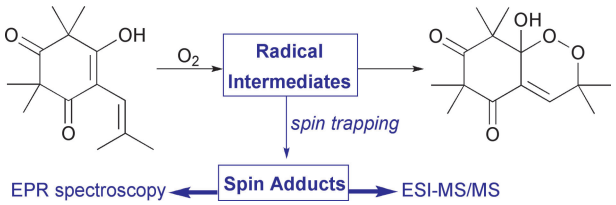
1351

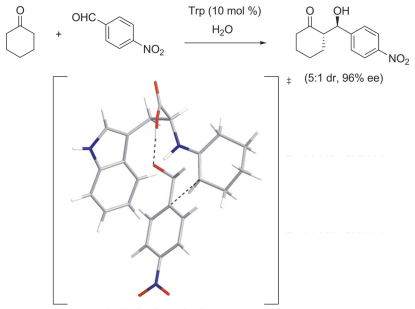


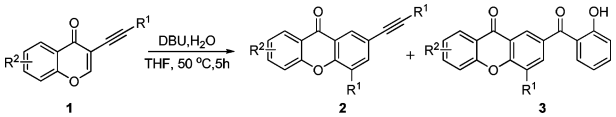
Exploring neoglycoprotein assembly through native chemical ligation using neoglycopeptide thioesters prepared *via* N→S acyl transfer

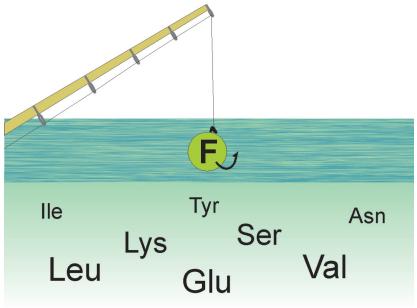
Jonathan P. Richardson, Chung-Hei Chan, Javier Blanc, Mona Saadi and Derek Macmillan*

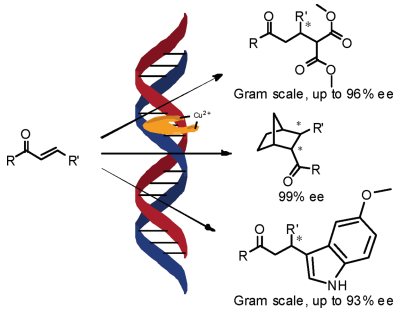
Sugars and simplified oligosaccharide "mimics" can be joined with protein fragments at pre-defined sites and assembled into potential neoglycoprotein therapeutics using native chemical ligation.

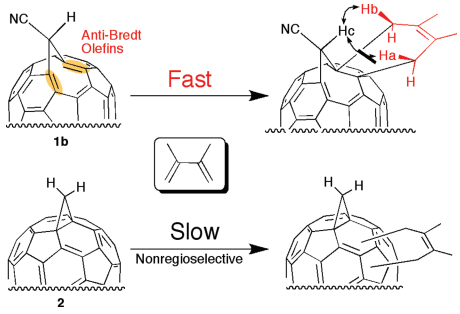


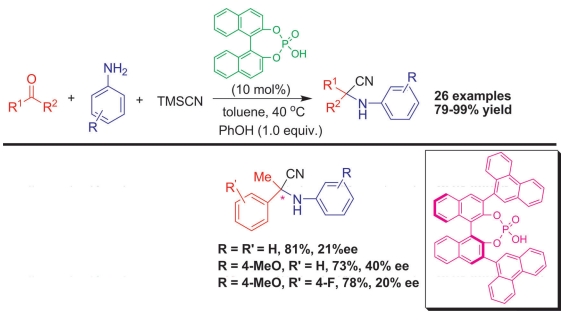


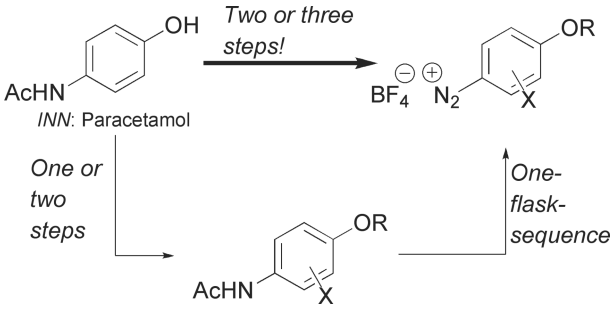












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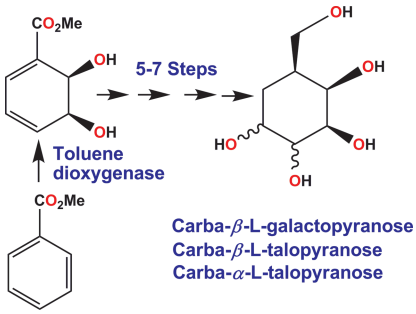
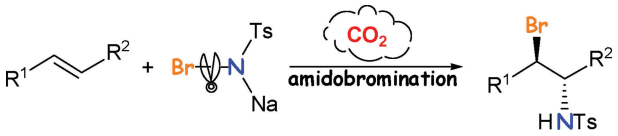


Chemoenzymatic synthesis of the carbasugars carba-β-L-galactopyranose, carba-β-L-talopyranose and carba-α-L-talopyranose from methyl benzoate

Derek R. Boyd,* Narain D. Sharma, Nigel I. Bowers, Gerard B. Coen, John F. Malone, Colin R. O'Dowd, Paul J. Stevenson and Christopher C. R. Allen

The *cis*-dihydrodiol metabolite from methyl benzoate has been used as a synthetic precursor of carba-β-L-galactopyranose, carba-β-L-talopyranose, carba-α-L-talopyranose and carba-β-L-galactopyranose.

1424

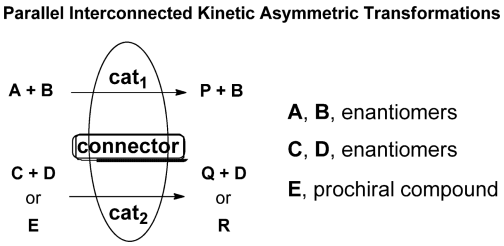


CO_2-induced amidobromination of olefins with bromamine-T

Junpei Hayakawa, Mitsuhiro Kuzuhara and Satoshi Minakata*

The carbon dioxide (CO_2)-induced amidobromination of olefins with bromamine-T is described. The method can be used in reactions with a wide range of olefins, leading to the regioselective formation of amidobrominated compounds.

1431

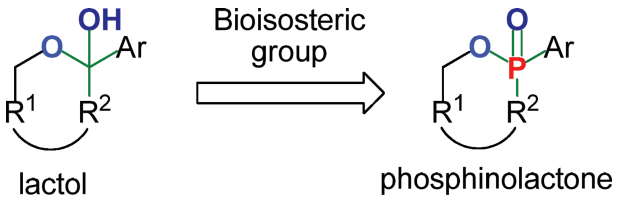


Biocatalysed concurrent production of enantioenriched compounds through parallel interconnected kinetic asymmetric transformations

Ana Rioz-Martínez, Fabricio R. Bisogno, Cristina Rodríguez, Gonzalo de Gonzalo, Iván Lavandera, Daniel E. Torres Pazmiño, Marco W. Fraaije and Vicente Gotor*

Examples of *parallel interconnected kinetic asymmetric transformations* are presented. In a *one-pot* reaction using two biocatalysts, optically active ketones, sulfoxides and *sec*-alcohols could *concurrently* be achieved in a strict *parallel* fashion.

1438



Drug discovery: phosphinolactone, *in vivo* bioisostere of the lactol group

Jean-Noël Volle,* Damien Filippini, Bartlomiej Krawczy, Nikolay Kaloyanov, Arie Van der Lee, Tangui Maurice, Jean-Luc Pirat and David Virieux*

In drug discovery, structural modifications over the lead molecule are often crucial for the development of a drug. Herein, we reported the first *in vivo* bioisosteric effect of phosphinolactone function in relation to the lactol group constituting the bioactive molecule: Hydroxybupropion.

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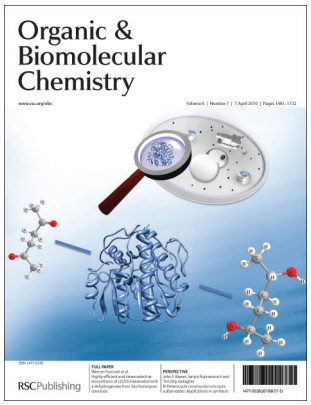
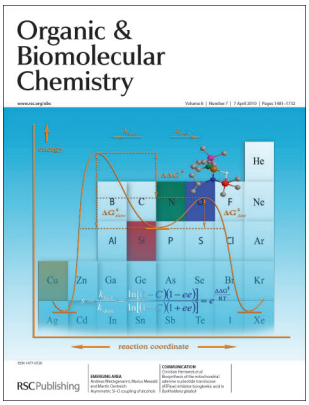
ISSN 1477-0520 CODEN OBCRAK 8(7) 1481–1732 (2010)



Cover

See Werner Hummel *et al.*, pp. 1540–1550.
Discovery of the bakers' yeast reductase responsible for the reduction of 2,5-hexanedione into enantiopure (2*S*,5*S*)-hexanediol. This diol serves as a building block for the production of various fine chemicals and pharmaceuticals.

Image reproduced by permission of Werner Hummel from *Org. Biomol. Chem.*, 2010, **8**, 1540.

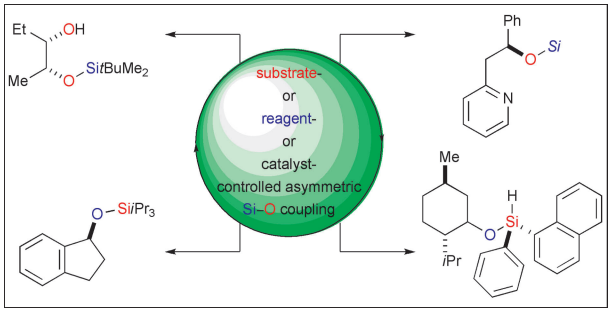


Inside cover

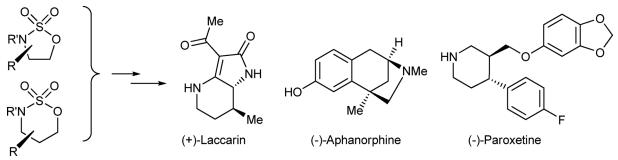
See Martin Oestreich *et al.*, pp. 1497–1504.
Stereoselective protection of alcohols is achieved through asymmetric Si–O coupling of silicon reagents and either chiral racemic alcohols (kinetic resolution) or prochiral alcohols (desymmetrisation).

Image reproduced by permission of Martin Oestreich from *Org. Biomol. Chem.*, 2010, **8**, 1497.

EMERGING AREA



PERSPECTIVE

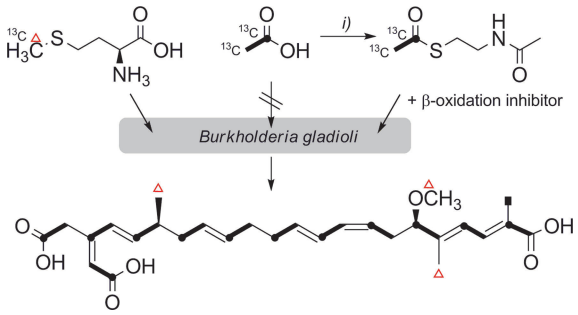


1520

Biosynthesis of the mitochondrial adenine nucleotide translocase (ATPase) inhibitor bongkrekic acid in *Burkholderia gladioli*

Barbara Rohm, Kirstin Scherlach and Christian Hertweck*

Biosynthetic studies with ^{13}C-labelled biosynthetic precursors revealed that the infamous, food-related toxin bongkrekic acid is a polyketide with acetate-derived β-branches and a carboxylate terminus derived from the methyl group of acetate.

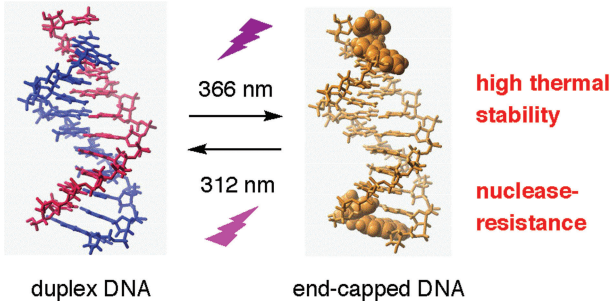


1523

Photoreversible DNA end capping for the formation of hairpin structures

Yoshinaga Yoshimura, Hajime Okada and Kenzo Fujimoto*

We describe a photoreversible DNA end capping *via* 3-cyanovinylcarbazole nucleoside. Doubly end-capped oligodeoxynucleotide (ODN) exhibits increased stability against snake venom phosphodiesterase and shows high thermal stability.

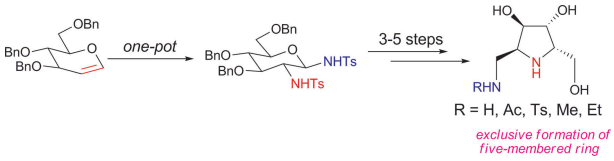


1527

Design and synthesis of new amino-modified iminocyclitols: selective inhibitors of α-galactosidase

Muthupandian Ganesan, Rekhawar V. Madhukarrao and Namakkal G. Ramesh*

A new and short synthesis of hitherto unreported stereo analogue of amino-modified five-membered iminocyclitols, that are selective inhibitors of α-galactosidase, is described.

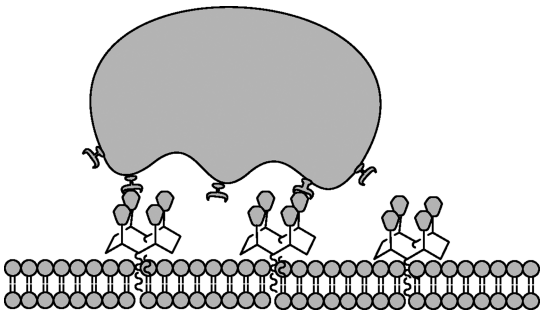


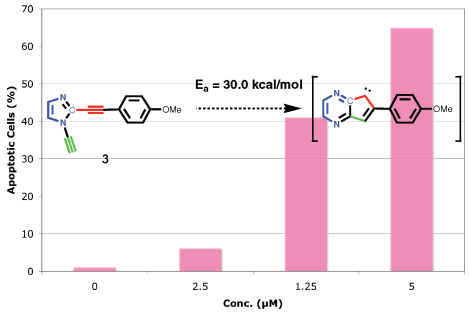
1531

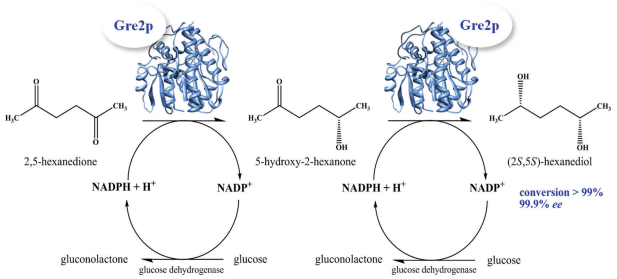
Cell adhesion through clustered ligand on fluid supported lipid bilayers

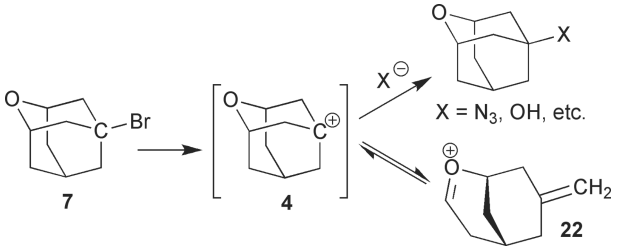
Ludivine Sandrin, Liliane Coche-Guérente, Amandine Bernstein, Hajra Basit, Pierre Labbé, Pascal Dumy* and Didier Boturyn*

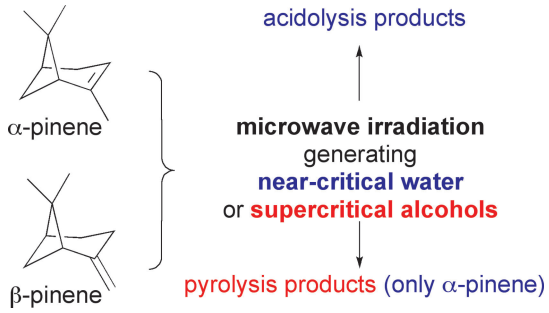
The complementary QCM-D and optical microscopy techniques were used for monitoring cell adhesion on a RGD-functionalized supported lipid bilayer. A critical interligand RGD spacing of nearly 80 nm was estimated for cell adhesion.



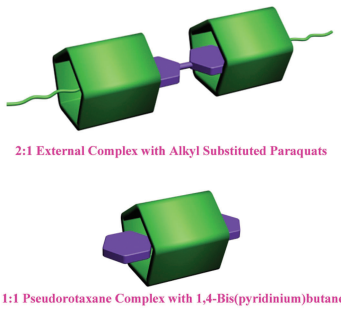








1568

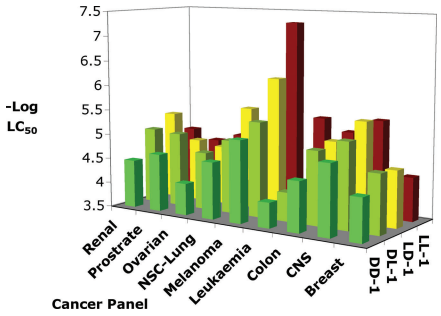


Complex interactions of pillar[5]arene with paraquats and bis(pyridinium) derivatives

Chunju Li,* Qianqian Xu, Jian Li, Feina Yao and Xueshun Jia*

The pillar[5]arene host forms 2 : 1 external complexes with alkyl-substituted paraquats, and it forms 1 : 1 pseudorotaxane-type inclusion complexes with methylene [–$(CH_2)_n$–] connected bis(pyridinium) derivatives.

1577

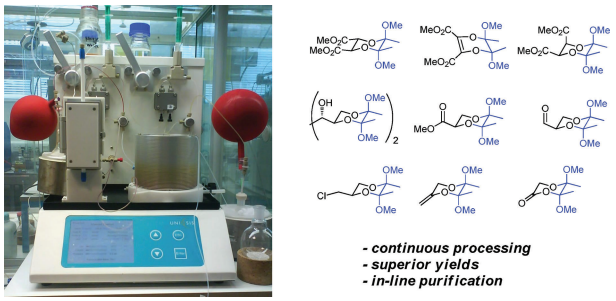


Triple molecular target approach to selective melanoma cytotoxicity

Edward B. Skibo,* Akmal Jamil, Brittany Austin, Douglas Hansen and Armand Ghodousi

Phenylalanine-linked pyrrolo[1,2-*a*]benzimidazole **LL1** was successfully designed to target melanoma cells *in vitro*; the design utilised three molecular targets: a phenylalanine pump, the reducing enzyme DT-diaphorase, and IMP dehydrogenase.

1588

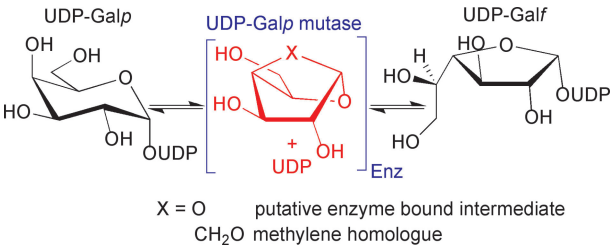


The continuous flow synthesis of butane-2,3-diacetal protected building blocks using microreactors

Catherine F. Carter, Ian R. Baxendale, John B. J. Pavey and Steven V. Ley*

The continuous flow syntheses of a family of butane-2,3-diacetal protected building blocks has been achieved using microreactors in concert with solid supported reagents and scavengers.

1596



The UDP-Gal*p* mutase catalyzed isomerization: synthesis and evaluation of 1,4-anhydro-β-D-galactopyranose and its [2.2.2] methylene homologue

Ali Sadeghi-Khomami, Tatiana J. Forcada, Claire Wilson, David A. R. Sanders and Neil R. Thomas*

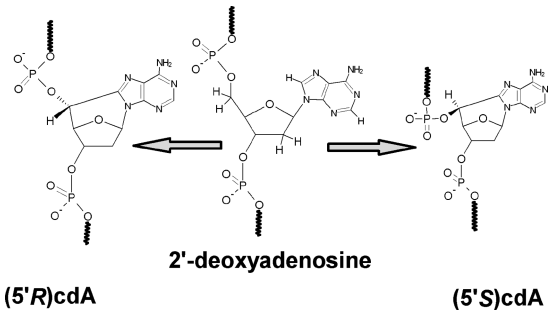
The synthesis of 1,4-anhydro-β-D-galactopyranose (1,5-anhydro-α-D-galactofuranose), a proposed intermediate in the ring contraction isomerisation catalyzed by UDP-galactopyranose mutase, together with its [2.2.2] bicyclic methylene homologue, synthesised as a possible competitive inhibitor or alternative substrate, are reported.

1603

Formation of 5′,8-cyclo-2′-deoxyadenosine in single strand DNA. Theoretical quantum mechanics study

Boleslaw T. Karwowski*

In the present study, for the first time, emphasis was placed on the investigation of the possible reaction of 2′-deoxyadenosine-3′,5′-diphosphate radicals, leading to the formation of the related 5′,8-cyclo-2′-deoxynucleotide-3′,5′-diphosphate.

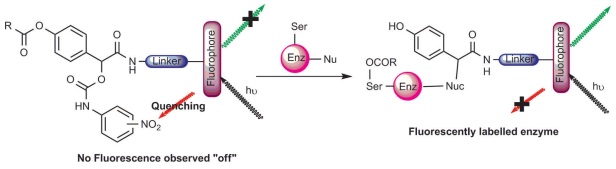


1610

Fluorescence quenched quinone methide based activity probes – a cautionary tale

Jonathan D. Sellars, Marie Landrum, Aileen Congreve, David P. Dixon, Jackie A. Mosely, Andrew Beeby, Robert Edwards* and Patrick G. Steel*

A carbamate linked quenching group coupled with a pro-quinone methide reactive core provides an effective tool for studying enzyme function without problems associated with background fluorescence. However protein labelling observations should be treated with caution.

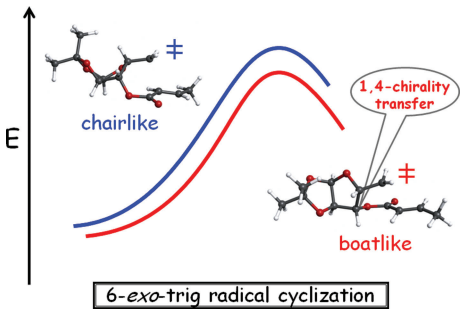


1619

Unravelling the stereoselectivity in 6-*exo*-trig radical cyclization of *α*,*β*-unsaturated ester-tethered sugars. A tale of two stereocenters

Marcelo T. de Oliveira,* Amary Cesar, Daniel H. S. Leal, Maria A. F. Prado, Thais H. Á. da Silva and Ricardo J. Alves

Based on insights gained from a DFT study on the 6-*exo*-trig radical cyclization of an *α*,*β*-unsaturated ester-tethered sugar, we demonstrate that the stereoselective reaction proceeds according to a 1,4-chirality transfer mechanism.

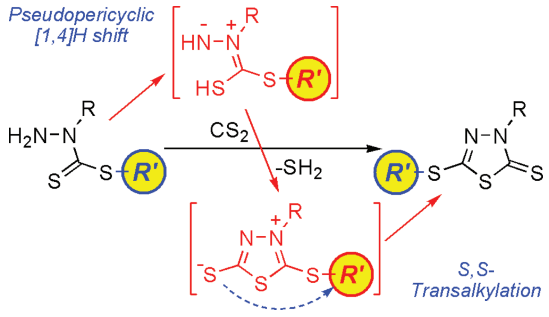


1623

Unexpected transalkylation on 3-alkyl-2-alkylthio-1,3,4-thiadiazolium-5-thiolates: A computational and experimental mechanistic study

Arturo Espinosa,* Rafaela García, Pedro Molina and Alberto Tárraga

The unprecedent pseudopericyclic [1,4]H *N*-to-*S* rearrangement of hydrazinecarbodithioate reagents, in the presence of carbon disulfide, affords thioxo-1,3,4-thiadiazolines involving a final intermolecular double *S*,*S*-transalkylation process.

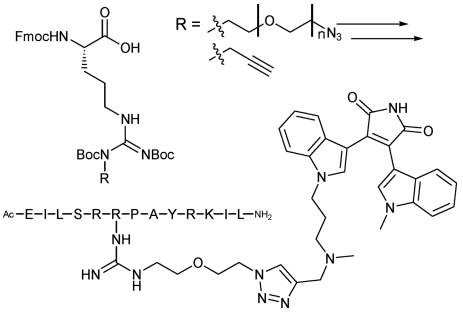


1629

Preparation of novel alkylated arginine derivatives suitable for click-cycloaddition chemistry and their incorporation into pseudosubstrate- and bisubstrate-based kinase inhibitors

Jeroen van Ameijde, Alex J. Poot, Loek T. M. van Wandelen, Angelique E. M. Wammes, Rob Ruijtenbeek, Dirk T. S. Rijkers and Rob M. J. Liskamp*

Novel modified arginine residues suitable for 'click' chemistry and their use in a PKC inhibitor are described.

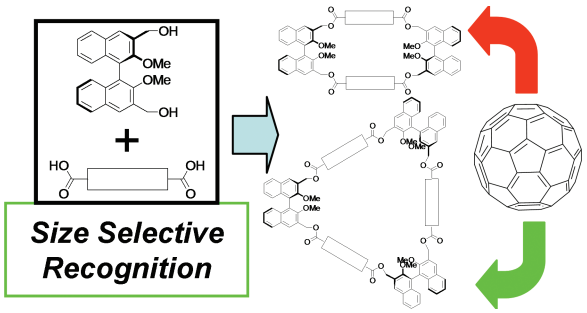


1640

Structurally-variable, rigid and optically-active D_2 and D_3 macrocycles possessing recognition properties towards C_{60}

Carmine Coluccini, Daniele Dondi, Marco Caricato, Angelo Taglietti, Massimo Boiocchi and Dario Pasini*

A straightforward route to chiral macrocycles is described. The larger [3 + 3] macrocycles possess the right cavity size for the complexation of C_{60}, with switchable stoichiometries in relation to the spacer shapes defining the cavities of the cyclic structures.

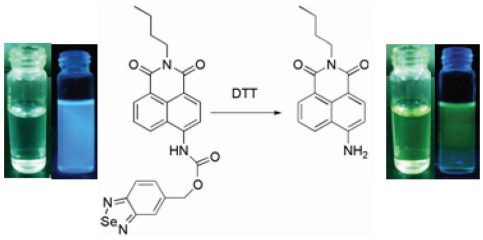


1650

A highly selective ratiometric fluorescent probe for 1,4-dithiothreitol (DTT) detection

Baocun Zhu, Xiaoling Zhang,* Hongying Jia, Yamin Li, Haipeng Liu and Weihong Tan*

A highly selective ratiometric fluorescent probe for 1,4-dithiothreitol (DTT) was designed and synthesized, which displays a 66 nm red-shift of fluorescence emission and the color changes from colorless to jade-green upon reaction with DTT.

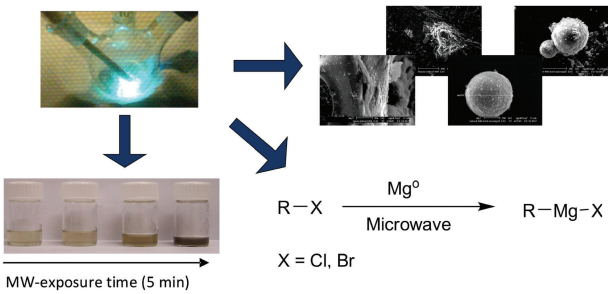


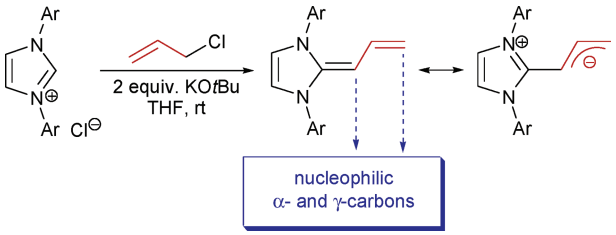
1655

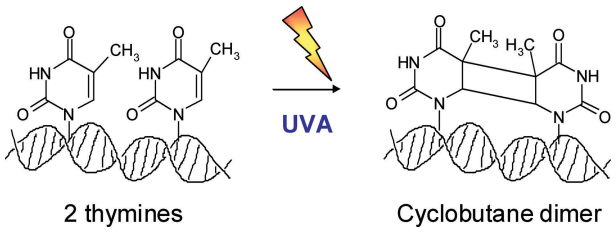
Synthesis of novel 2,5-diarylselenophenes from selenation of 1,4-diarylbutane-1,4-diones or methanol/arylacetylenes

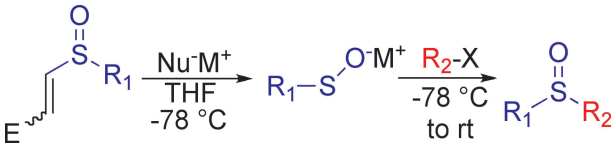
Guoxiong Hua, John B. Henry, Yang Li, Andrew R. Mount, Alexandra M. Z. Slawin and J. Derek Woollins*

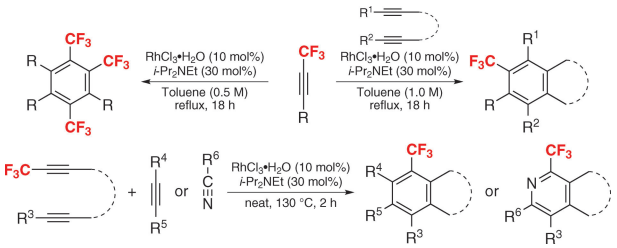
2,5-Diarylselenophenes can be prepared by reaction of *O*-methyl *Se*-hydrogen phenylphosphonodiselenoate with arylacetylenes or by direct reaction of Woollins' reagent with 1,4-diarylbutane-1,4-diones.

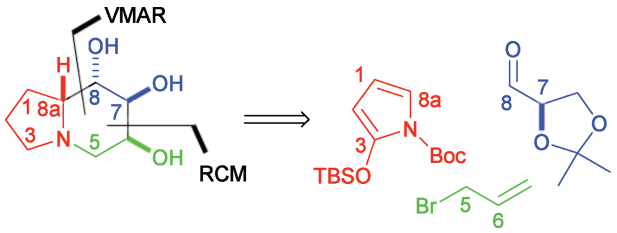












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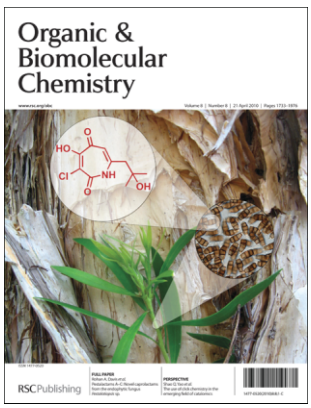
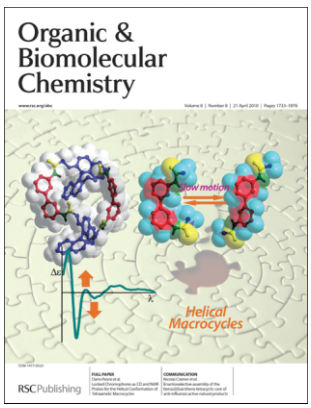


Cover

See Rohan A. Davis *et al.*, pp. 1790–1796.
Chemical investigations of a fermentation culture from the endophytic fungus *Pestalotiopsis* sp. yielded three novel natural products, pestalactams A–C. This fungus was isolated from the Australian plant *Melaleuca quinquenervia*.

Image reproduced by permission of Rohan A. Davis from *Org. Biomol. Chem.*, 2010, **8**, 1785.

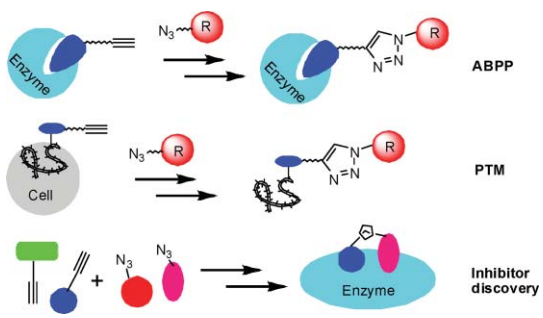


Inside cover

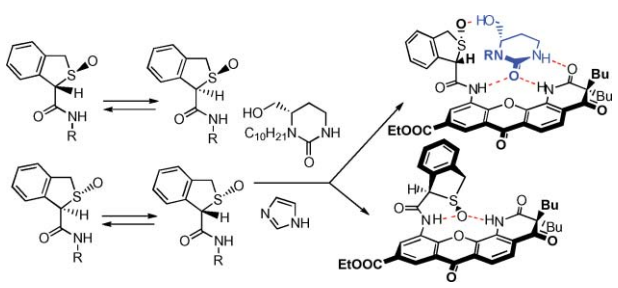
See Dario Pasini, pp. 1815–1819.
Chiral macrocycles adopt an unusual helical shape when the internal rigidification induced by hydrogen bonding is counterbalanced by flexible spacers.

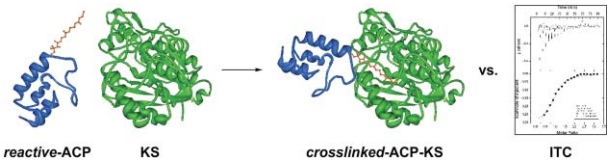
Image reproduced by permission of Dario Pasini from *Org. Biomol. Chem.*, 2010, **8**, 1807.

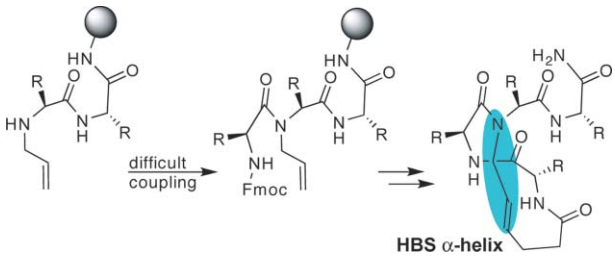
PERSPECTIVE

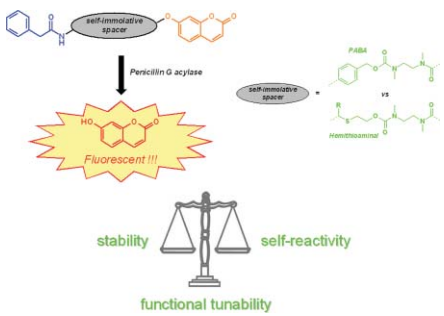


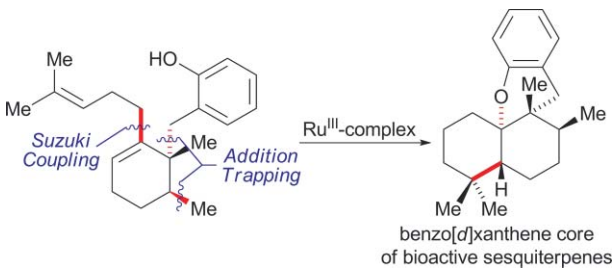
COMMUNICATIONS



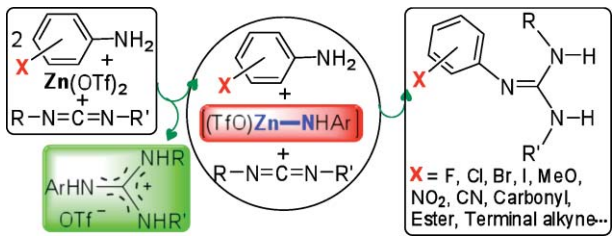








1816

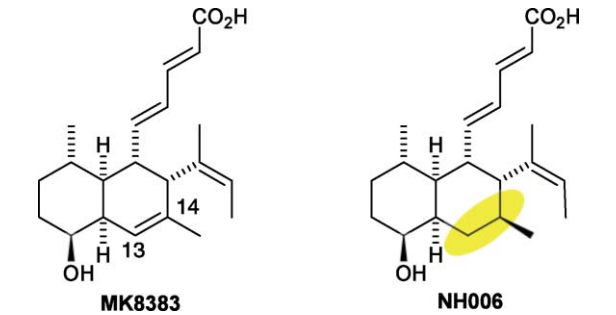


$Zn(OTf)_2$-catalyzed addition of amines to carbodiimides: efficient synthesis of guanidines and unpredicted formation of Zn–N amido species

Dongzhen Li, Jie Guang, Wen-Xiong Zhang,* Yang Wang and Zhenfeng Xi*

$Zn(OTf)_2$ acts as an excellent catalyst precursor for addition of various amines to carbodiimides under an atmosphere of air, offering a convenient synthesis of guanidines with high functional-group tolerance. A Zn–N amido species acts as the active species.

1821

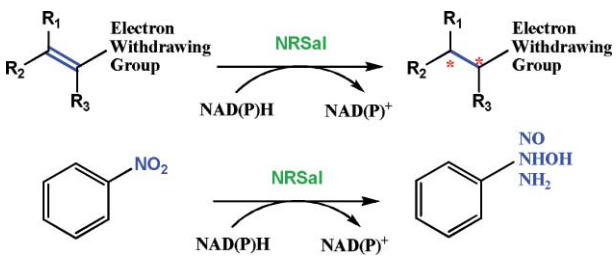


Synthesis of NH006—a photostable fungicide effective against *Botrytis cinerea*—according to the asymmetric total synthesis of MK8383

Nobuyuki Hayashi, Kentaro Yamamoto, Nobuto Minowa, Masaaki Mitomi and Masahisa Nakada*

We report the synthesis of NH006, an MK8383 derivative with a saturated C13-14 double bond and (*S*) configuration at C14, based on the asymmetric total synthesis of MK8383. NH006 exhibits good photostability and potent antifungal activity against *B. cinerea*.

1826

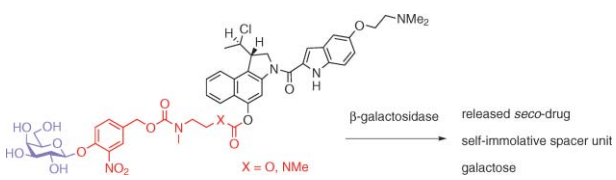


Nitroreductase from *Salmonella typhimurium*: characterization and catalytic activity

Yanto Yanto, Mélanie Hall and Andreas S. Bommarius*

Nitroreductase NRSal from *Salmonella typhimurium* displays both nitroreductase and enoate reductase activity in the asymmetric reduction of C=C bonds and aromatic nitro compounds. It also demonstrated the first single isolated enzyme-catalyzed reduction of nitrobenzene to aniline.

1833

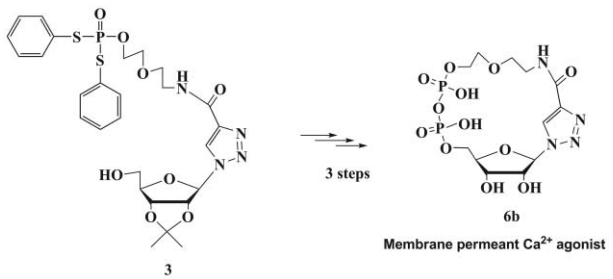


Synthesis of the first spacer containing prodrug of a duocarmycin analogue and determination of its biological activity

Heiko J. Schuster, Birgit Krewer, J. Marian von Hof, Kianga Schmuck, Ingrid Schuberth, Frauke Alves and Lutz F. Tietze*

The synthesis of a spacer prodrug is presented, which allows selective activation at the tumour site releasing the cytostatic after sufficient self-immolation of an introduced spacer unit with an $IC_{50} = 750$ pM.

1843

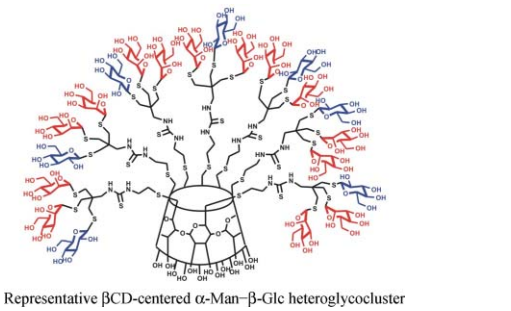


Novel nucleobase-simplified cyclic ADP-ribose analogue: A concise synthesis and Ca^{2+}-mobilizing activity in T-lymphocytes

Lingjun Li, Cornelia C. Siebrands, Zhenjun Yang, Liangren Zhang, Andreas H. Guse and Lihe Zhang*

A purine nucleobase-simplified cyclic ADP ribose (cADPR) analogue was synthesized. It exhibits calcium release activity in intact T-lymphocytes, and indicates that it is a membrane-permeable cADPR mimic.

1849

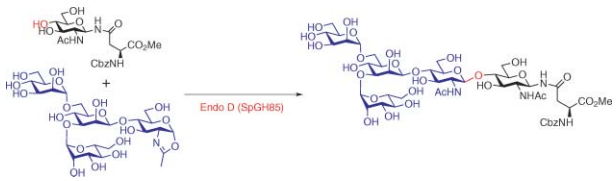


Comparative studies on lectin–carbohydrate interactions in low and high density homo- and heteroglycoclusters

Marta Gómez-García, Juan M. Benito, Ricardo Gutiérrez-Gallego, Alfredo Maestre, Carmen Ortiz Mellet, José M. García Fernández and José L. Jiménez Blanco*

A versatile synthetic procedure to construct a series of high- and low-density homo- and heteroglycoclusters is reported. The binding properties of these multivalent glycoconjugates to Con A, a model lectin, have been assessed by using a range of competitive and non-competitive binding assays including ELLA, ITC and SPR.

1861

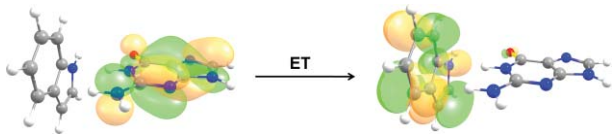


Streptococcus pneumoniae endohexosaminidase D; feasibility of using *N*-glycan oxazoline donors for synthetic glycosylation of a GlcNAc-asparagine acceptor

Thomas B. Parsons, Mitul K. Patel, Alisdair B. Boraston, David J. Vocadlo and Antony J. Fairbanks*

Endohexosaminidase D, a family 85 glycoside hydrolase from *S. pneumoniae*, catalyses the glycosylation of a GlcNAc-bearing glycosyl amino acceptor using *N*-glycan oxazoline oligosaccharides as donors, demonstrating the synthetic potential of this enzyme as a biocatalyst for the synthesis of defined glycoconjugates.

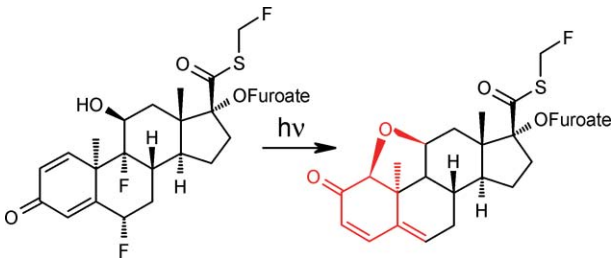
1870

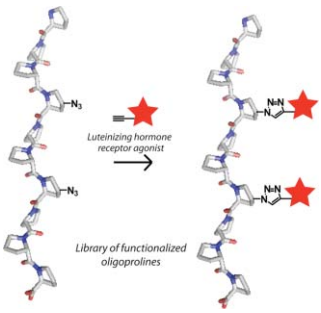


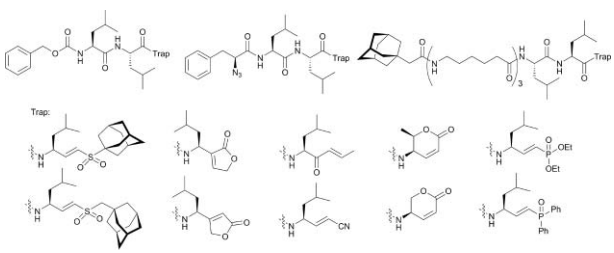
Electron transfer from aromatic amino acids to guanine and adenine radical cations in π stacked and T-shaped complexes

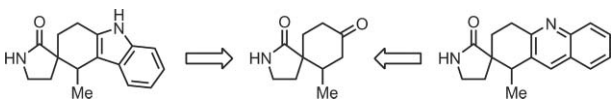
Cristina Butchosa, Sílvia Simon* and Alexander A. Voityuk*

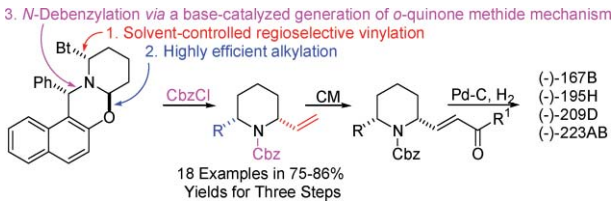
Efficient electron transfer (ET) from aromatic amino acid residues to guanine and adenine radical cations has been found in T-shaped complexes. Thus, π stacking of the donor and acceptor sites is not required for the repair of oxidized nucleobases.

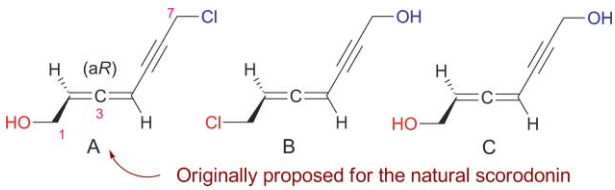


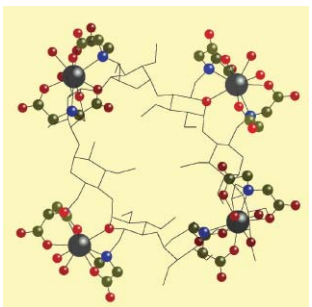


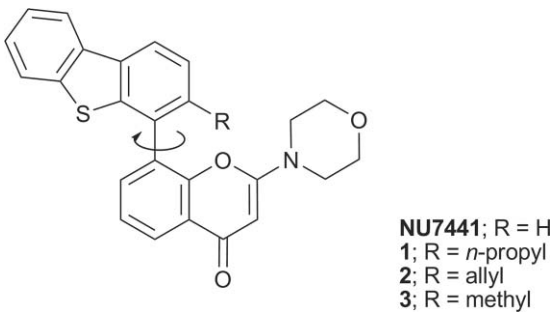




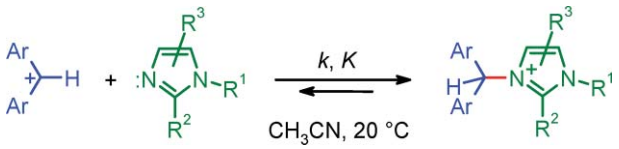








1929

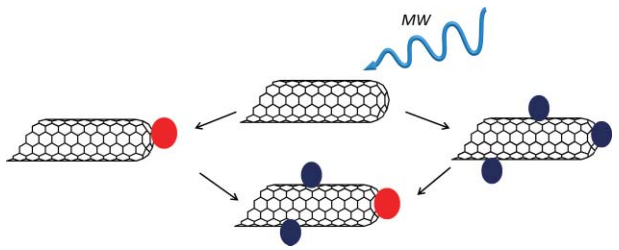


Nucleophilicities and Lewis basicities of imidazoles, benzimidazoles, and benzotriazoles

Mahiuddin Baidya, Frank Brotzel and Herbert Mayr*

Determination of rate and equilibrium constants: imidazoles and benzimidazoles are much weaker nucleophiles than expected from their Lewis and Brønsted basicities.

1936

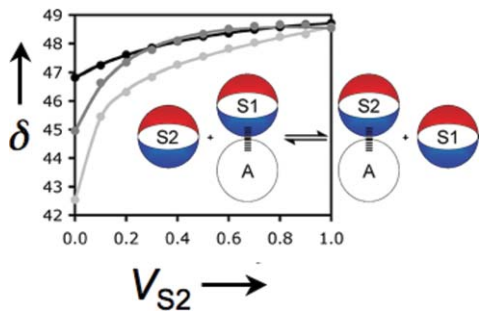


Versatile microwave-induced reactions for the multiple functionalization of carbon nanotubes

Noelia Rubio, M. Antonia Herrero, Antonio de la Hoz, Moreno Meneghetti, Maurizio Prato* and Ester Vázquez*

Doubly functionalized CNTs, obtained *via* microwave activation, can serve as multipurpose, versatile synthons.

1943

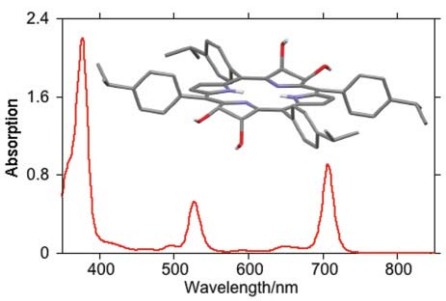


A thermodynamic study of selective solvation in solvent mixtures

Rafel Cabot and Christopher A. Hunter*

The ^{31}P NMR chemical shift of nBu$_3$PO provides a probe of selective solvation in solvent mixtures, allowing characterisation of solvation equilibria and quantification of the H-bond properties of non-polar solvents.

1951



Syntheses, structures, modification, and optical properties of *meso*-tetraaryl-2,3-dimethoxychlorin, and two isomeric *meso*-tetraaryl-2,3,12,13-tetrahydroxybacteriochlorins

Lalith P. Samankumara, Matthias Zeller, Jeanette A. Krause and Christian Brückner*

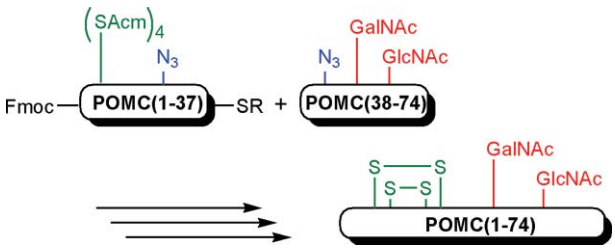
The refined syntheses, modification, and first X-ray structural characterization of *meso*-tetraarylporphyrin-derived β-tetraolbacteriochlorins are described.

1966

Chemical synthesis of mouse pro-opiomelanocortin(1–74) by azido-protected glycopeptide ligation *via* the thioester method

Hidekazu Katayama,* Hironobu Hojo,* Ichiko Shimizu, Yuko Nakahara and Yoshiaki Nakahara

The use of azidopeptide as a building block facilitated the chemoselective peptide ligation by the thioester method. A glycoprotein was successfully synthesized by this method.



* Indicates the author for correspondence: see article for details.

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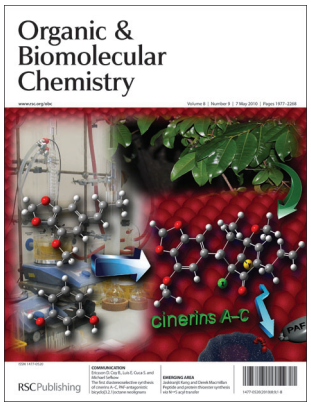


Cover
See Michael Sefkow *et al.*, pp. 2003–2005.
The first total synthesis of PAF-antagonistic cinerins A–C, isolated from the leaves of *Pleurothyrium cinereum*, is reported by Coy *et al.* on page 2003.

Image reproduced by permission of Michael Sefkow from *Org. Biomol. Chem.*, 2010, **8**, 2003.

Inside cover
See Werner M. Nau *et al.*, pp. 2037–2042.
Cucurbiturils are promising macrocycles for drug delivery, which have now been shown to display very low, if not negligible, toxicity in cell and animal studies.

Image reproduced by permission of Werner M. Nau from *Org. Biomol. Chem.*, 2010, **8**, 2037.

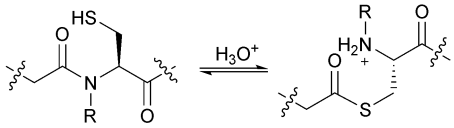
EMERGING AREA

1993

Peptide and protein thioester synthesis *via* N→S acyl transfer

Jaskiranjit Kang and Derek Macmillan*

Peptide thioesters are playing an increasingly prominent role in the chemical toolbox for protein assembly and modification through Native Chemical Ligation (NCL). In this article we highlight recent developments in thioester production through selective disruption of amide bonds.



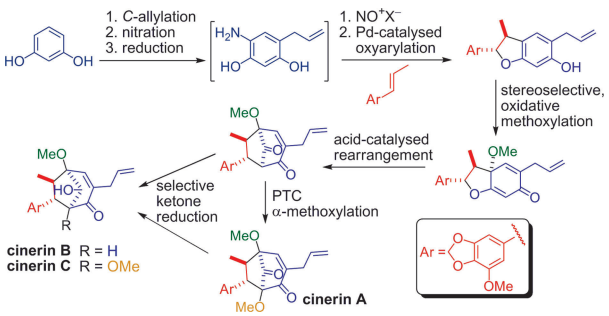
COMMUNICATIONS

2003

The first diastereoselective synthesis of cinerins A–C, PAF-antagonistic macrophyllin-type bicyclo[3.2.1]octane neolignans, using a novel Pd-catalysed oxyarylation

Ericsson D. Coy B.,* Luis E. Cuca S. and Michael Sefkow*

The first diastereoselective synthesis of PAF-antagonistic cinerins A–C, macrophyllin-type bicyclo[3.2.1]octane neolignans from *Pleurothyrium cinereum*, has been accomplished using a novel Pd-catalysed oxyarylation to afford a 2,3-dihydrobenzofuran as the key intermediate.

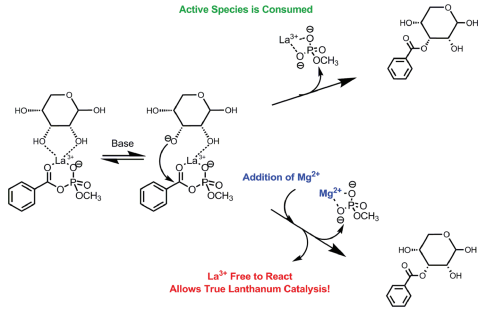


2006

Magnesium ion enhances lanthanum-promoted monobenzoylation of a monosaccharide in water

Raj S. Dhiman and Ronald Kluger*

Monobenzoylation of sugars is promoted by lanthanum triflate. Addition of magnesium ion produces a precipitate from the phosphate monoester by-product that allows lanthanum to function at low catalyst loading.

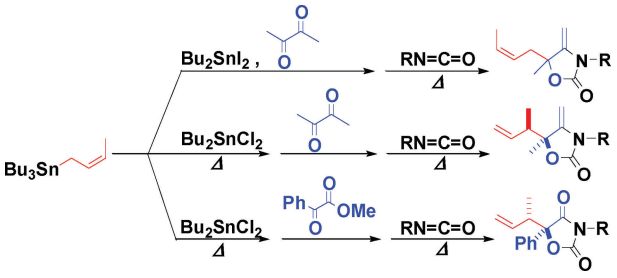


2009

Synthesis of oxazolidinones initiated by regio- and diastereo-controlled crotylation of α-dicarbonyl compounds

Ikuya Shibata,* Ryota Kojima, Shinji Tsunoi, Takashi Nozaki, Tomonari Watanabe, Atsushi Ninomiya, Makoto Yasuda and Akio Baba

One-pot synthesis of oxazolidinones was established initiated by allylation of α-dicarbonyl compounds, accompanying regio- and diastereo-controlled carbon–carbon bond formation on the side chains of the oxazolidinones.

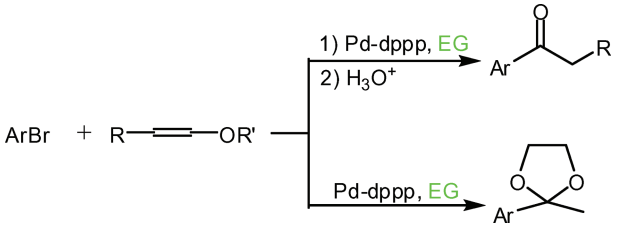


2012

Efficient synthesis of alkyl aryl ketones & ketals *via* palladium-catalyzed regioselective arylation of vinyl ethers

Mingcui Liu, Zeynab Hyder, Yawei Sun, Weijun Tang, Lijin Xu* and Jianliang Xiao

The combination of $Pd(OAc)_2$ with 1,3-bis(diphenylphosphino)propane in ethylene glycol constitutes a high-performance catalytic system for highly regioselective arylation of a range of electron-rich vinyl ethers by aryl bromides to provide, upon hydrolysis, alkyl aryl ketones and cyclic ketals in good yields with up to 3.75×10^5 TON and 15625 h^{-1} TOF.

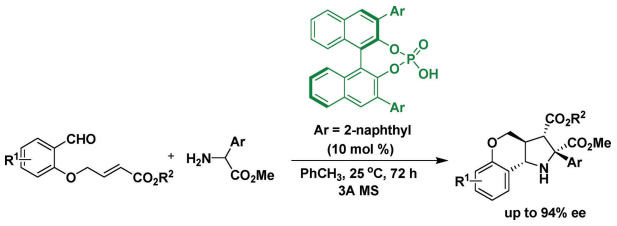


2016

Organocatalytic asymmetric intramolecular [3+2] cycloaddition: A straightforward approach to access multiply substituted hexahydrochromeno[4,3-b]pyrrolidine derivatives in high optical purity

Nan Li, Jin Song, Xi-Feng Tu, Bin Liu, Xiao-Hua Chen and Liu-Zhu Gong*

Asymmetric organocatalytic intramolecular 1,3-dipolar cycloaddition of 4-(2-formylphenoxy)butenoates with amino esters provides hexahydromeno[4,3-b]pyrrolidine derivatives in high ee (up to 94% ee).

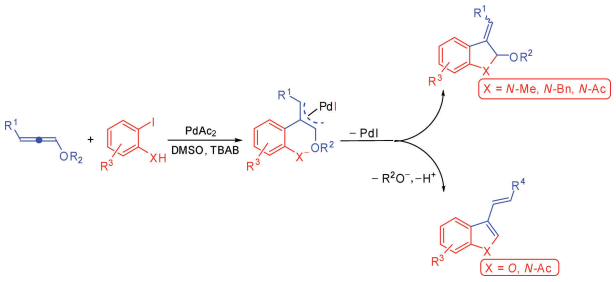


2020

Heck reaction on protected 3-alkyl-1,2-dien-1-ols: an approach to substituted 3-alkenylindoles, 2-alkoxy-3-alkylidene-2,3-dihydrobenzofuranes and -indolidines

Tommaso Boi, Annamaria Deagostino,* Cristina Prandi, Silvia Tabasso, Antonio Toppino and Paolo Venturello

Two different heterocyclic frameworks were obtained in the benzoannulation of 3-alkyl-1,2-dienols and *o*-iodophenols or protected *o*-iodoanilines, in dependence of the nucleophilic properties of the attaching heteroatom.

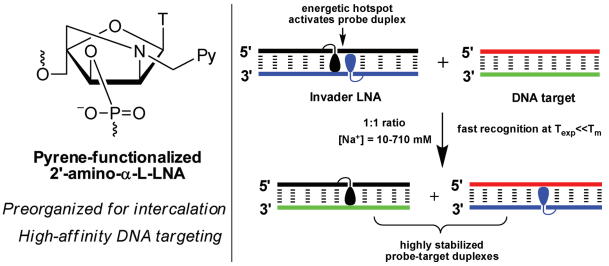


2028

Invader LNA: Efficient targeting of short double stranded DNA

Sujay P. Sau, T. Santhosh Kumar and Patrick J. Hrdlicka*

Energetically activated double stranded Invader LNA probes enable recognition of short isosequential dsDNA-targets at low experimental temperatures, at a variety of ionic strengths, and with good mismatch discrimination.

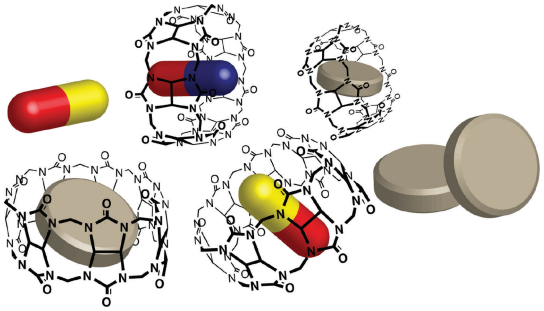


2037

Toxicity of cucurbit[7]uril and cucurbit[8]uril: an exploratory *in vitro* and *in vivo* study

Vanya D. Uzunova, Carleen Cullinane, Klaudia Brix, Werner M. Nau* and Anthony I. Day*

The molecular container cucurbit[7]uril shows a low cytotoxicity (IC_{50} = 0.53 mM) and high tolerated intravenous and oral dosage of at least 250 mg kg^{-1}, which makes it an ideal candidate for potential pharmaceutical applications.

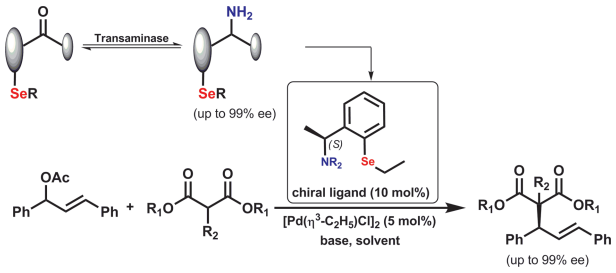


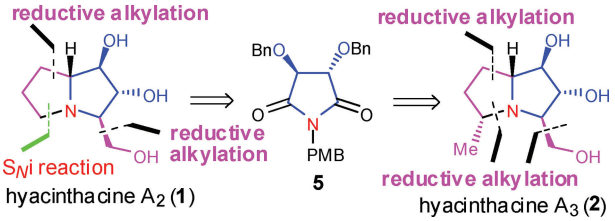
2043

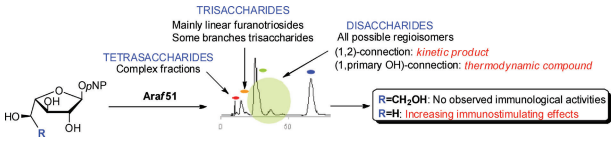
ω-Transaminases as efficient biocatalysts to obtain novel chiral selenium-amine ligands for Pd-catalysis

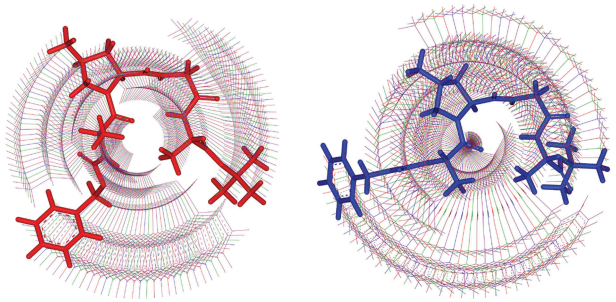
Leandro H. Andrade,* Alexandre V. Silva, Priscila Milani, Dominik Koszelewski and Wolfgang Kroutil

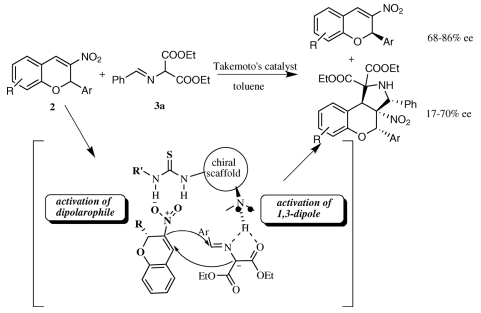
Modulated chiral selenium-amines were efficiently synthesized by using ω-transaminases as tools for asymmetric induction. New chiral selenium compounds were evaluated as ligands in the palladium-catalyzed asymmetric alkylation.

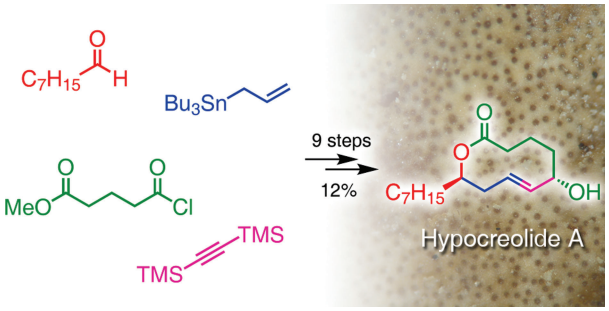


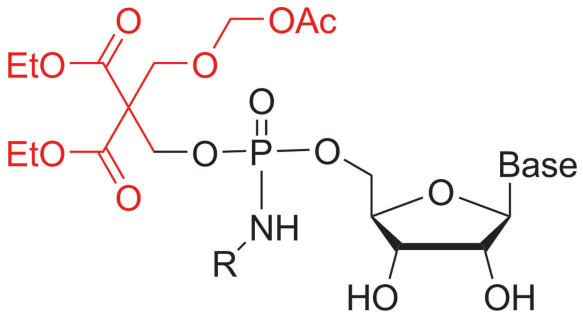


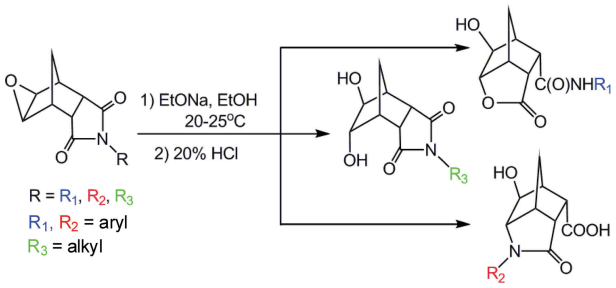


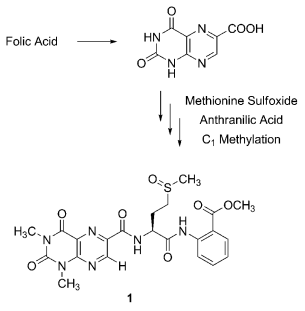


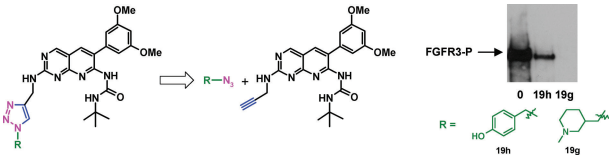


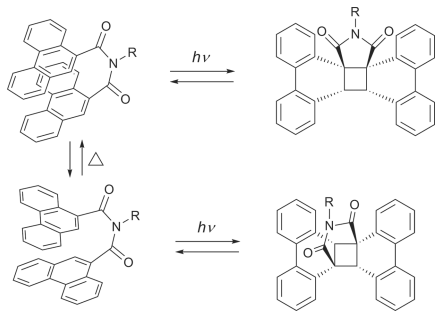


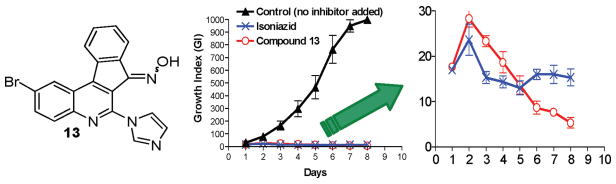


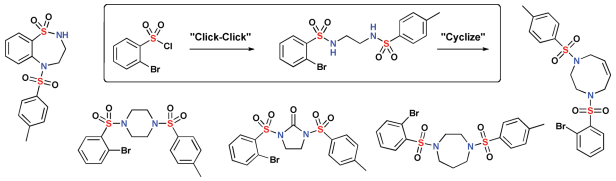












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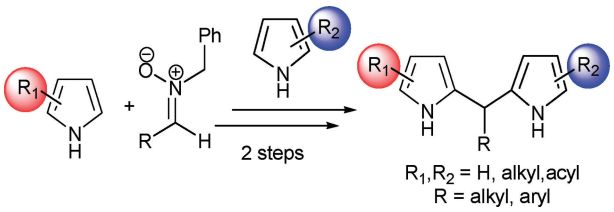
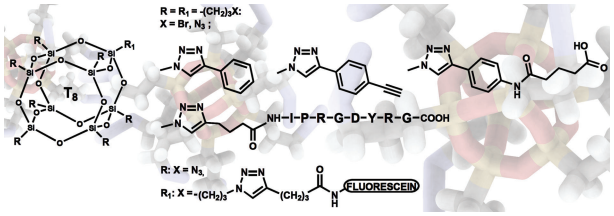


An efficient method for the synthesis of unsymmetrical 2,2′-bis(pyrrolyl)alkanes

Marie Laure Murat-Onana, Christophe Berini, Frédéric Minassian,* Nadia Pelloux-Léon* and Jean-Noël Denis

A new strategy for the preparation of unsymmetrical 2,2′-bis(pyrrolyl)alkanes has been developed, and it has also been extended to the synthesis of tripyrromethanes and *N*-confused dipyrromethanes.

2212

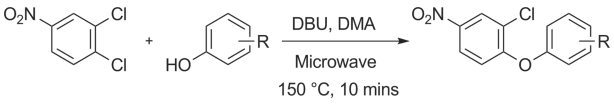


Towards click bioconjugations on cube-octameric silsesquioxane scaffolds

Sebastian Fabritz, Dirk Heyl, Viktor Bagutski, Martin Empting, Eckhard Rikowski, Holm Frauendorf, Ildiko Balog, Wolf-Dieter Fessner, Jörg. J. Schneider, Olga Avrutina and Harald Kolmar*

Synthesis and click conjugations on octaazido octasilsesquioxane scaffold without cage rearrangements are described, including effective transformation into an octaalkyne POSS framework and an octaconjugate of a fully unprotected functional peptide.

2219

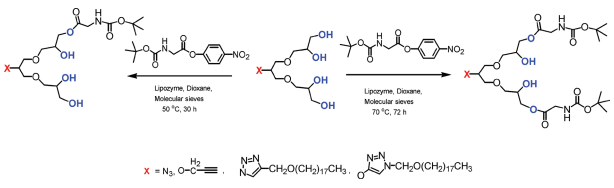


The application of stop-flow microwave technology to scaling-out S_NAr reactions using a soluble organic base

Jameel A. Marafie and Jonathan D. Moseley*

Substituted diaryl ethers have been prepared by S_NAr reaction in combination with a soluble organic base, with productivities of >0.5 kg per day using an automated stop-flow microwave reactor.

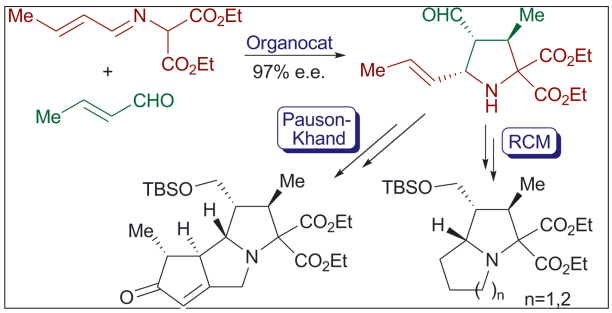
2228

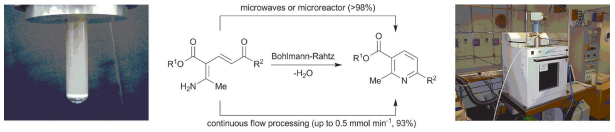


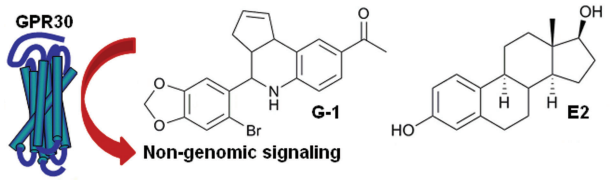
Novel chemoenzymatic methodology for the regioselective glycine loading on polyhydroxy compounds

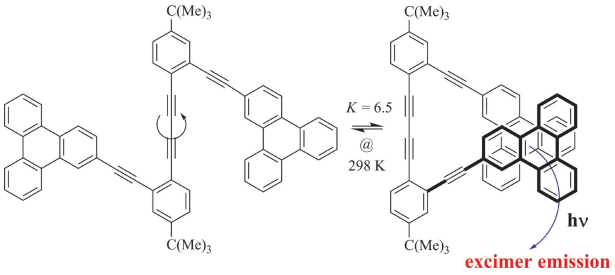
Shashwat Malhotra, Marcelo Calderón, Ashok K. Prasad, Virinder S. Parmar* and Rainer Haag*

We present a temperature-dependent chemo-enzymatic methodology which offers efficient and controlled loading of amino acid (glycine) on polyhydroxy compounds and represents a platform for the selective amino acid attachment (decoration) to the dendritic polyglycerol (PG) scaffolds.









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IN THIS ISSUE

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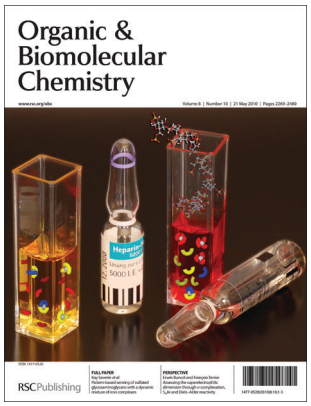
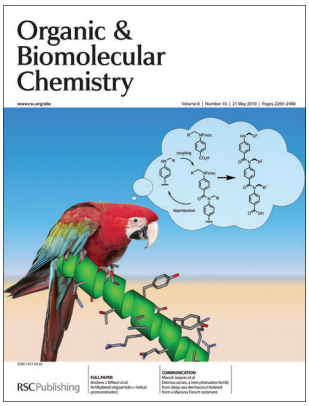


Cover
See Kay Severin *et al.*, pp. 2327–2331.
A dynamic mixture of iron complexes can be used as a colorimetric sensor for sulfated glycosaminoglycans such as heparin.

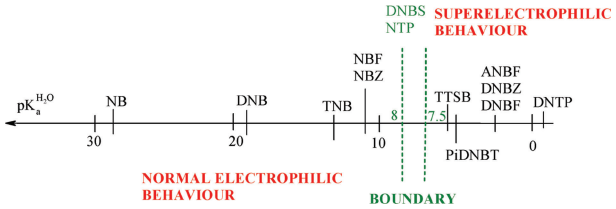
Image reproduced by permission of Kay Severin from *Org. Biomol. Chem.*, 2010, **10**, 2327.



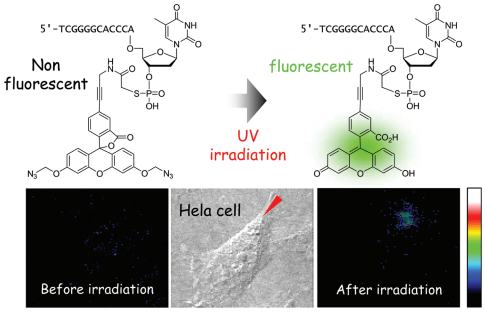
Inside cover
See Andrew J. Wilson *et al.*, pp. 2344–2351.
'Who's a pretty helix?' On page 2344 of this issue, Wilson and co-workers describe the solid-phase synthesis of a novel series of oligobenzamide a-helix mimetics shown to act as potent inhibitors of the p53-hDM2 interaction.

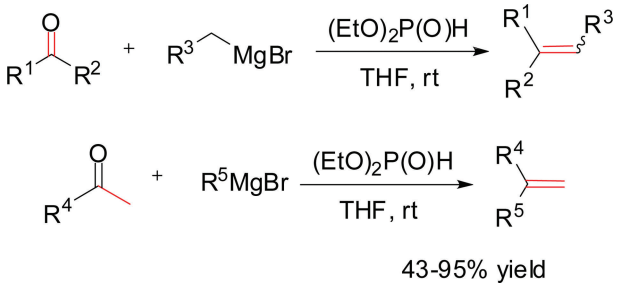
Image reproduced by permission of Andrew J. Wilson from *Org. Biomol. Chem.*, 2010, **10**, 2344.

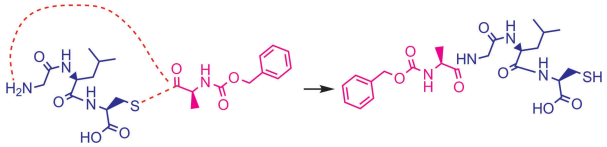
PERSPECTIVE

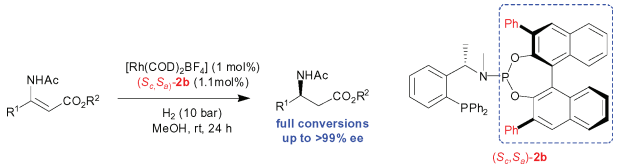


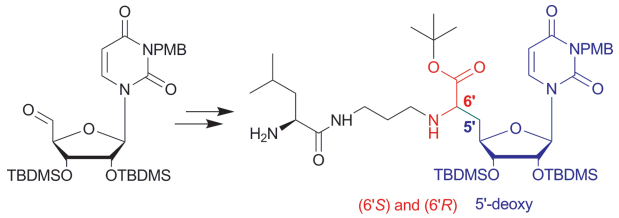
COMMUNICATIONS

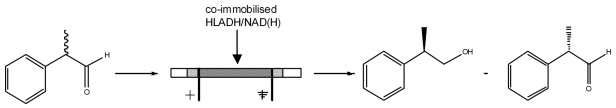


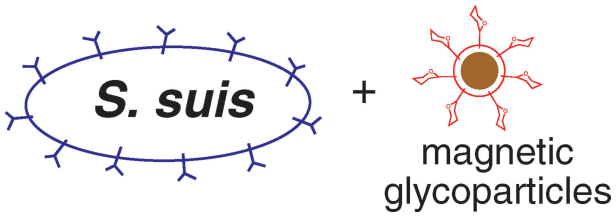


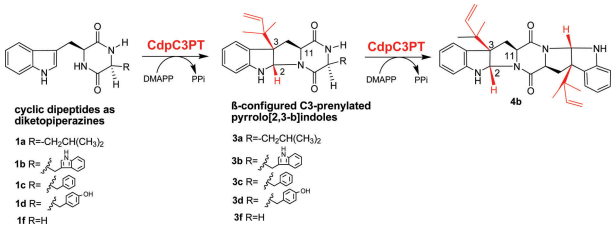


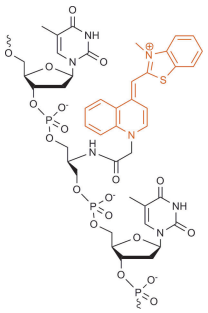


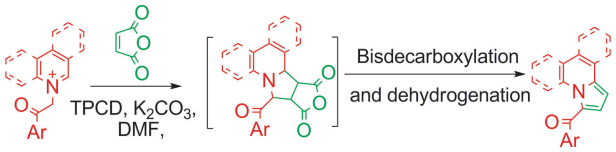


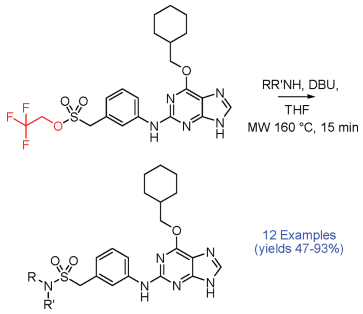


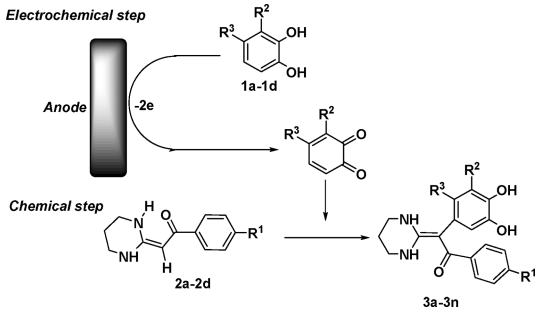


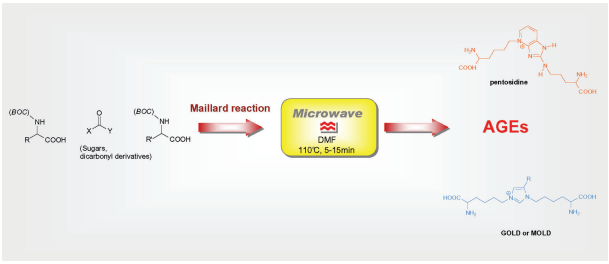












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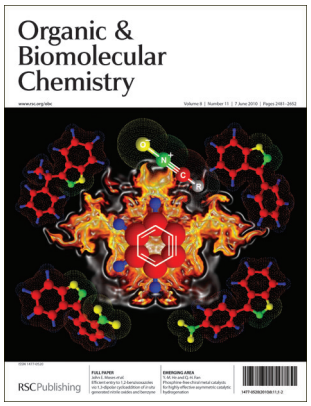
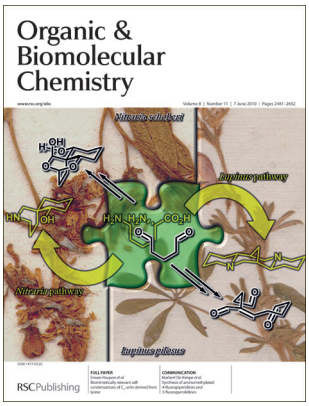


Cover

See John E. Moses *et al.*, pp. 2537–2542.
An improved synthesis of a range of 1,2-benzisoxazoles *via* 1,3-dipolar cycloaddition of *in situ* generated reactive intermediates: nitrile oxides and benzyne is described.

Image reproduced by permission of John E. Moses from *Org. Biomol. Chem.*, 2010, **8**, 2537.

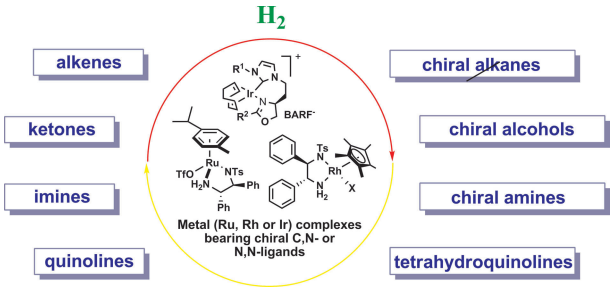


Inside cover

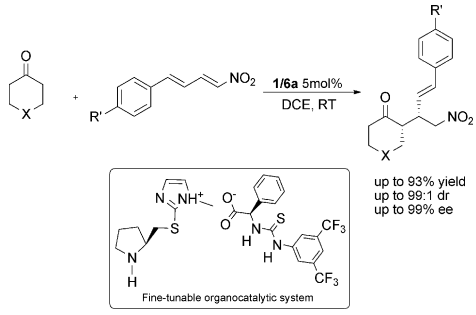
See Erwan Poupon *et al.*, pp. 2522–2528.
Self-condensations of C_5 reactive units enabled the synthesis of skeletons reminiscent to that of alkaloids known to be biosynthesized *via* the lysine pathway (images of the Linnaeus' herbarium courtesy of the Museum of Natural History, Stockholm, Sweden).

Image reproduced by permission of Erwan Poupon from *Org. Biomol. Chem.*, 2010, **8**, 2522.

EMERGING AREA



COMMUNICATIONS

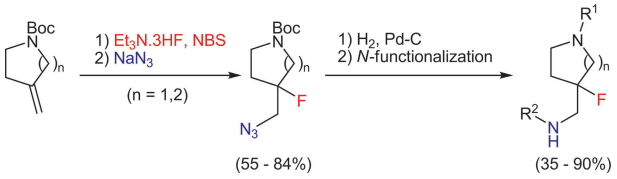


2509

Synthesis of aminomethylated 4-fluoropiperidines and 3-fluoropyrrolidines

Guido Verniest, Karel Piron, Eva Van Hende, Jan Willem Thuring, Gregor Macdonald, Frederik Deroose and Norbert De Kimpe*

A short and efficient synthesis of 4-aminomethyl-4-fluoropiperidines and 3-aminomethyl-3-fluoropyrrolidines is described. These fluorinated azaheterocycles are of specific interest as bifunctional building blocks for fluorinated pharmaceutical compounds.

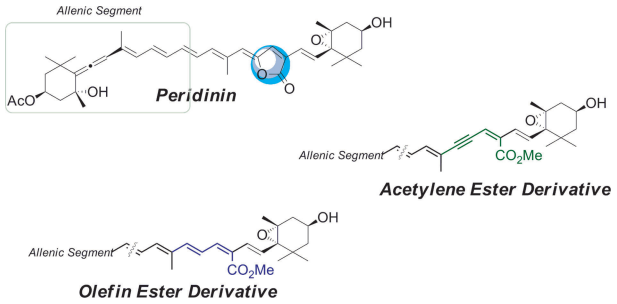


2513

Syntheses of ylidenbutenolide-modified derivatives of peridinin and their stereochemical and spectral characteristics

Takayuki Kajikawa, Kazuyoshi Aoki, Takashi Iwashita, Dariusz M. Niedzwiedzki, Harry A. Frank and Shigeo Katsumura*

We describe the syntheses of two ylidenbutenolide-modified derivatives of peridinin and the results of their stereochemical and spectral characteristics toward elucidation of the exact role of the ylidenbutenolide function.

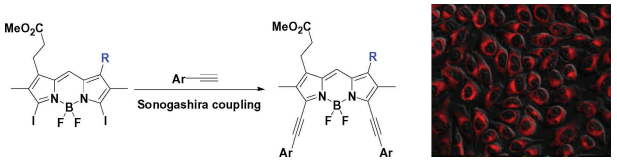


2517

Long wavelength red fluorescent dyes from 3,5-diiodo-BODIPYs

Lijuan Jiao,* Changjiang Yu, Timsy Uppal, Mingming Liu, Yan Li, Yunyou Zhou, Erhong Hao, Xiaoke Hu and M. Graça H. Vicente*

Amphiphilic and long wavelength red fluorescent dyes have been efficiently synthesized from the Sonogashira coupling reactions of 3,5-diiodo-BODIPYs. One of these compounds showed low dark cytotoxicity and accumulated preferentially within the ER of HEp2 cells.

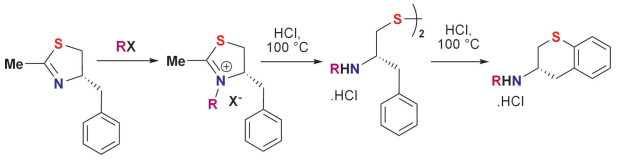


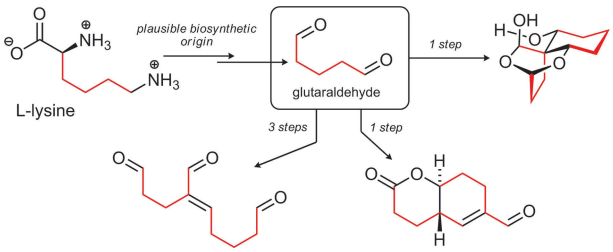
2520

Synthesis of 3-amino-thiochromanes from 4-benzyl 2-thiazolines, *via* an unprecedented intramolecular electrophilic aromatic substitution

Guillaume Mercey, Remi Legay, Jean-François Lohier, Jana Sopkova-de Oliveira Santos, Jocelyne Levillain, Annie-Claude Gaumont and Mihaela Gulea*

A one-pot synthesis of various *N*-substituted 3-amino-thiochromanes from 4-benzyl-2-methyl thiazoline is described. The reaction involves the formation of a disulfide, which subsequently takes part in an unprecedented intramolecular electrophilic aromatic substitution.

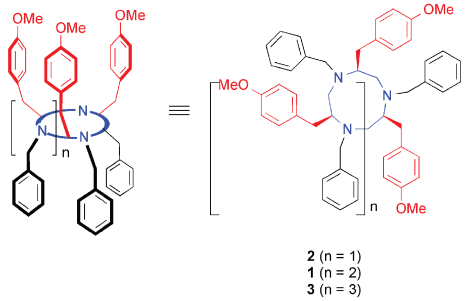




Biomimetically relevant self-condensations of C_5 units derived from lysine

Rim Salame, Edmond Gravel, Pascal Retailleau and Erwan Poupon*

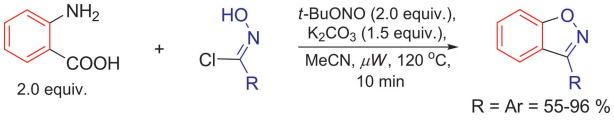
In various and simple conditions, dimerization of pentanedial-derived units gives rise to interesting skeletons, which are reminiscent of alkaloids known to be biosynthesized in Nature *via* lysine metabolism.



Synthesis of chiral polyazamacrocycles of variable ring size

Seiji Kamioka, Sakae Sugiyama, Takashi Takahashi and Takayuki Doi*

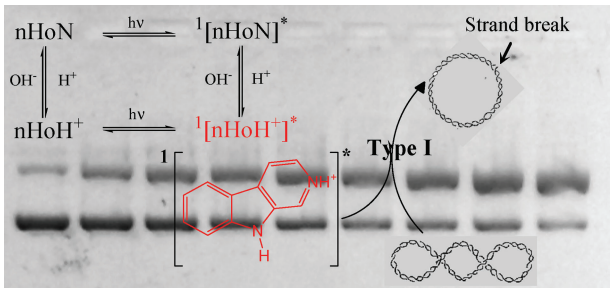
Optically active tri-, tetra-, and penta-azamacrocycles having 4-methoxyphenyl pendants were synthesized. Tri-azamacrocycle **2** does not mainly have a vase-type conformation as tetra-azamacrocycle **1** does but penta-azamacrocycle **3** has a vase-type conformation in $CDCl_3$ and in CD_2Cl_2.



An efficient entry to 1,2-benzisoxazoles *via* 1,3-dipolar cycloaddition of *in situ* generated nitrile oxides and benzyne

Christian Spiteri, Christopher Mason, Fengzhi Zhang, Dougal J. Ritson, Pallavi Sharma, Steve Keeling and John E. Moses*

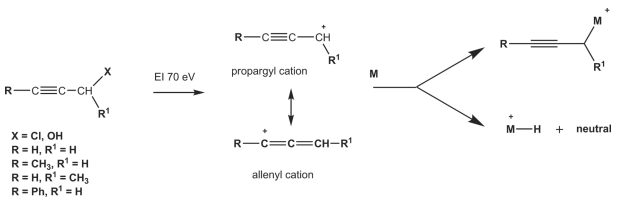
An efficient protocol for the synthesis of a range of 1,2-benzisoxazoles using an improved 1,3-dipolar cycloaddition of nitrile oxides and benzyne is described. Key to the procedure is the *in situ* generation of the reactive nitrile oxide and benzyne reactants simultaneously.

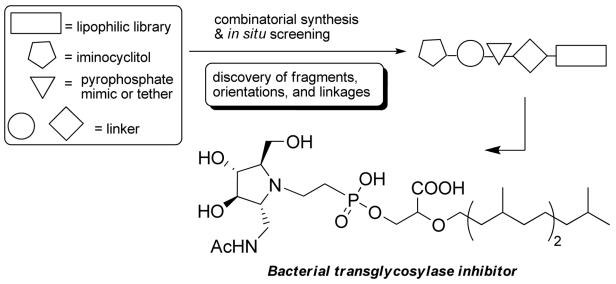


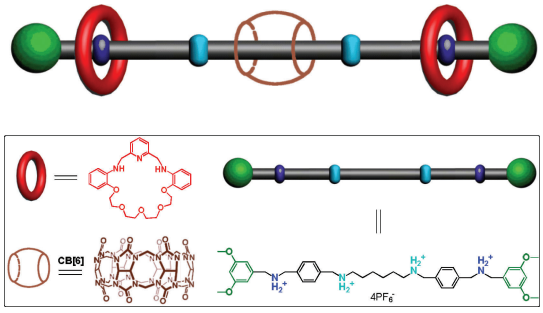
Photosensitized cleavage of plasmidic DNA by norharmane, a naturally occurring β-carboline

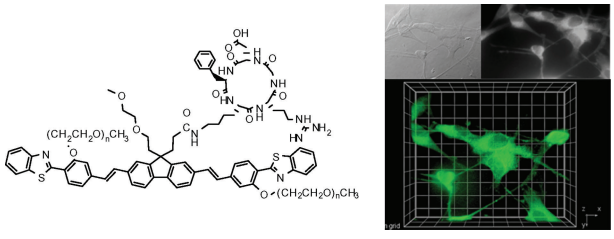
M. Micaela Gonzalez, Magali Pellon-Maison, Matias A. Ales-Gandolfo, Maria R. Gonzalez-Baró, Rosa Erra-Balsells* and Franco M. Cabrerizo*

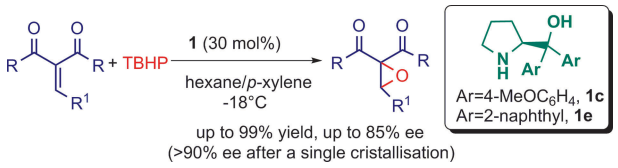
In air-equilibrated aqueous solution, under both pH conditions, the photosensitized cleavage of plasmidic DNA occurs mainly *via* Type I mechanism (electron transfer) from the single excited state (S_1) of the protonated form of norharmane (^{1}[nHoH$^+$]*).

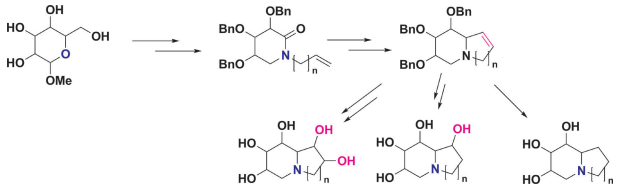












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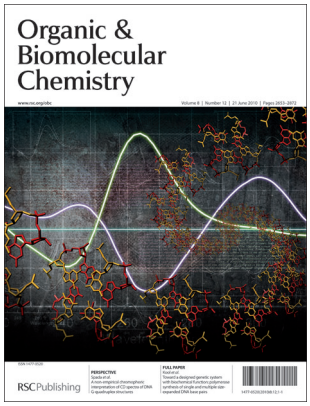

Cover
See Gian Piero Spada *et al.*, pp. 2683–2692.
Why does the different strand folding in G4-DNAs give rise to different circular dichroism spectra? In this perspective article, the most relevant CD features are rationalised in terms of different stacking orientation between adjacent G-quartets.

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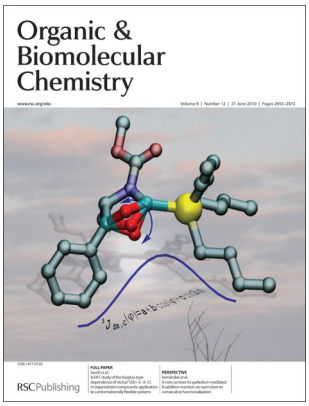

Inside cover
See Giacomo Saielli *et al.*, pp. 2711–2718.
Relativistic DFT calculations, including population analysis, highlight several unexpected features of the Karplus-type dependence of vicinal (Sn–C–X–C) spin-spin couplings in organotin(IV) synthetic intermediates.

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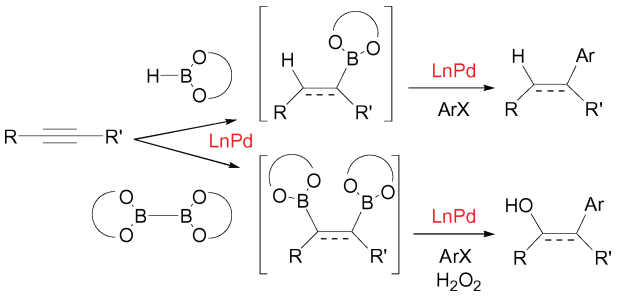

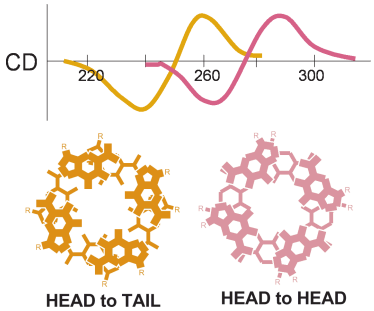

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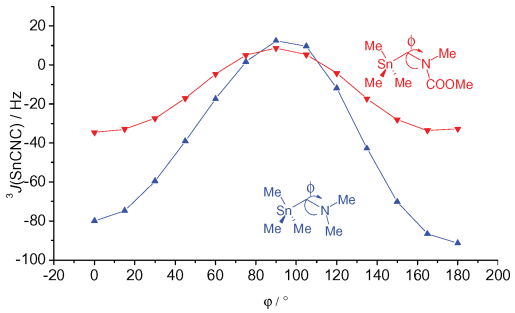
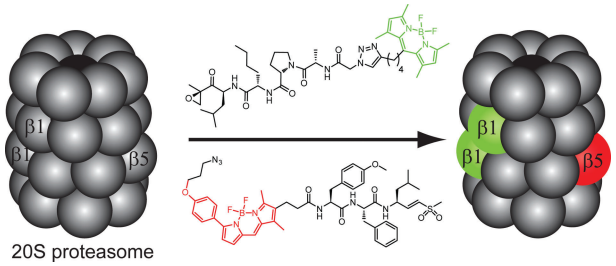
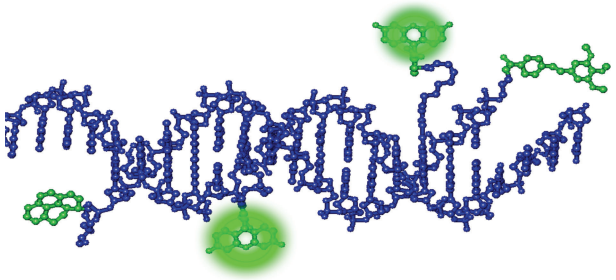
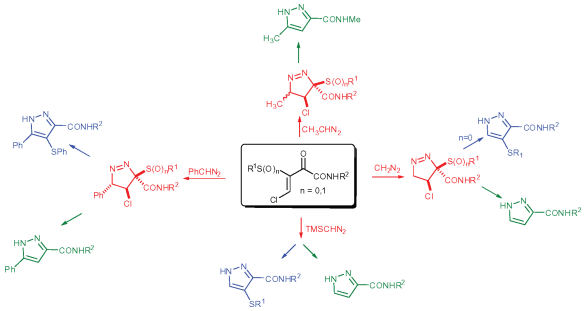
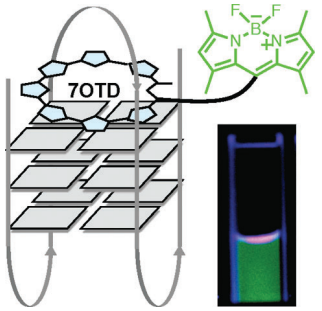
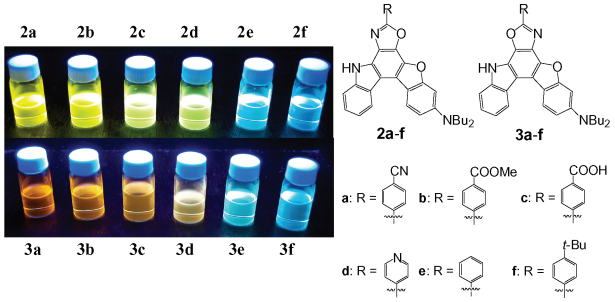


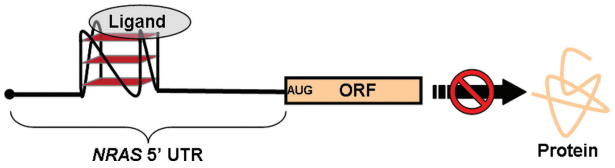


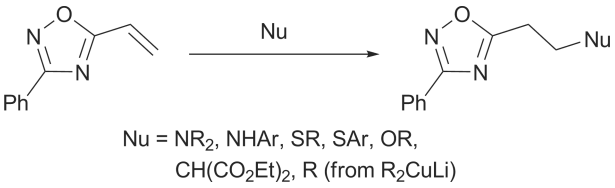


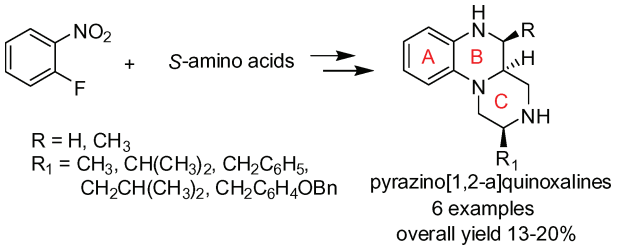


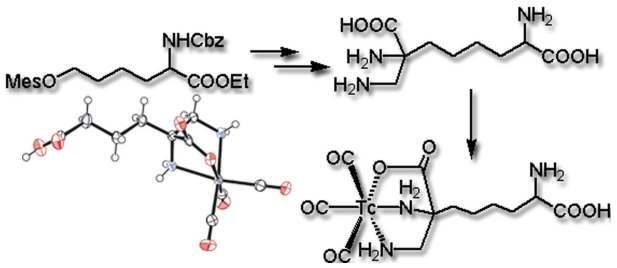


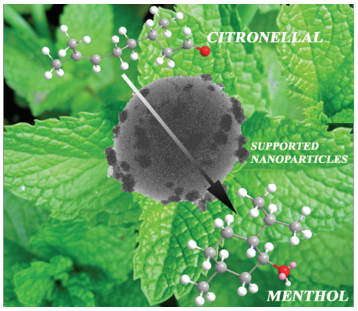










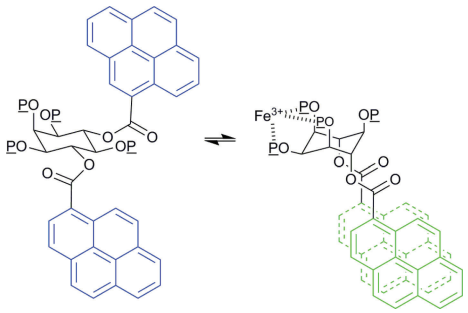


2850

Conformational analysis of the natural iron chelator *myo*-inositol 1,2,3-trisphosphate using a pyrene-based fluorescent mimic

D. Mansell, N. Rattray, L. L. Etchells, C. H. Schwalbe, A. J. Blake, J. Torres, C. Kremer, E. V. Bichenkova, C. J. Barker and S. Freeman*

The selective interaction of Fe^{3+} with a *myo*-inositol phosphate containing the natural antioxidant 1,2,3-trisphosphate motif has been monitored using a pyrene-based fluorescent probe: the penta-equatorial chair (blue fluorescence) ring flips to the unstable penta-axial conformation (green excimer fluorescence) upon binding Fe^{3+}.

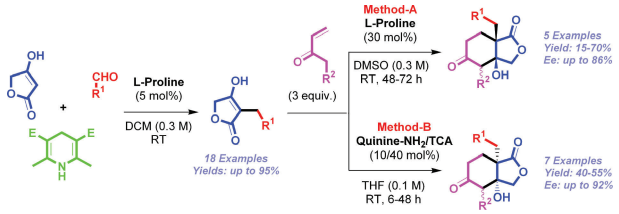


2859

Direct catalytic asymmetric synthesis of highly functionalized tetronic acids/tetrahydro-isobenzofuran-1,5-diones *via* combination of cascade three-component reductive alkylations and Michael-aldol reactions

Dhevalapally B. Ramachary* and Mamillapalli Kishor

A general process for the synthesis of tetrahydro-isobenzofuran-1,5-diones was achieved for the first time through asymmetric cascade Michael-aldol reaction of 4-hydroxy-3-alkyl-5*H*-furan-2-ones with alkyl vinyl ketones in the presence of a catalytic amount of L-proline or Q-NH_2/TCA



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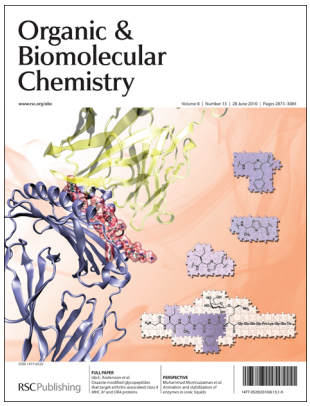

Cover

See Andersson *et al.*, pp. 2931–2940. Oxazole-modified glycopeptides that probe interactions with class II MHC proteins and T-cell receptors associated with autoimmune arthritis.

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Inside cover

See Wang *et al.*, pp. 2923–2925. New aminonaphthalimide imidazolium podands as luminescence chemosensors were prepared for selectively sensing nucleoside polyphosphates ADP and ATP in living cells.

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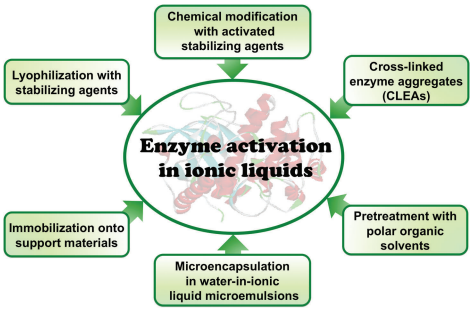
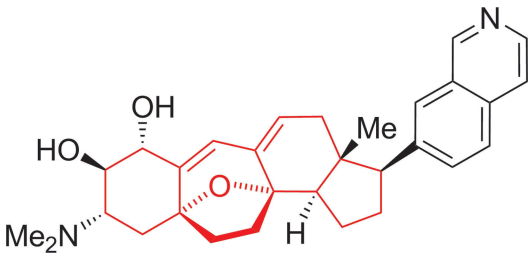
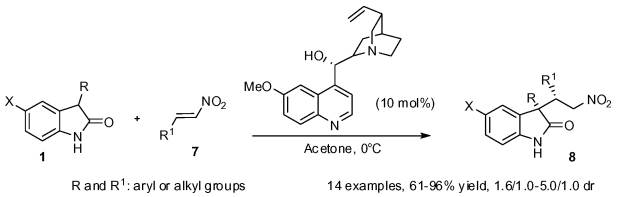
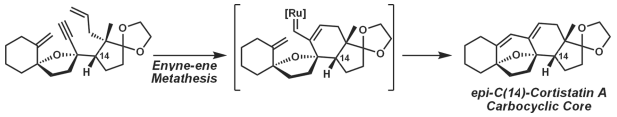
PERSPECTIVES

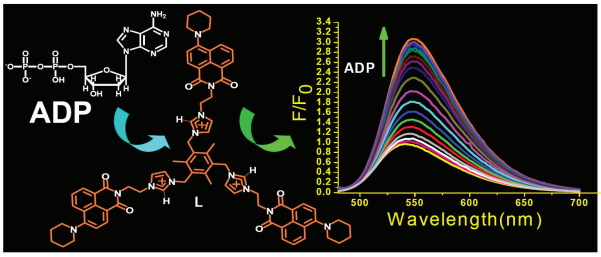


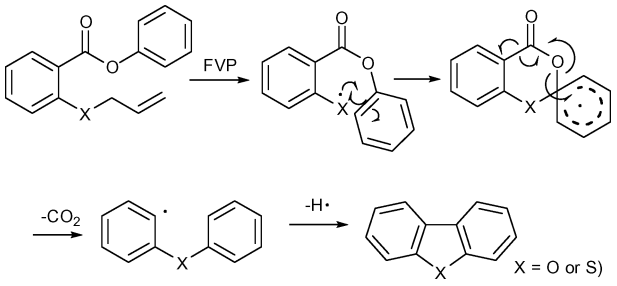


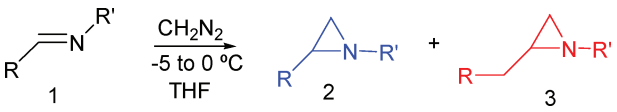
Cortistatin A

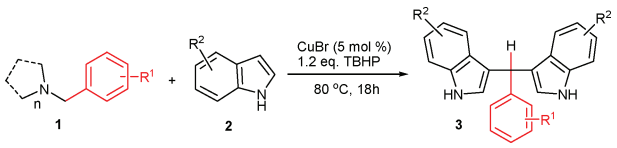


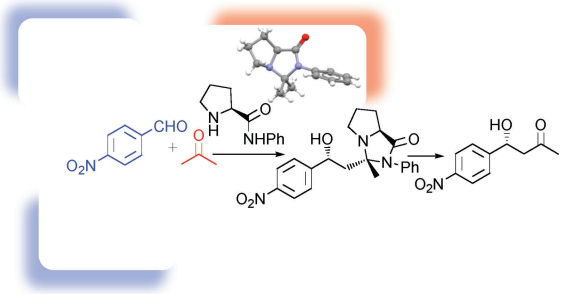


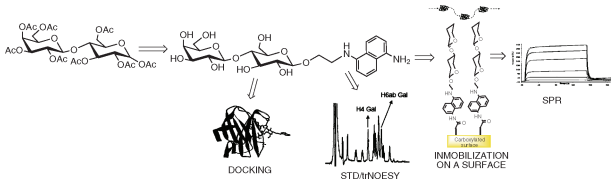


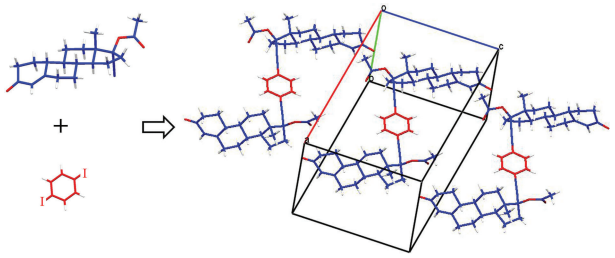


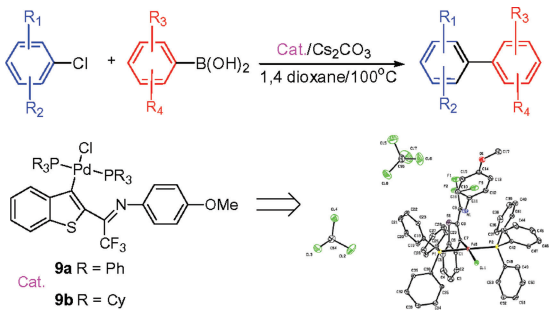


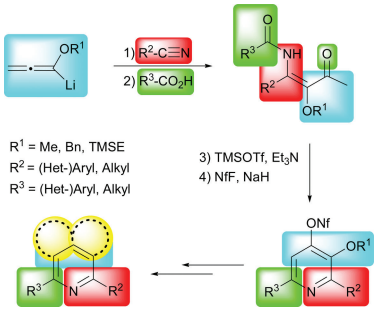


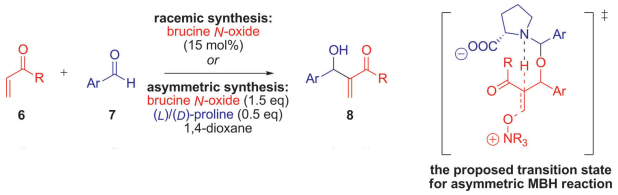








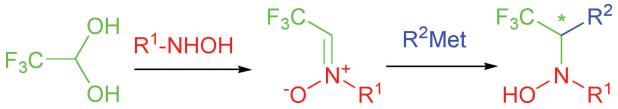




Brucine *N*-oxide-catalyzed Morita–Baylis–Hillman reaction of vinyl ketones: a mechanistic implication of dual catalyst system with proline

Kyungsoo Oh,* Jian-Yuan Li and Jinhyang Ryu

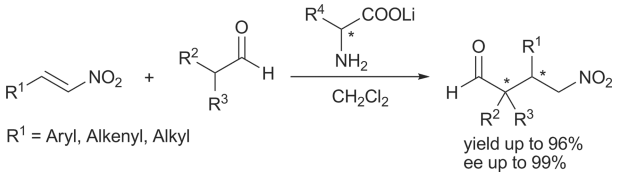
The asymmetric Morita–Baylis–Hillman reaction of vinyl ketones with electron-deficient aromatic aldehydes was catalyzed by proline in the presence of co-catalyst, brucine *N*-oxide.



Trifluoromethyl nitrones: from fluoral to optically active hydroxylamines

Thierry Milcent, Nathan Hinks, Danièle Bonnet-Delpon and Benoit Crousse*

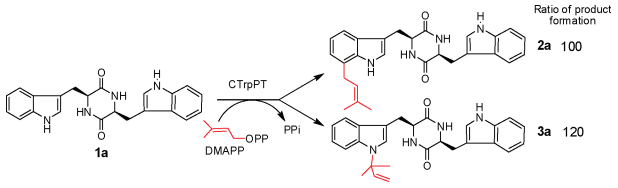
We present the nucleophilic diastereoselective additions of organometallic reagents to trifluoromethyl nitrones, affording the corresponding optically active trifluoroethyl hydroxylamines in good yields.



Asymmetric Michael addition of aldehydes to nitroalkenes using a primary amino acid lithium salt

Masanori Yoshida,* Atsushi Sato and Shoji Hara

Enantioselective Michael addition of aldehydes to nitroalkenes catalysed by L-phenylalanine lithium salt gave γ-nitroaldehydes in good yields with high enantioselectivity.

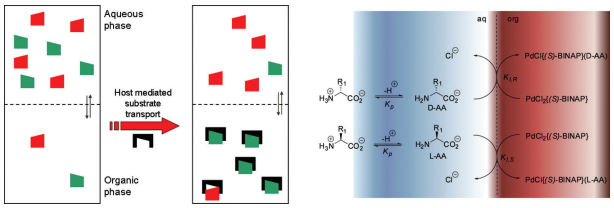


Simultaneous C7- and N1-prenylation of cyclo-L-Trp-L-Trp catalyzed by a prenyltransferase from *Aspergillus oryzae*

Hui-Xi Zou, Xiu-Lan Xie, Uwe Linne, Xiao-Dong Zheng and Shu-Ming Li*

A recombinant prenyltransferase His_6-CTrpPT from *Aspergillus oryzae* catalyzes simultaneously the regular C7- and reverse N1-prenylation of tryptophan-containing cyclic dipeptides, as demonstrated by using cyclo-L-Trp-L-Trp.

3045

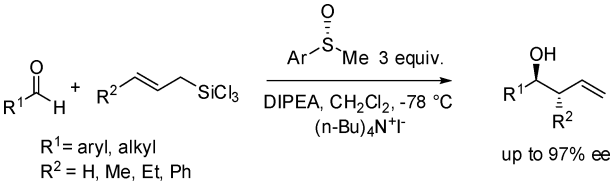


Chiral separation of substituted phenylalanine analogues using chiral palladium phosphine complexes with enantioselective liquid–liquid extraction

Bastiaan J. V. Verkuijl, Boelo Schuur, Adriaan J. Minnaard,* Johannes G. de Vries* and Ben L. Feringa*

Chiral palladium phosphine complexes have been employed in the chiral separation of amino acids and phenylalanine analogues in particular.

3055

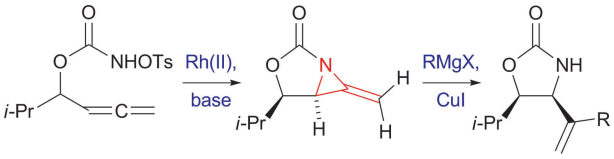


Chiral sulfoxides as activators of allyl trichlorosilanes in the stereoselective allylation of aldehydes

Vincenzo De Sio, Antonio Massa* and Arrigo Scettri*

Chiral aryl methyl sulfoxides proved to be efficient activators in the asymmetric allylation of aldehydes with allyl trichlorosilanes. High enantioselectivity was found in the case of electron-poor aldehydes. The high levels of diastereoselectivity and the detection of nonlinear effects have allowed the elucidation of some mechanistic aspects of the reaction.

3060

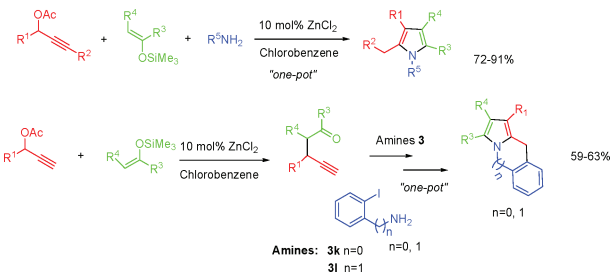


Structure and reactivity of bicyclic methylene aziridines prepared by intramolecular aziridination of allenes

Jeremy Robertson,* George C. Feast, Louise V. White, Victoria A. Steadman (née Doughty) and Timothy D. W. Claridge

The Rh(II)-catalyzed intramolecular aziridination of allenyl-substituted *N*-tosyloxycarbamates leads to bicyclic methylene aziridines that undergo formal S_NV ring-opening with organocuprates.

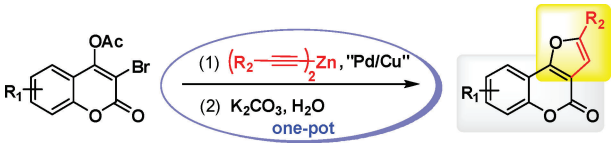
3064

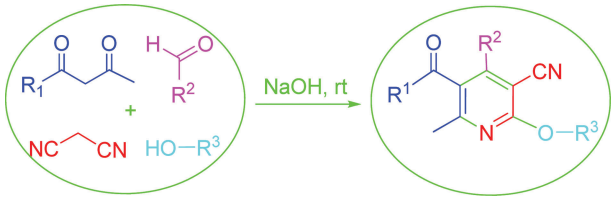


One-pot highly efficient synthesis of substituted pyrroles and *N*-bridgehead pyrroles by zinc-catalyzed multicomponent reaction

Xiao-tao Liu, Lu Hao, Min Lin, Li Chen and Zhuang-ping Zhan*

A convenient zinc-catalyzed multicomponent process has been developed for the synthesis of substituted pyrroles. The protocol developed has been extended to the synthesis of *N*-bridgehead pyrroles containing polycyclic fragments.





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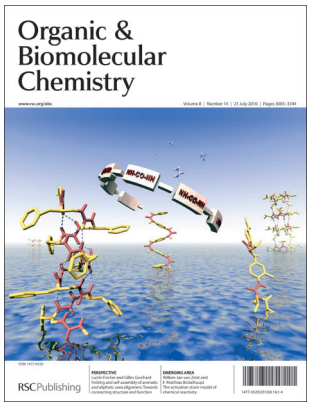
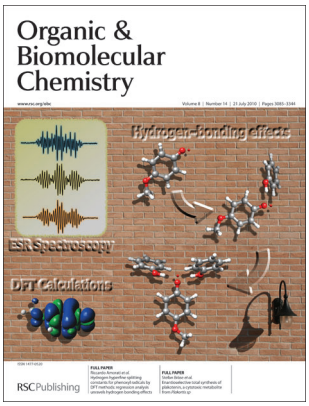


Cover

See Lucile Fischer and Gilles Guichard, pp. 3101–3117.
Just like their oligoamide congeners, aromatic and aliphatic urea-based oligomers show high propensity to fold and to self-assemble. Ultimately, structural knowledge is providing a basis for *function*

Image reproduced by permission of Gilles Guichard from *Org. Biomol. Chem.*, 2010, **8**, 3101.

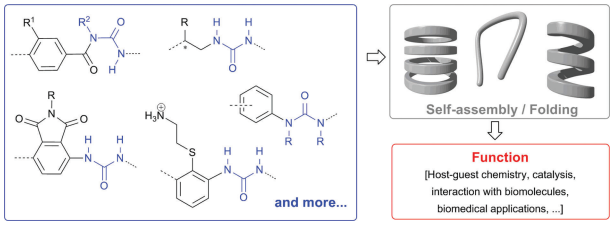


Inside cover

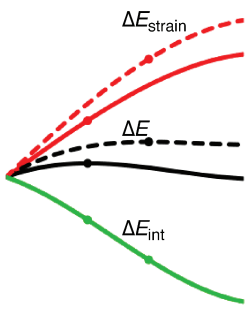
See Riccardo Amorati *et al.*, pp. 3136–3141.
Joint ESR spectroscopic measures and DFT theoretical calculations shed new light on hydrogen bonds formation between phenols and biologically relevant phenoxyl radicals

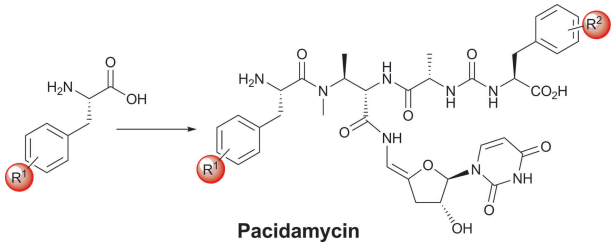
Image reproduced by permission of Riccardo Amorati from *Org. Biomol. Chem.*, 2010, **8**, 3136.

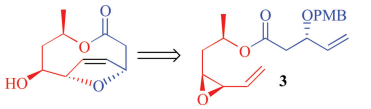
PERSPECTIVE



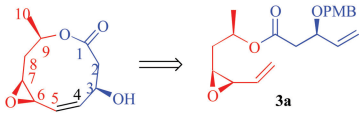
EMERGING AREA



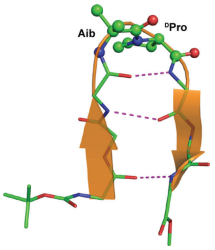


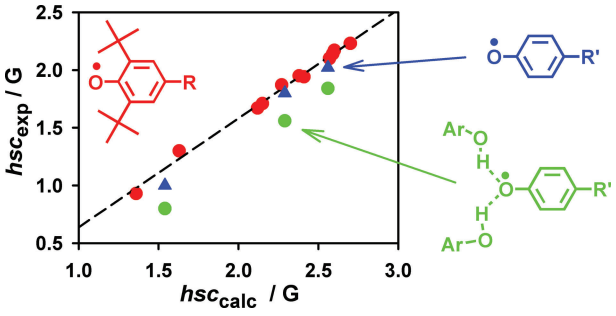


Decarestrictine I (**1**)



Botryolide B (**1a**)





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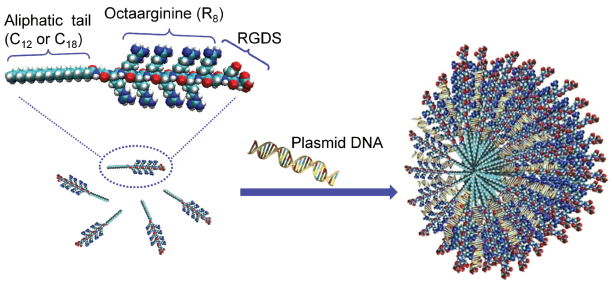
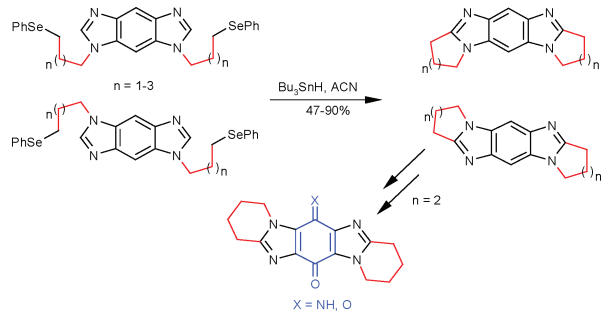


Amphiphilic cationic lipopeptides with RGD sequences as gene vectors

Jing-Xiao Chen, Hui-Yuan Wang, Chang-Yun Quan, Xiao-Ding Xu, Xian-Zheng Zhang* and Ren-Xi Zhuo

Two kinds of arginine-rich amphiphilic lipopeptides with hydrophobic aliphatic tails were designed and synthesized as functional gene vectors. Due to the incorporation of RGD sequences, these two amphiphilic lipopeptides exhibited improved transfection efficiency in HeLa cells.

3149

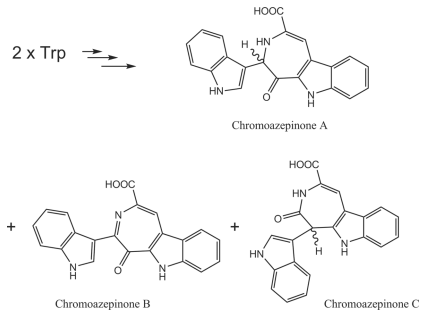


One-pot double intramolecular homolytic aromatic substitution routes to dialicyclic ring fused imidazobenzimidazolequinones and preliminary analysis of anticancer activity

Vincent Fagan, Sarah Bonham, Michael P. Carty and Fawaz Aldabbagh*

New quinone and iminoquinone anticancer agents that show specificity towards cervical and prostate cancer cell lines were prepared *via* double alkyl radical cyclizations onto imidazobenzimidazoles.

3157

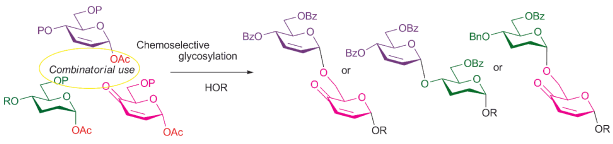


Novel tryptophan metabolites, chromoazepinone A, B and C, produced by a blocked mutant of *Chromobacterium violaceum*, the biosynthetic implications and the biological activity of chromoazepinone A and B

Takaaki Mizuoka, Kazufumi Toume, Masami Ishibashi and Tsutomu Hoshino*

The chemical mutagenesis of *Chromobacterium violaceum* afforded novel tryptophan metabolites, named chromoazepinone A~C. The biosynthetic pathways for the novel compounds are proposed and the inhibition effect of Wnt signal transcriptional activity is reported.

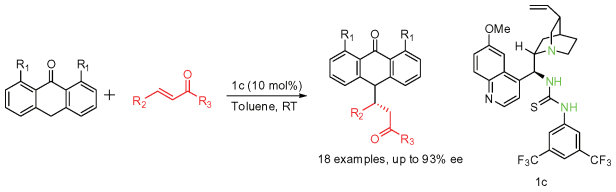
3164

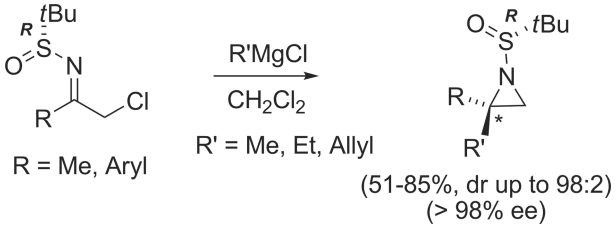


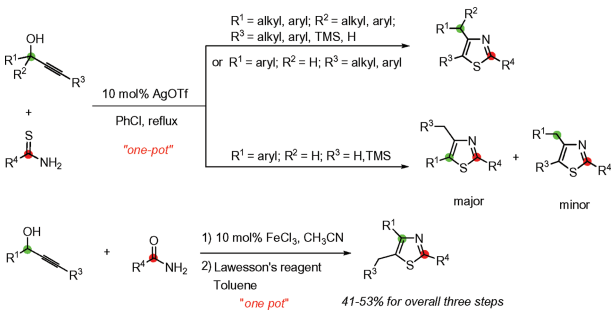
Effective and chemoselective glycosylations using 2,3-unsaturated sugars

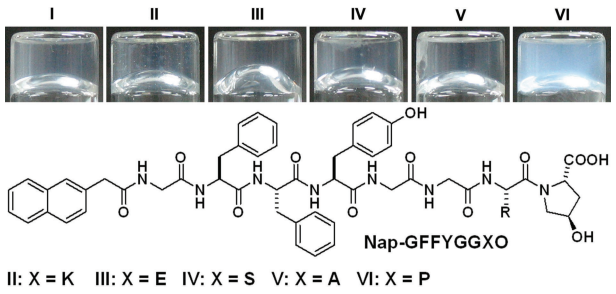
Shunichi Kusumi, Kaname Sasaki, Sainan Wang, Tatsuya Watanabe, Daisuke Takahashi and Kazunobu Toshima*

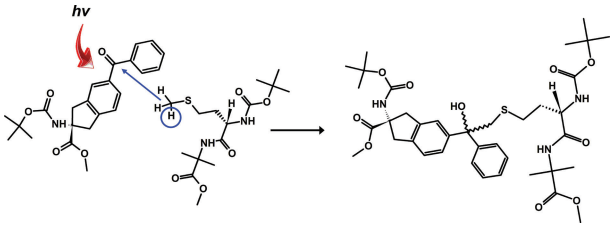
The 2,3-unsaturated glycosyl donors were found to exhibit high reactivity, while the corresponding 2,3-unsaturated-4-keto glycosyl donors showed low reactivity, under several conditions. These findings make it possible to realize chemoselective glycosylations *via* combinatorial uses of 2,3-unsaturated, 2,3-unsaturated-4-keto, and 2,3-dideoxy glcosyl donors providing various types of deoxyoligosaccharides in short-steps.

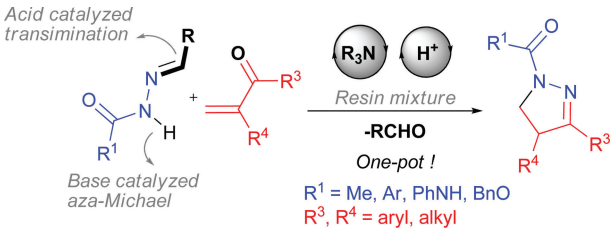


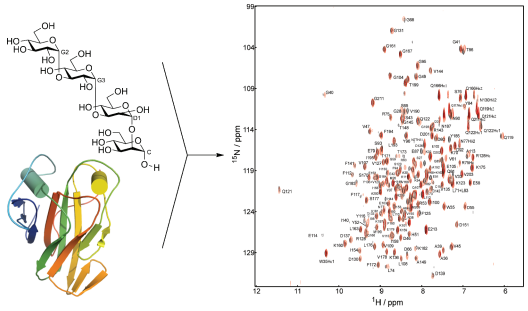












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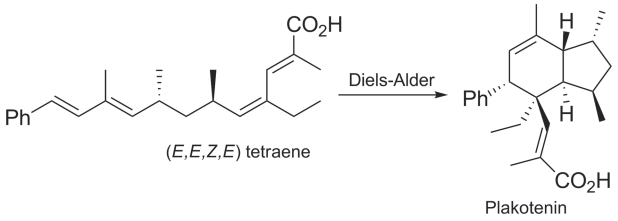
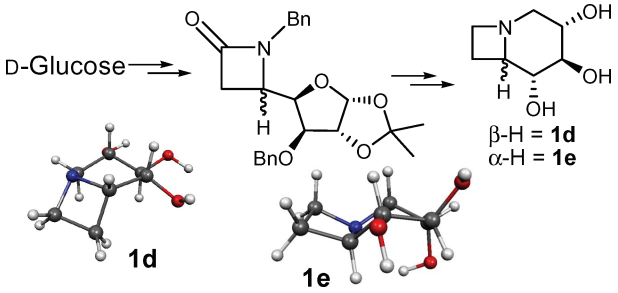


Enantioselective total synthesis of plakotenin, a cytotoxic metabolite from *Plakortis sp*

Stephanie Arzt, Emmanuel Bourcet, Thierry Muller and Stefan Bräse*

The first total enantioselective synthesis of plakotenin is described, proving the relative and absolute stereochemistry of natural plakotenin. A biomimetic intramolecular Diels–Alder reaction served as a key step in the total synthesis.

3307

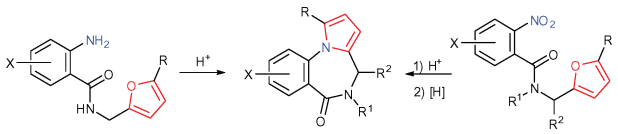


Synthesis, computational study and glycosidase inhibitory activity of polyhydroxylated conidine alkaloids—a bicyclic iminosugar

Shrihari P. Sanap, Sougata Ghosh, Amit M. Jabgunde, Rahul V. Pinjari, Shridhar P. Gejji, Shailza Singh, Balu A. Chopade and Dilip D. Dhavale*

A short and efficient synthesis of two hitherto unreported conidine iminosugars, one of which is selective inhibitor of α-mannosidase, and their conformational study by ^{1}H NMR, DFT calculations and molecular docking is described.

3316

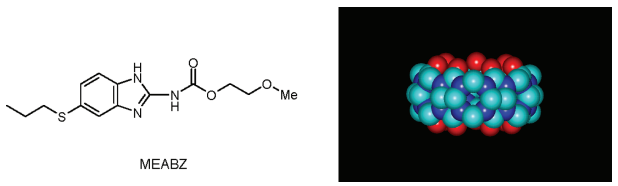


Furan ring opening–pyrrole ring closure: a new synthetic route to aryl(heteroaryl)-annulated pyrrolo[1,2-*a*][1,4]diazepines

Alexander V. Butin,* Tatyana A. Nevolina, Vitaly A. Shcherbinin, Igor V. Trushkov, Dmitry A. Cheshkov and Gennady D. Krapivin

Two new routes to pyrrolo[1,2-*a*][1.4]diazepines are proposed which are based on intramolecular furan recyclization.

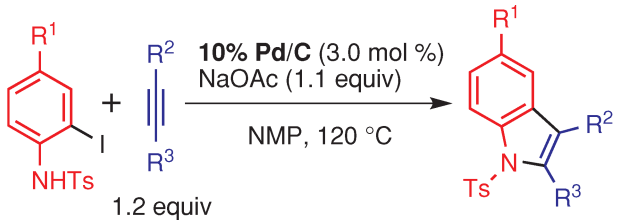
3328



Enhanced cytotoxicity of benzimidazole carbamate derivatives and solubilisation by encapsulation in cucurbit[*n*]uril

Yunjie Zhao, Mohammad H. Pourgholami, David L. Morris, J. Grant Collins* and Anthony I. Day*

A new highly cytotoxic benzimidazole carbamate drug (MEABZ) has been synthesized, and encapsulation of the drug in the macrocycle cucurbit[*n*]uril (picture) significantly increased its water solubility.



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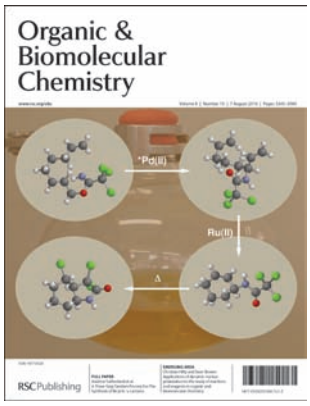
IN THIS ISSUE

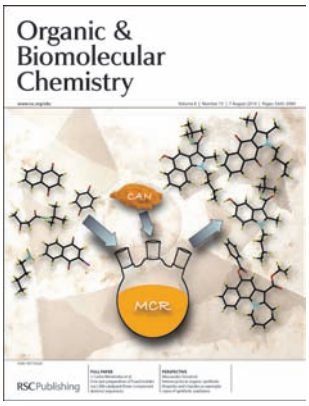
ISSN 1477-0520 CODEN OBCRAK 8(15) 3345–3580 (2010)



Cover

See Sutherland *et al.*, pp. 3418–3425.
A one-pot, three-step tandem process involving an Overman rearrangement, a ring closing metathesis reaction and a Kharasch cyclisation has been developed for the asymmetric synthesis of bicyclic γ-lactams.

Image reproduced by permission of Fiona I. McGonagle, Lindsay Brown, Andrew Cooke and Andrew Sutherland from *Org. Biomol. Chem*, 2010, **8**, 3418.

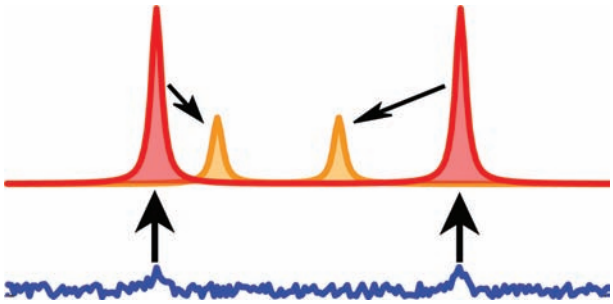


Inside cover

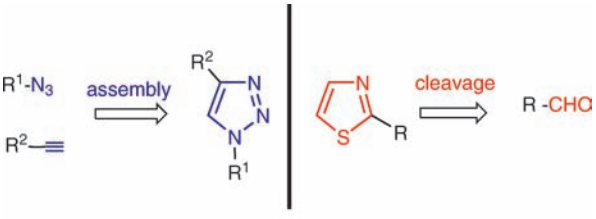
See Menéndez *et al.*, pp. 3426–3436.
The inside cover picture shows the range of structurally diverse indole-related nitrogen heterocycles that can be synthesized on the basis of a CAN-catalyzed three-component reaction between primary amines, β-dicarbonyl compounds and (2-bromo)naphthoquinones.

Image reproduced by permission of Padmakar A. Suryavanshi, Vellaisamy Sridharan and J. Carlos Menéndez from *Org. Biomol. Chem.*, 2010, **8**, 3426.

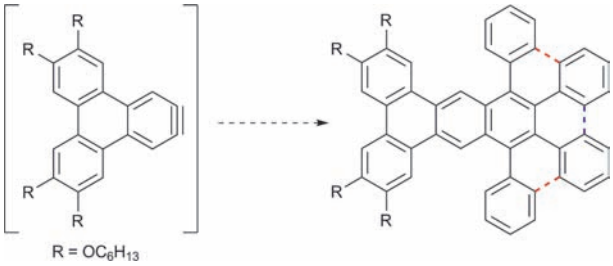
EMERGING AREA

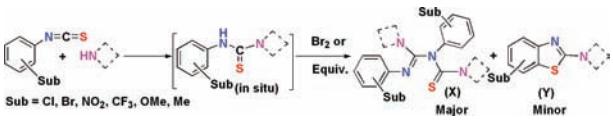


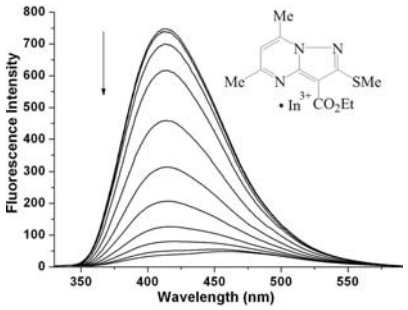
PERSPECTIVE

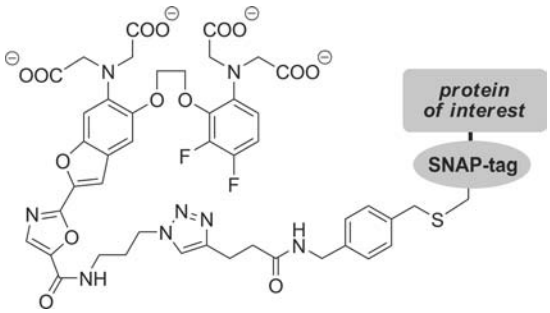


triazole serves as a linker while thiazole is a masked functionality



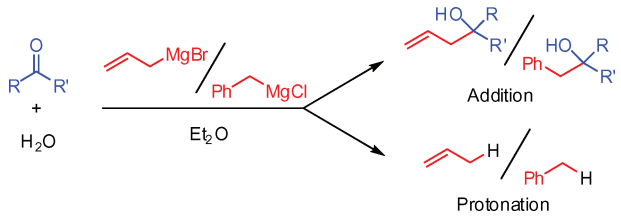






COMMUNICATIONS

3402



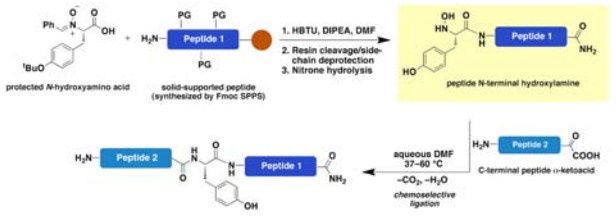
Ultrafast Grignard addition reactions in the presence of water

Gyorgyi Osztrovszky, Torkil Holm* and Robert Madsen*

For two highly reactive Grignard reagents (allylMgBr and benzylMgCl) the rate of carbonyl addition is comparable to the rate of protonation by water.

PAPERS

3405

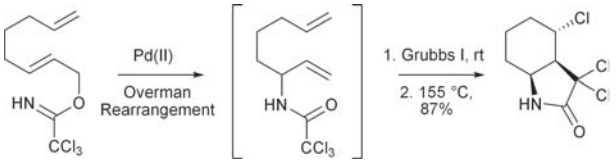


Nitrone protecting groups for enantiopure *N*-hydroxyamino acids: synthesis of N-terminal peptide hydroxylamines for chemoselective ligations

S. Irene Medina, Jian Wu and Jeffrey W. Bode*

Enantiopure peptide N-terminal hydroxylamines are key substrates for a chemoselective ligation with α-ketoacids to form native peptide bonds. A robust method for their synthesis in enantiopure form *via* *N*-benzylidene nitrone protected intermediates is described. This procedure provides intermediates and protocols compatible with Fmoc-based solid phase peptide synthesis.

3418

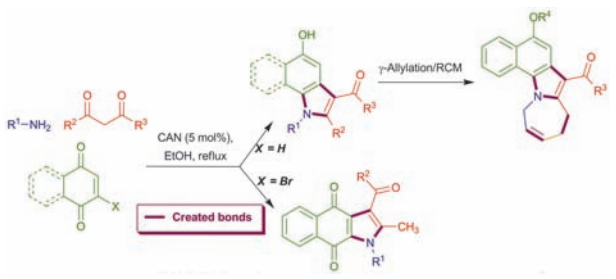


A three-step tandem process for the synthesis of bicyclic γ-lactams

Fiona I. McGonagle, Lindsay Brown, Andrew Cooke and Andrew Sutherland*

A one-pot, three-step tandem process has been developed for the direct synthesis of functionalised bicyclic [3.3.0], [4.3.0] and [5.3.0] γ-lactams from simple allylic trichloroacetimidates.

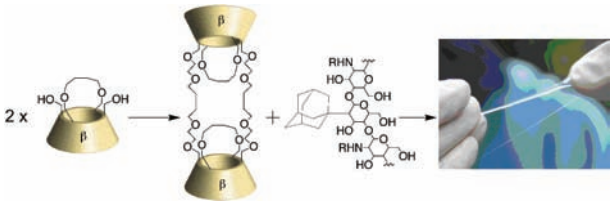
3426

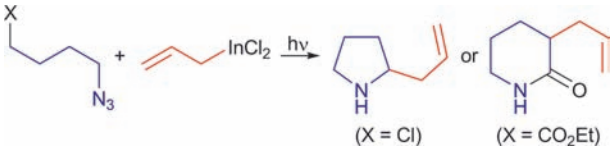


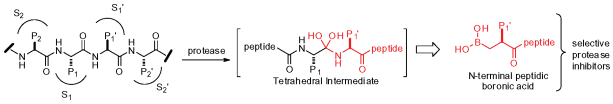
Expedient, one-pot preparation of fused indoles *via* CAN-catalyzed three-component domino sequences and their transformation into polyheterocyclic compounds containing pyrrolo[1,2-*a*]azepine fragments

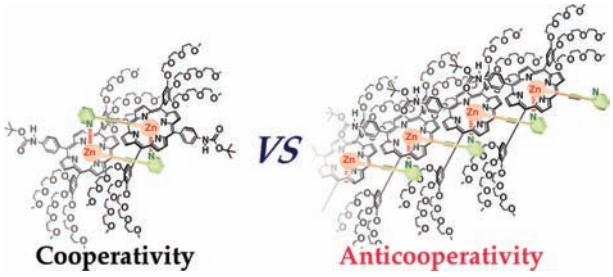
Padmakar A. Suryavanshi, Vellaisamy Sridharan and J. Carlos Menéndez*

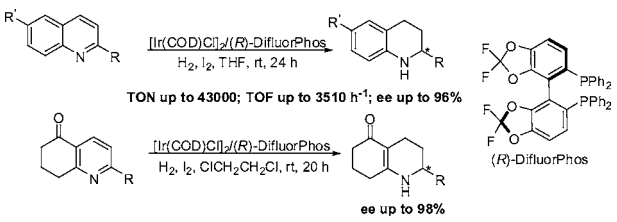
The CAN-catalyzed three-component reaction between primary amines, β-dicarbonyl compounds and naphthoquinones or 2-bromonaphthoquinones afforded, respectively, 5-hydroxybenzo[*g*]indoles and benzo[*f*]indole-4,9-diones. Further transformations were also studied.

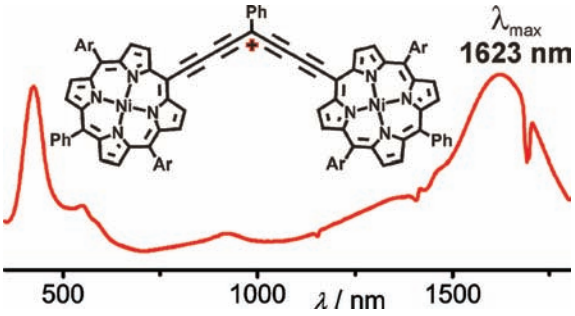


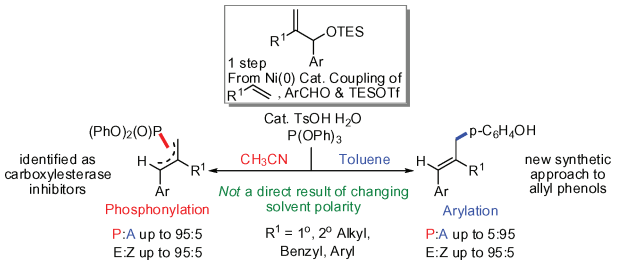


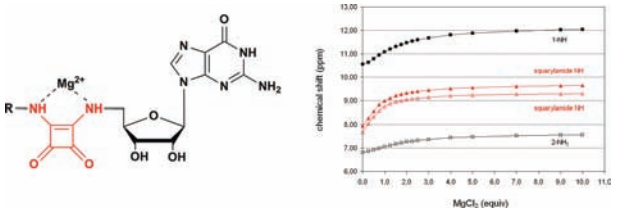


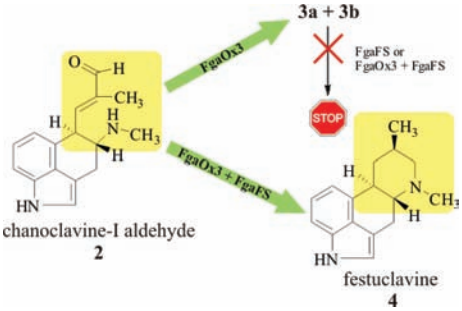








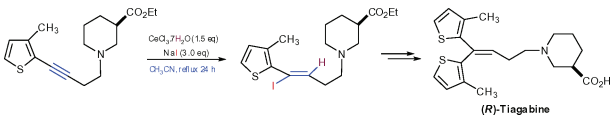




Ergot alkaloid biosynthesis in *Aspergillus fumigatus*: Conversion of chanoclavine-I aldehyde to festuclavine by the festuclavine synthase FgaFS in the presence of the old yellow enzyme FgaOx3

C. Wallwey, M. Matuschek, X.-L. Xie and S.-M. Li*

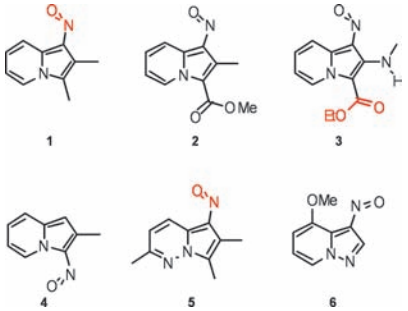
The conversion of chanoclavine-I aldehyde (**2**) to festuclavine (**4**) was demonstrated by using old yellow enzyme FgaOx3 and festuclavine synthase FgaFS. In the absence of FgaFS, **2** was converted by FgaOx3 to two shunt products **3a** and **3b**, which were not accepted by FgaFS as substrates.



A convergent approach to (*R*)-Tiagabine by a regio- and stereocontrolled hydroiodination of alkynes

Giuseppe Bartoli, Roberto Cipolletti, Giustino Di Antonio, Riccardo Giovannini, Silvia Lanari, Mauro Marcolini and Enrico Marcantoni*

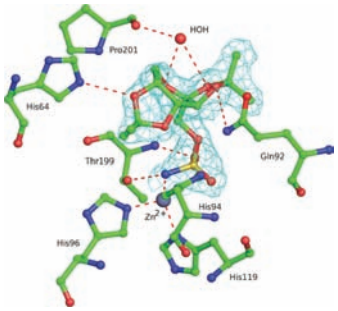
An efficient methodology for the iodofunctionalization of carbon–carbon triple bonds has efficiently been applied to the preparation of (*R*)-Tiagabine, a GABA uptake inhibitor marketed from the treatment of epilepsy.



Conformational equilibria and barriers to rotation in some novel nitroso derivatives of indolizines and 3- and 5-azaindolizines – an NMR and molecular modeling study

Ion Ghiviriga,* Bahaa El-Dien M. El-Gendy, Henry Martinez, Dmytro Fedoseyenko, Eric P. Metais, Aziz Fadli and Alan R. Katritzky*

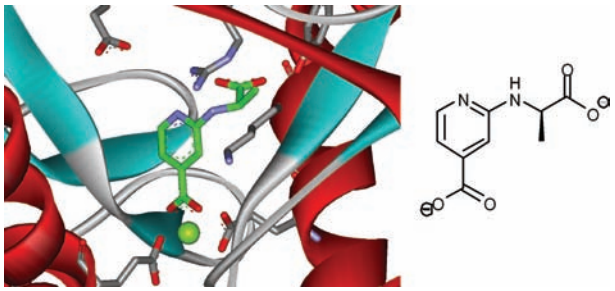
The conformational preferences of compounds **1**–**6** have been identified by NMR and explained by molecular modeling.

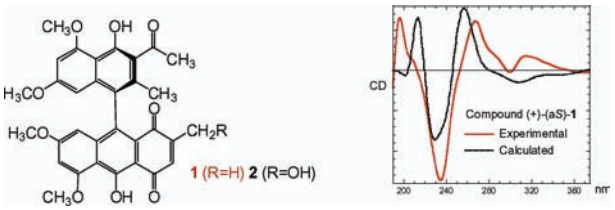


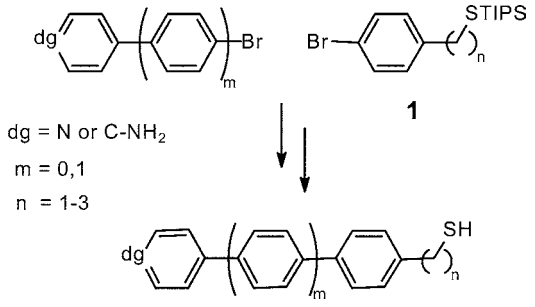
The first example of a significant active site conformational rearrangement in a carbonic anhydrase-inhibitor adduct: the carbonic anhydrase I–topiramate complex

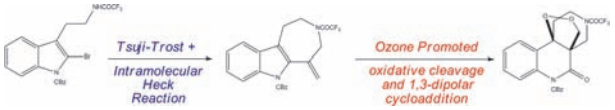
Vincenzo Alterio, Simona Maria Monti, Emanuela Truppo, Carlo Pedone, Claudiu T. Supuran* and Giuseppina De Simone*

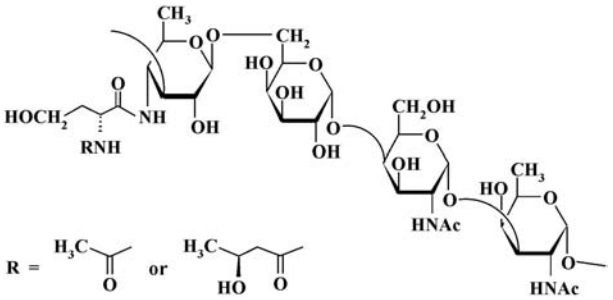
The crystallographic structure of the adduct which **TPM**, a widely used antiepileptic drug, forms with human Carbonic Anhydrase (CA) I, has been reported, showing for the first time a significant conformational rearrangement of the CA active site upon binding of the inhibitor.











* Indicates the author for correspondence: see article for details.

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IN THIS ISSUE

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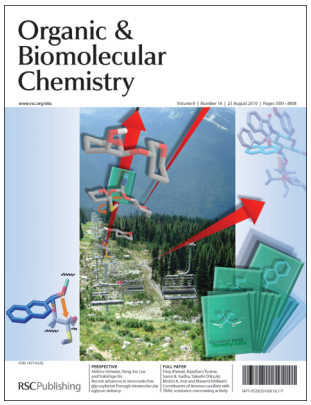
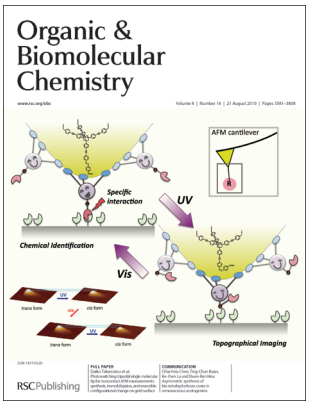


Cover
See Akihiro Ishiwata *et al.*, pp. 3596–3608.
The article by Ishiwata *et al.* describes invention and evolution of intramolecular aglycon delivery (IAD) approach which has proven powerful in giving a variety of *O*-glycosides stereoselectively.

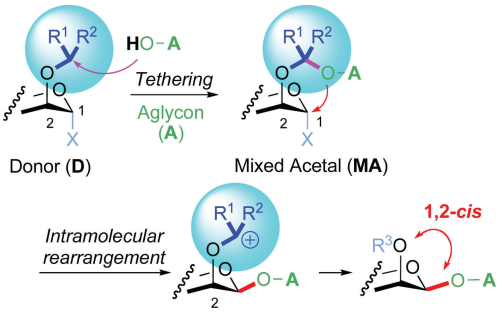
Image reproduced by permission of Akihiro Ishiwata and Yukishige Ito from *Org. Biomol. Chem.*, 2010, **8**, 3596.

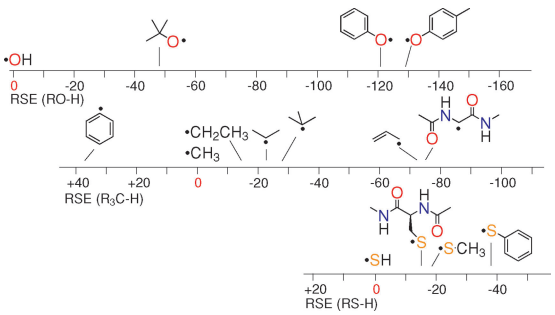


Inside cover
See Daiko Takamatsu *et al.*, pp. 3655–3664.
Robust, stationary, and photoswitchable tripods were synthesized as single molecule AFM tips for combined chemical force microscopy and topographical imaging.

Image reproduced by permission of Yoko Yamakoshi from *Org. Biomol. Chem.*, 2010, **8**, 3655.

PERSPECTIVES



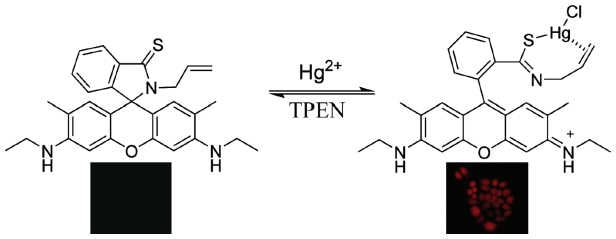


3618

A reversible fluorescent Hg^{2+} chemosensor based on a receptor composed of a thiol atom and an alkene moiety for living cell fluorescence imaging

Weiying Lin,* Xiaowei Cao, Yundi Ding, Lin Yuan and Quanxing Yu

A novel reversible fluorescence turn-on Hg^{2+} chemosensor was constructed based on a new receptor for fluorescence imaging in living cells.

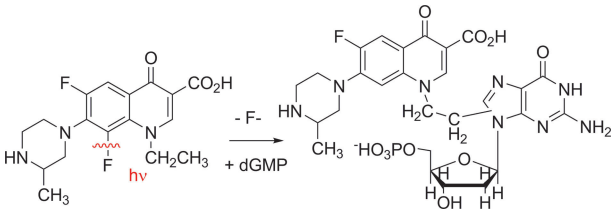


3621

Fluoroquinolones as potential photochemotherapeutic agents: covalent addition to guanosine monophosphate

Elisa Fasani,* Ilse Manet, Massimo L. Capobianco, Sandra Monti,* Luca Pretali and Angelo Albini*

The aryl cation photochemically generated from 8-fluoroquinolones forms a covalent bond with guanosine monophosphate ($k_r > 10^9$ $M^{-1}s^{-1}$).

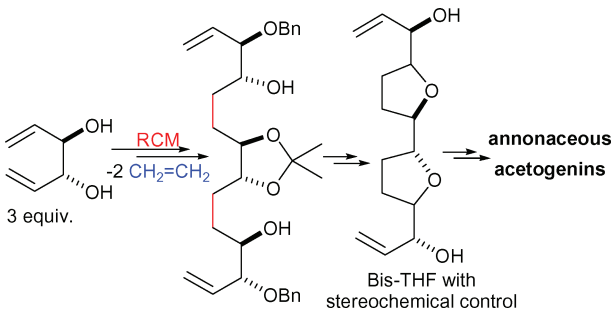


3624

Asymmetric synthesis of bis-tetrahydrofuran cores in annonaceous acetogenins

Chia-Hsiu Chen, Ting-Chun Kuan, Ke-Jhen Lu and Duen-Ren Hou*

The bis-THF cores were synthesized from (3*R*,4*R*)-1,5-hexadiene-3,4-diol, and the methylene acetal function was developed as a new linker for RCM.

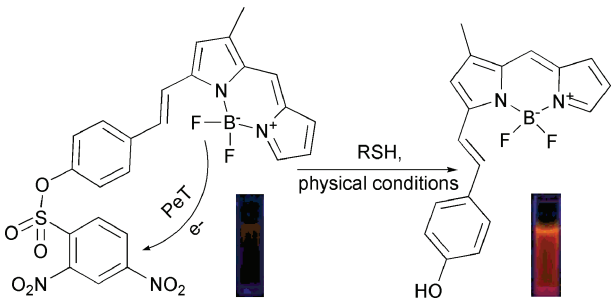


3627

Design and synthesis of a highly selective fluorescent turn-on probe for thiol bioimaging in living cells

Xin Li, Shijing Qian, Qiaojun He, Bo Yang, Jia Li and Yongzhou Hu*

A highly-selective fluorescent turn-on probe for the rapid optical sensing of thiols has been designed, synthesized and applied to imaging of thiols in living cells.



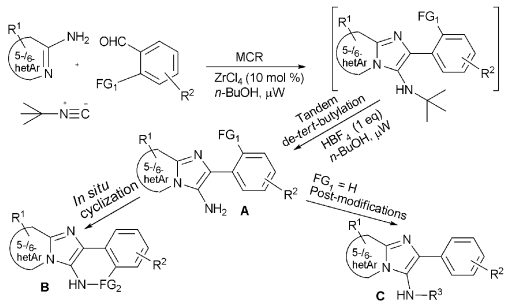
COMMUNICATIONS

3631

Towards molecular diversity: dealkylation of *tert*-butyl amine in Ugi-type multicomponent reaction product establishes *tert*-butyl isocyanide as a useful convertible isonitrile

Sankar K. Guchhait* and Chetna Madaan

Development of a novel tandem de-*tert*-butylation in an Ugi-type MCR product afforded for the first time *tert*-butyl isocyanide as a useful convertible isonitrile towards the generation of molecular diversity of N-fused imidazoles (**A**, **B** and **C**).

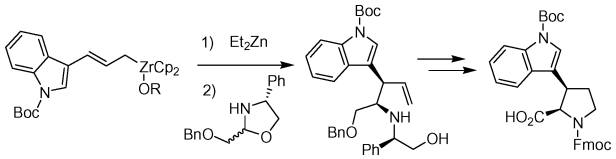


3635

Asymmetric synthesis of proline-based conformationally constrained tryptophan mimetic

Pierre-Olivier Delaye, Jean-Luc Vasse* and Jan Szymoniak

The stereoselective synthesis of a constrained tryptophan mimetic is described, based on the generation of an unprecedented indole-containing allylmetal.



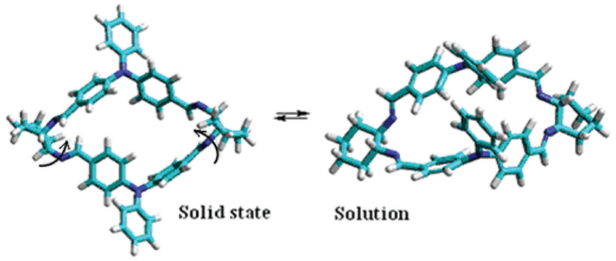
PAPERS

3638

Triphenylamine-based rhombimine macrocycles with solution interconvertable conformation

Mircea Grigoras,* Loredana Vacareanu, Teofilia Ivan and Gabriela Liliana Ailiesei

Three rhombimine macrocycles have been synthesized by [2+2] cyclocondensation reaction between (R,R)-1,2-diaminocyclohexane and 4,4′-*bis*formyl triphenylamine derivatives. Evidence from ^{1}H-NMR and UV suggests that there is a rotamer inversion in solution arising from the rotation of triphenylamine group around cyclohexyl–N single bonds.

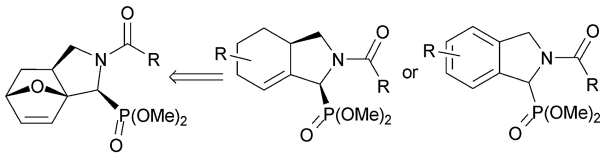


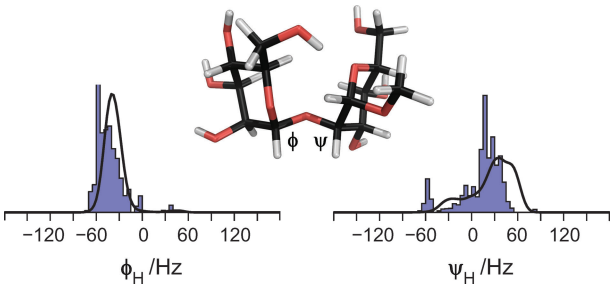
3644

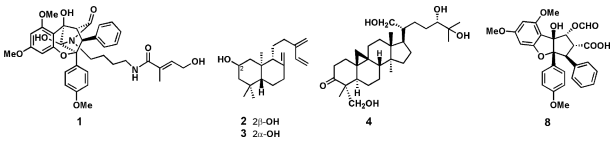
Experimental and computational study of the ring opening of tricyclic oxanorbornenes to polyhydro isoindole phosphonates

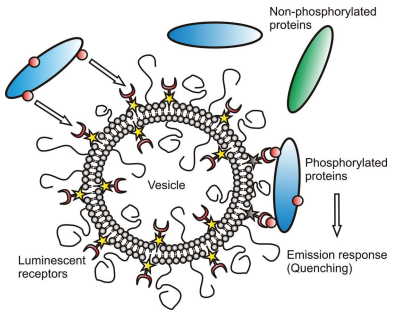
Diederica D. Claeys, Christian V. Stevens,* Bart I. Roman, Pieter Van De Caveye, Michel Waroquier and Veronique Van Speybroeck*

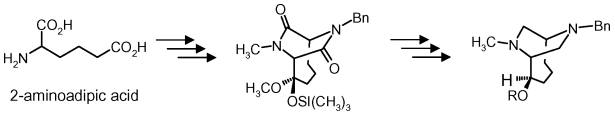
Experimental and molecular modelling study of the ring opening of tricyclic α-amino phosphonates with Lewis-acid and clay-based catalysts.

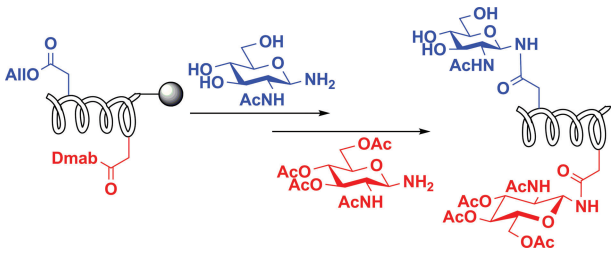


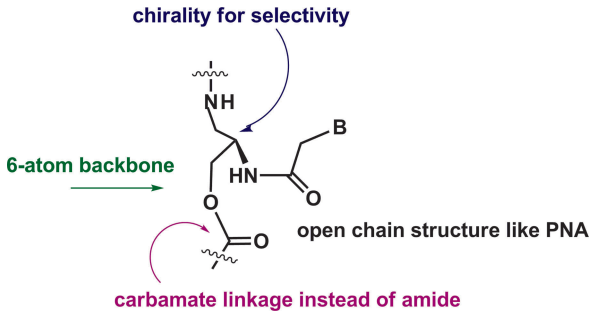


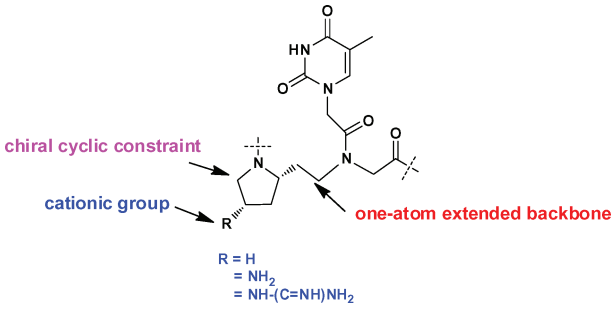


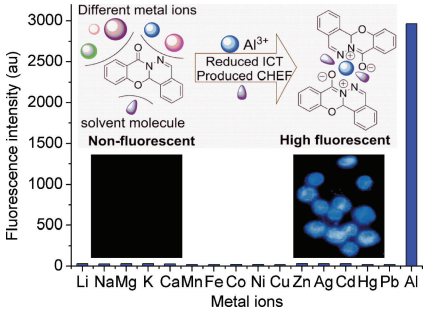


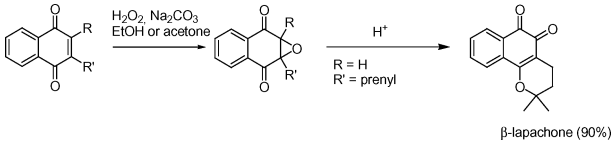


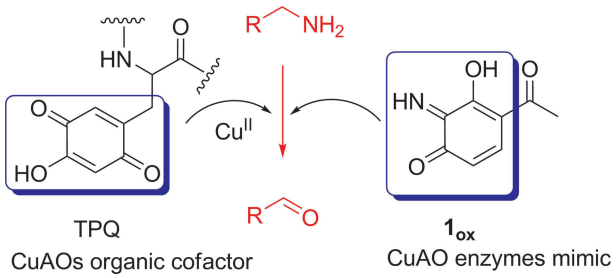


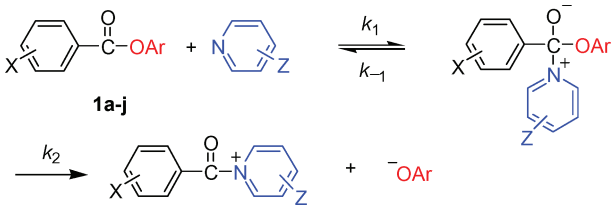












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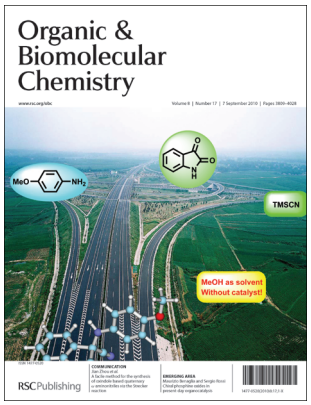
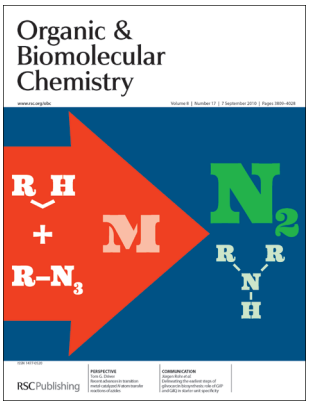
ISSN 1477-0520 CODEN OBCRAK 8(17) 3809–4028 (2010)



Cover
See Jian Zhou *et al.*, pp. 3847–3850.
The direct α-cyanoamination of isatins using TMSCN was accomplished in methanol without any catalyst.

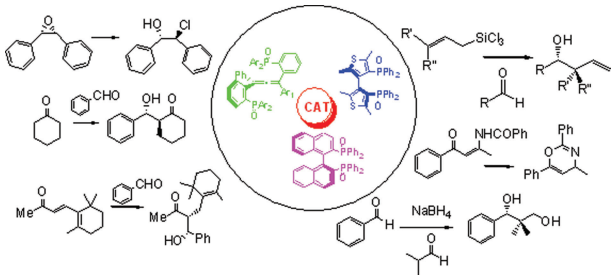
Image reproduced by permission of Yun-Lin Liu, Feng Zhou, Jun-Jie Cao, Cong-Bin Ji, Miao Ding and Jian Zhou from *Org. Biomol. Chem*, 2010, **8**, 3847.



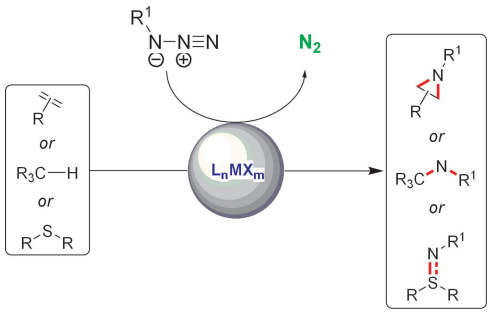
Inside cover
See Tom G. Driver, pp. 3831–3846.
Azides are useful progenitors of metal nitrene species that transform simple starting materials into complex, functionalized products. Cover art designed and prepared by Benjamin Kiel of House Industries.

Image reproduced by permission of Tom G. Driver from *Org. Biomol. Chem*, 2010, **8**, 3831.

EMERGING AREA



PERSPECTIVE

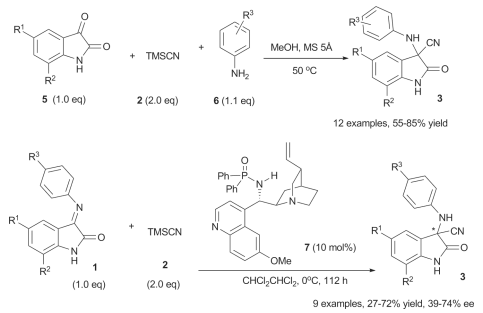


3847

A facile method for the synthesis of oxindole based quaternary α-aminonitriles *via* the Strecker reaction

Yun-Lin Liu, Feng Zhou, Jun-Jie Cao, Cong-Bin Ji, Miao Ding and Jian Zhou*

The direct α-cyanoamination of isatins using TMSCN has been developed, which is carried out in methanol without any catalyst. A new bifunctional cinchona alkaloid-based phosphinamide catalyst **7** could promote the Strecker reaction of isatins derived ketimine with TMSCN in up to 74% ee.

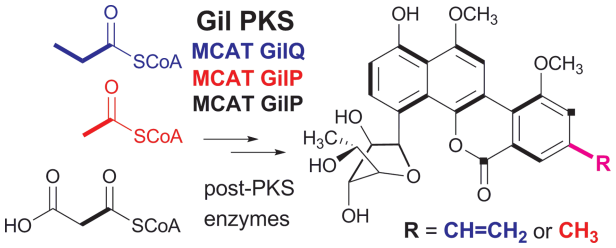


3851

Delineating the earliest steps of gilvocarcin biosynthesis: role of GilP and GilQ in starter unit specificity

Micah D. Shepherd, Madan K. Kharel, Lili L. Zhu, Steven G. van Lanen and Jürgen Rohr*

Unusual MCAT-type activities, not a distinct KASIII analogue, steer gilvocarcin biosynthesis toward preferentially priming with propionate over acetate starter units.

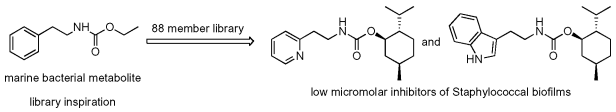


3857

Synthesis and bacterial biofilm inhibition studies of ethyl *N*-(2-phenethyl) carbamate derivatives

Steven A. Rogers, Daniel C. Whitehead, Trey Mullikin and Christian Melander*

An 88 member library based upon the marine bacterial metabolite ethyl *N*-(2-phenethyl) carbamate was evaluated for bacterial biofilm inhibition against a panel of medically relevant strains.

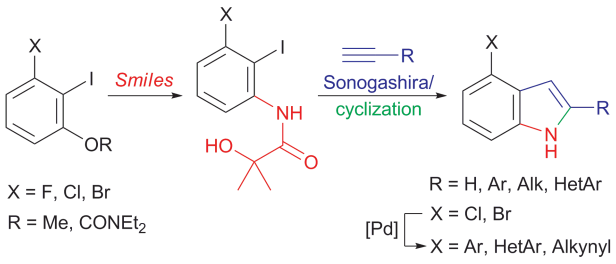


3860

Synthesis of 4-functionalized-1*H*-indoles from 2,3-dihalophenols

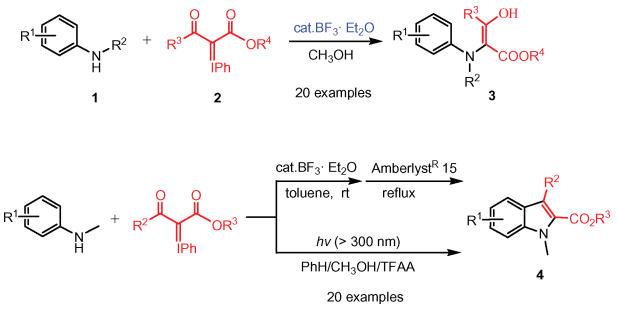
Roberto Sanz,* Verónica Guilarte and Nuria García

A new synthesis of 4-halo-1*H*-indoles has been developed from easily available 2,3-dihalophenol derivatives. The key steps are Smiles rearrangement and a one-pot or stepwise Sonogashira coupling/NaOH-mediated cyclization. Subsequent functionalization allows access to a wide variety of 2,4- or 2,3,4-regioselectively functionalized indoles.



COMMUNICATIONS

3865



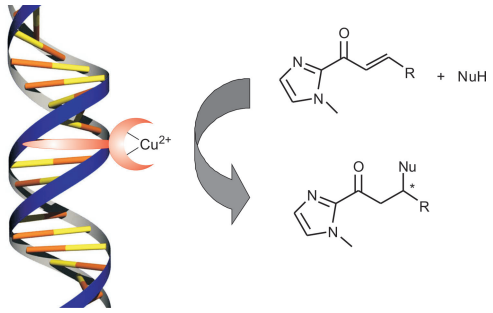
The acid-promoted reactions of phenyliodonium ylides with substituted anilines and their applications to the synthesis of indoles

Xianpei Wang, Bing Han, Junyan Wang and Wei Yu*

The reactions of phenyliodonium ylides with substituted anilines constitute a new protocol for the synthesis of indoles.

PAPERS

3868

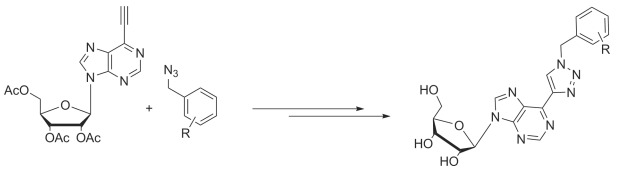


On the Role of DNA in DNA-based Catalytic Enantioselective Conjugate Addition Reactions

Ewold W. Dijk, Arnold J. Boersma, Ben L. Feringa* and Gerard Roelfes*

DNA significantly affects the reaction rates of DNA-based catalytic enantioselective Friedel–Crafts alkylation and Michael addition reactions.

3874

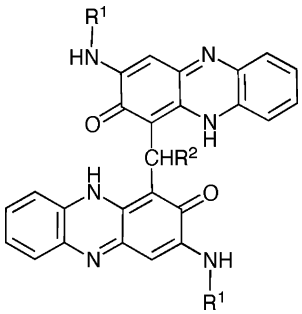


Expeditious synthesis and biological evaluation of new C-6 1,2,3-triazole adenosine derivatives A1 receptor antagonists or agonists

S. C. Mathew, Y. By, A. Berthault, M.-A. Virolleaud, L. Carrega, G. Chouraqui, L. Commeiras, J. Condo, M. Attolini, A. Gaudel-Siri, J. Ruf, J. Rodriguez,* J.-L. Parrain* and R. Guieu*

An expeditious synthesis and biological evaluation of new C-6 1,2,3-triazole adenosine derivatives A1 receptor antagonists or agonists are described.

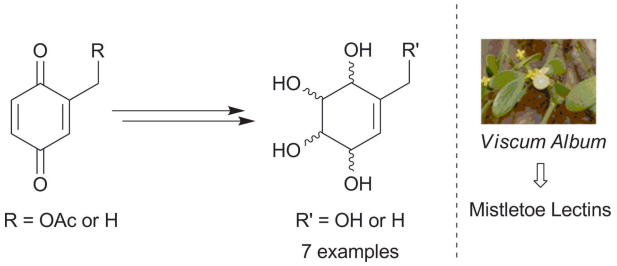
3882

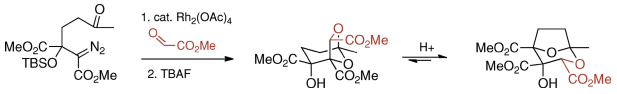


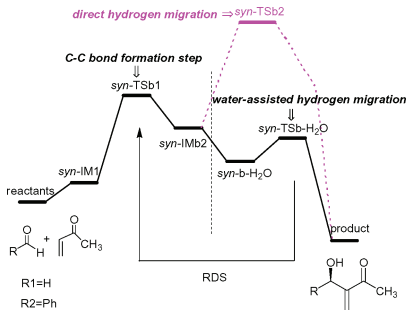
New class of highly stable nonaromatic tautomers

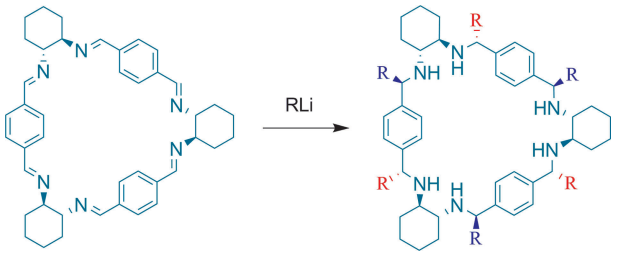
Claire Seillan, Philippe Marsal and Olivier Siri*

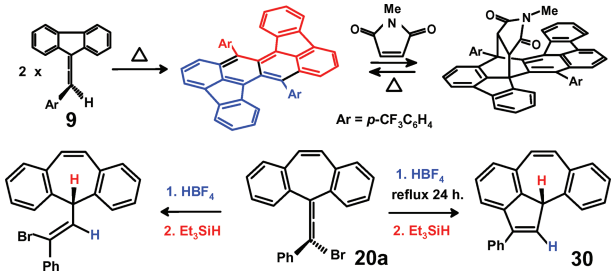
A new and efficient one-pot synthesis of unprecedented dimers which sacrifice by prototropic rearrangement their aromatic character (OH form) in favor of a new class of highly stable nonaromatic NH tautomers is described (either in solution or in solid-state).

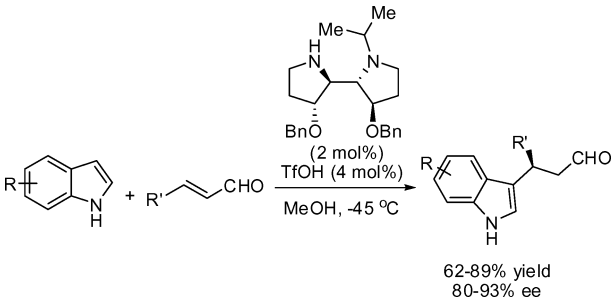


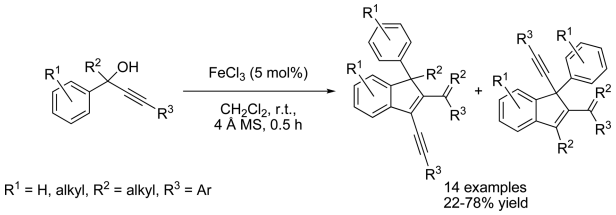












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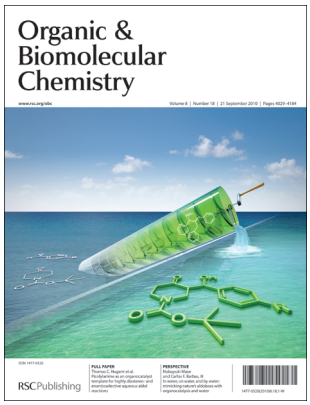
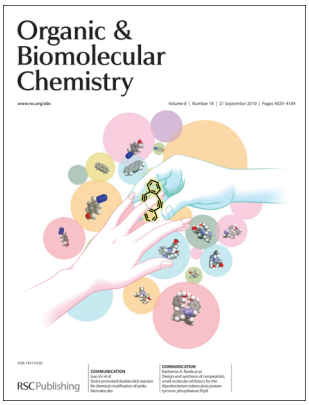


Cover

See Thomas C. Nugent *et al.*, pp. 4085–4089

Archimedes' screw, an ingenious device synonymous with water transport, is depicted here as the water active 1,2-diamine catalyst converting low value starting materials into high value multifunctional aldol products. Graphic Art Credit: Michael Holt (Bremen, Germany).

Image reproduced by permission of Thomas C. Nugent from *Org. Biomol. Chem.*, 2010, **8**, 4085.



Inside cover

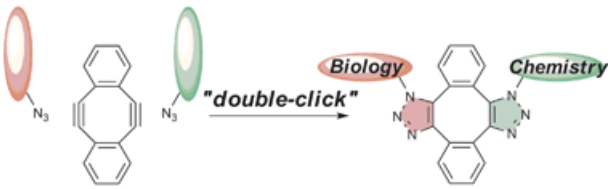
See Isao Kii *et al.*, pp. 4051–4055.

The wedding ring. He is putting the Sondheimer diyne on her finger and they are covalently joined together. This wedding ring provides a novel convergent method, "strain-promoted double-click reaction" enabling us to modify azido-biomolecules with a small reporter azide.

Image reproduced by permission of Takamitsu Hosoya from *Org. Biomol. Chem.*, 2010, **8**, 4051.

PERSPECTIVE

COMMUNICATIONS



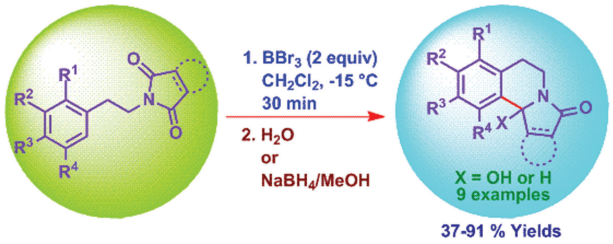
The Sondheimer diyne acts as a matchmaker between chemistry and biology.

4056

An unusual reactivity of BBr_3: Accessing tetrahydroisoquinoline units from *N*-phenethylimides

Jayaraman Selvakumar, Alexandros Makriyannis and Chinnasamy Ramaraj Ramanathan*

A simple methodology to construct the tetrahydroisoquinoline containing skeleton through electrophilic activation of imide carbonyl group of *N*-phenethylimides using BBr_3 as Lewis acid is developed.

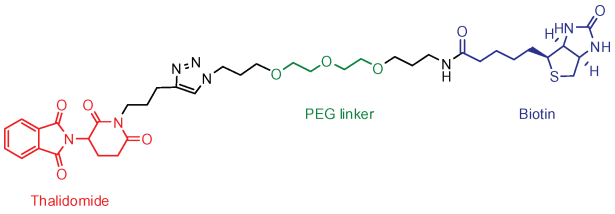


4059

Efforts toward elucidating Thalidomide's molecular target: an expedient synthesis of the first Thalidomide biotin analogue

Scott G. Stewart,* Carlos J. Braun, Marta E. Polomska, Mahdad Karimi, Lawrence J. Abraham and Keith A. Stubbs

The synthesis of the first Thalidomide–biotin analogue is described *via* a Huisgen 1,3-dipolar cycloaddition (click reaction) as the key synthetic step. This compound will help unlock investigations into the as yet unknown molecular mode of action of Thalidomide.

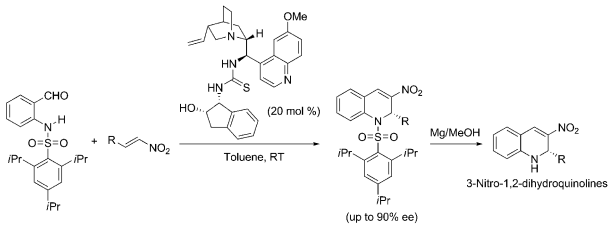


4063

Bifunctional thiourea-promoted cascade aza-Michael-Henry-dehydration reactions: asymmetric preparation of 3-nitro-1,2-dihydroquinolines

Xiaoqian Liu and Yixin Lu*

A cascade aza-Michael-Henry-dehydration reaction led to a one-step preparation of 3-nitro-1,2-dihydroquinolines in high yields and up to 90% ee.

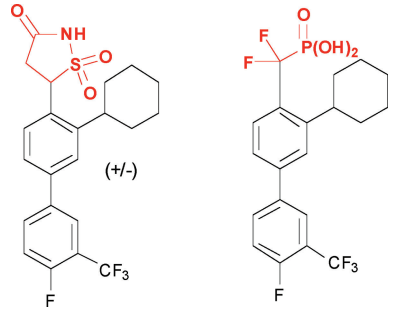


4066

Design and synthesis of nonpeptidic, small molecule inhibitors for the *Mycobacterium tuberculosis* protein tyrosine phosphatase PtpB

Katherine A. Rawls, Christoph Grundner and Jonathan A. Ellman*

The design and synthesis of small molecules with low micromolar inhibition of *Mycobacterium tuberculosis* protein tyrosine phosphatase PtpB is described.



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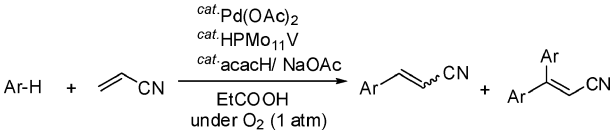
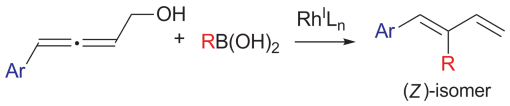


Direct oxidative coupling of benzenes with acrylonitriles to cinnamonitriles catalyzed by $Pd(OAc)_2/HPMoV/O_2$ system

Yasushi Obora,* Yoshihisa Okabe and Yasutaka Ishii*

A facile direct synthesis of cinnamonitriles from acrylonitriles and benzenes is successfully achieved by using $Pd(OAc)_2/HPMoV/O_2$ catalyst system *via* the direct C–H bond activation of benzenes using molecular oxygen as a terminal oxidant.

4074

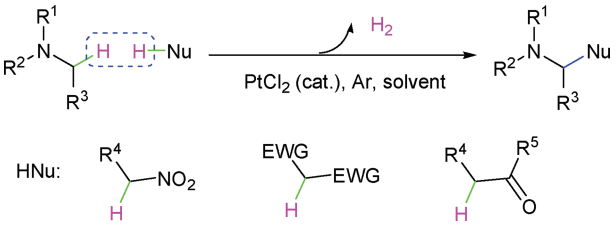


Stereoselective synthesis of vinyl-substituted (*Z*)-stilbenes by rhodium-catalysed addition of arylboronic acids to allenic alcohols

Tomoya Miura, Hiroshi Shimizu, Tomohiro Igarashi and Masahiro Murakami*

The reaction of 4-arylbuta-2,3-dien-1-ols with arylboronic acids in the presence of a rhodium(I) catalyst gave vinylsubstituted (*Z*)-stilbenes stereoselectively.

4077

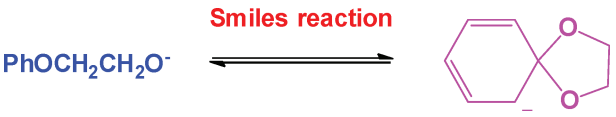


Platinum-catalyzed cross-dehydrogenative coupling reaction in the absence of oxidant

Xing-Zhong Shu, Yan-Fang Yang, Xiao-Feng Xia, Ke-Gong Ji, Xue-Yuan Liu and Yong-Min Liang*

A third strategy for cross-dehydrogenative coupling reaction has been reported *via* platinum catalysis in the absence of oxidant.

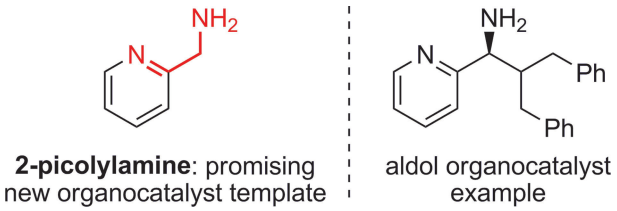
4080

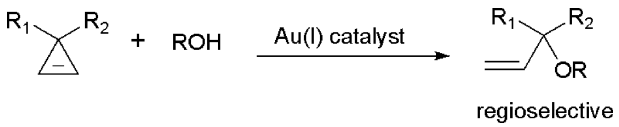


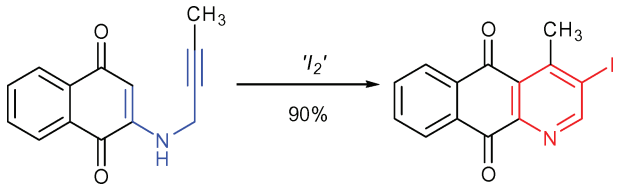
The gas phase Smiles rearrangement of anions $PhO(CH_2)_nO^-$ ($n = 2$–4). A joint theoretical and experimental approach

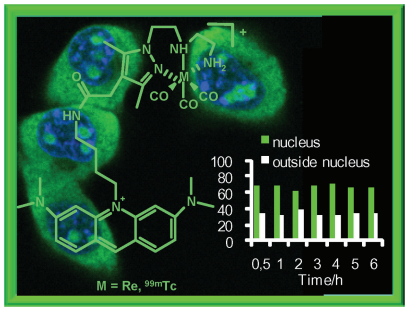
Tianfang Wang, Nico M. M. Nibbering and John H. Bowie*

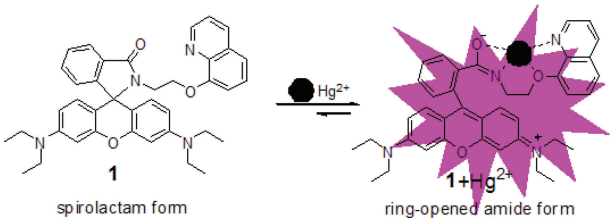
A combination of theory and experiment shows that energized $PhOCH_2CH_2O^-$ exclusively undergoes the Smiles rearrangement.

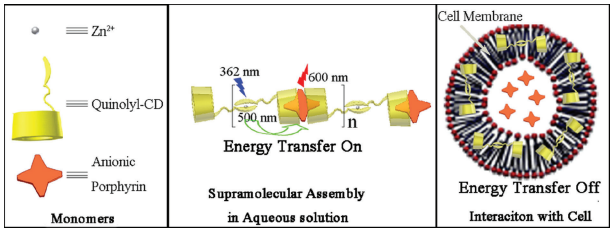


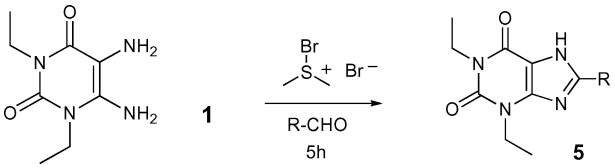


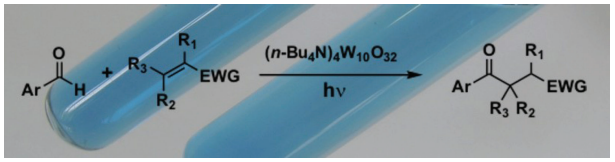










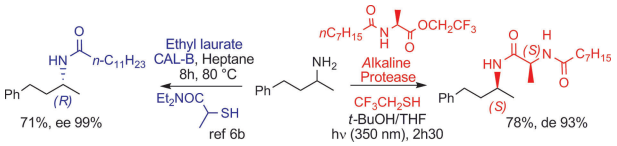


4165

Switching from (*R*)- to (*S*)-selective chemoenzymatic DKR of amines involving sulfanyl radical-mediated racemization

Lahssen El Blidi, Nicolas Vanthuyne, Didier Siri, Stéphane Gastaldi,* Michèle P. Bertrand* and Gérard Gil*

Chemoenzymatic dynamic kinetic resolution of amines involving sulfanyl radical-induced racemization happened to be the very first switchable DKR process allowing the synthesis of either (*R*)- or (*S*)-amides.

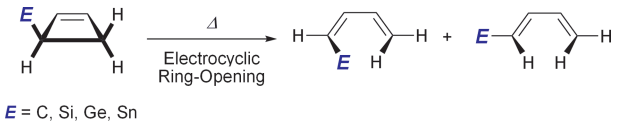


4169

Substituent effect of group 14 elements on the ring-opening reaction of cyclobutene

Munehiro Hasegawa, Ippei Usui, Soichiro Konno and Masahiro Murakami*

A series of cyclobutenes bearing group 14 elements at the 3-position were synthesized, and their rotational behaviors in the thermal ring-opening reaction are discussed.

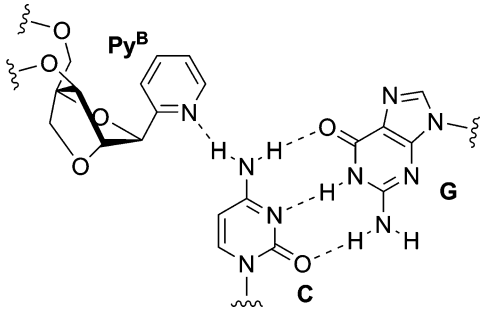


4176

2′,4′-BNA bearing a 2-pyridine nucleobase for CG base pair recognition in the parallel motif triplex DNA

Yoshiyuki Hari,* Sachiko Matsugu, Hiroyasu Inohara, Yuri Hatanaka, Masaaki Akabane, Takeshi Imanishi and Satoshi Obika*

2′,4′-BNA bearing a 2-pyridine nucleobase (Py^B, see picture) in triplex-forming oligonucleotides was able to recognize a CG base pair within dsDNA with high sequence-selectivity and strong binding affinity.



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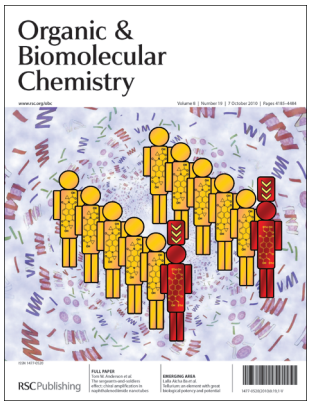
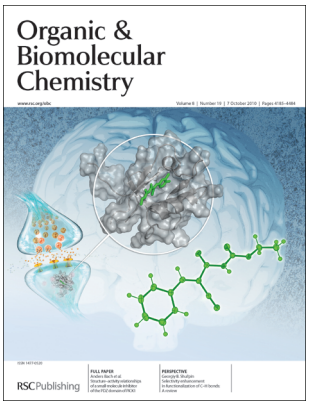
ISSN 1477-0520 CODEN OBCRAK 8(19) 4185–4484 (2010)



Cover
See Anderson *et al.*, pp. 4274–4280.
Chiral naphthalenediimide-based monomers impose a helical supramolecular structure upon achiral monomers much like sergeants organising soldiers in rank and file.

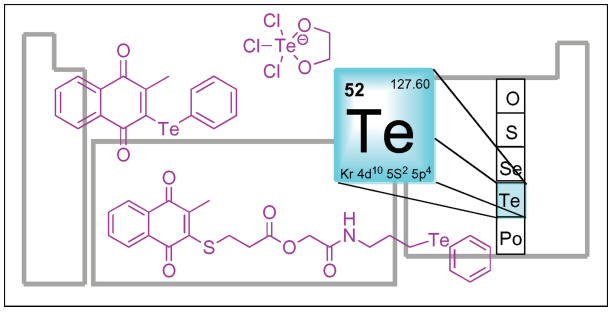
Image reproduced by permission of G. Dan Pantoş from *Org. Biomol. Chem.*, 2010, **8**, 4274.



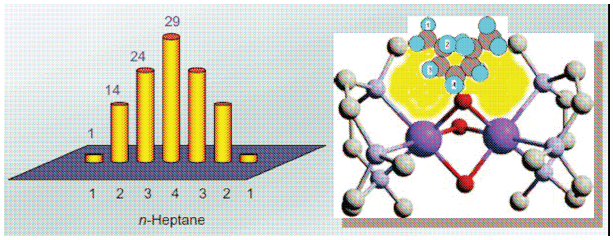
Inside cover
See Bach *et al.*, pp. 4281–4288.
Structure-activity relationships of the first small-molecule inhibitor of the PDZ domain of PICK1, an important protein in the brain, have been explored.

Image reproduced by permission of Ulrik Gether and Kristian Strømgaard from *Org. Biomol. Chem.*, 2010, **8**, 4281.

EMERGING AREA



PERSPECTIVE

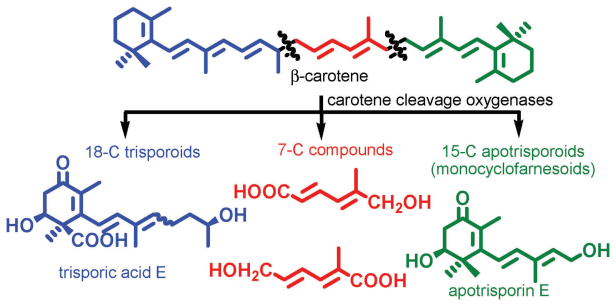


4229

Splitting of β-carotene in the sexual interaction of *Phycomyces*

Silvia Polaino, M. Mar Herrador, Enrique Cerdá-Olmedo and Alejandro F. Barrero*

The new C7 natural products **1–2** are the result of enzymatic carotene degradation during the sexual interaction.

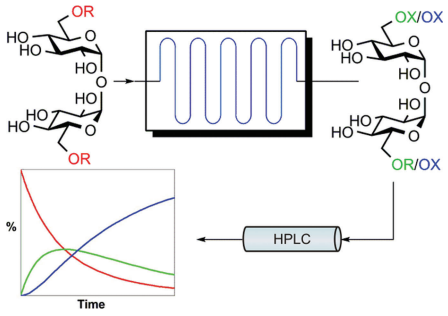


4232

Flow chemistry kinetic studies reveal reaction conditions for ready access to unsymmetrical trehalose analogues

Mitul K. Patel and Benjamin G. Davis*

Trehalose functionalization was studied in a microreactor, furnishing kinetic data that allowed the development of a synthetic route for large scale desymmetrizations.

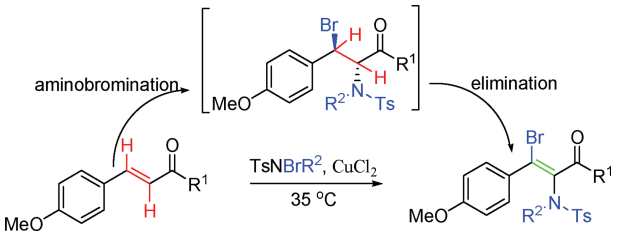


4236

Copper-catalyzed aminobromination/elimination process: an efficient access to α,β-unsaturated vicinal haloamino ketones and esters

Hao Sun, Guangqian Zhang, Sanjun Zhi, Jianlin Han,* Guigen Li and Yi Pan*

A novel copper-catalyzed aminobromination-elimination process has been developed, which provides an easy access to α,β-unsaturated vicinal haloamindes derivatives.

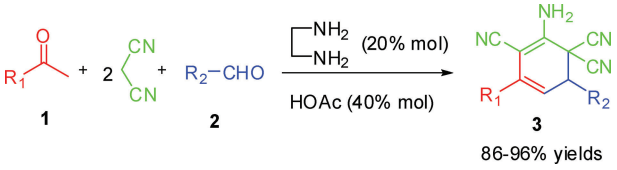


4240

Primary 1,2-diamine catalysis III: an unexpected domino reaction for the synthesis of multisubstituted cyclohexa-1,3-dienamines

Junfeng Wang, Qin Li, Chao Qi, Yi Liu, Zemei Ge* and Runtao Li*

Primary 1,2-diamine was employed in the first organocatalyzed multicomponent domino reactions of aryl ketones, aldehydes and malononitrile, affording multisubstituted cyclohexa-1,3-dienamines **3** in satisfactory results.

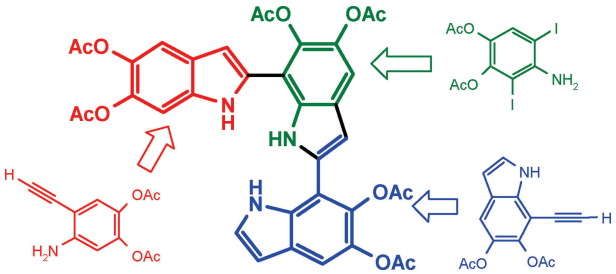


4243

First synthetic entry to the trimer stage of 5,6-dihydroxyindole polymerization: *ortho*-alkynylaniline-based access to the missing 2,7′:2′,7″-triindole

Luigia Capelli, Paola Manini,* Alessandro Pezzella and Marco d'Ischia

An *ortho*-alkynylaniline-based strategy allowed the first access to a 5,6-dihydroxyindole trimer, 5,5′,5″,6,6′,6″-hexaacetoxy-2,7′:2′,7″-triindole, *via* a sequence of Sonogashira coupling and metal cation catalyzed intramolecular cyclization.

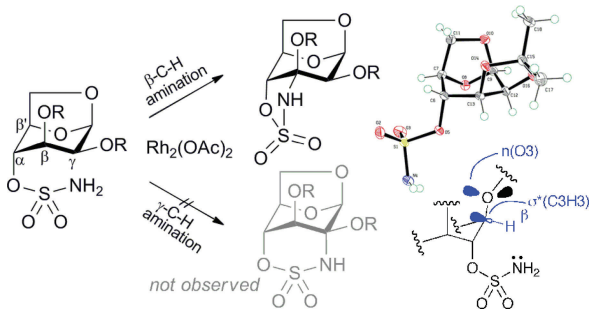


4246

Inverted regioselectivity of C–H amination: Unexpected oxidation at β- rather than γ-C–H

Filip J. Wyszynski, Amber L. Thompson and Benjamin G. Davis*

From derivatives of 1,6-anhydro-β-D-mannopyranose, five-membered sulfamidates were formed in preference to the typical six-membered oxathiazinane intramolecular insertion products.

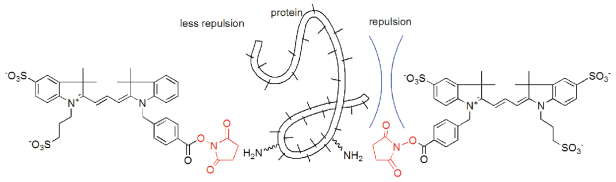


4249

Asymmetric trimethine 3*H*-indocyanine dyes: efficient synthesis and protein labeling

Fengling Song, Li Wang, Xiaoqiang Qiao, Bingshuai Wang, Shiguo Sun, Jiangli Fan, Lihua Zhang and Xiaojun Peng*

To achieve better protein labeling performance, sulfo groups should be away from the NHS ester end.

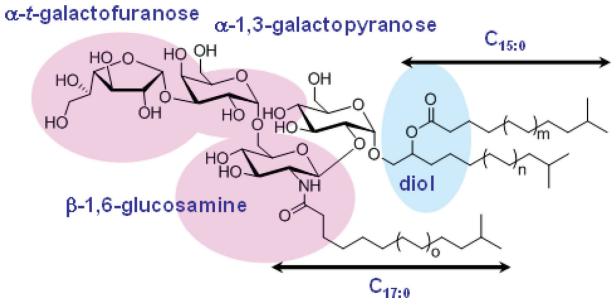


4252

Structural variation of glycolipids from *Meiothermus taiwanensis* ATCC BAA-400 under different growth temperatures

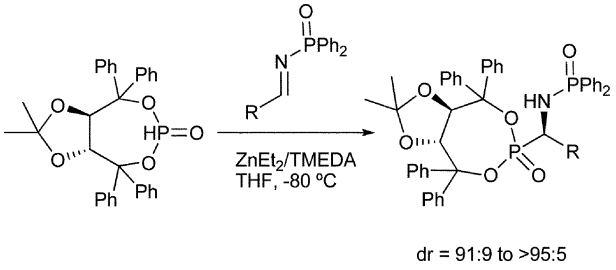
Yu-Liang Yang, Feng-Ling Yang, Zih-You Huang, Yu-Hsuan Tsai, Wei Zou and Shih-Hsiung Wu*

Structural variation of membrane glycolipids (including lipid and carbohydrate) under different growth temperature was revealed in thermophilic bacteria. The variation is assumed to stabilize membrane structure for survival in harsh environment.



COMMUNICATIONS

4255

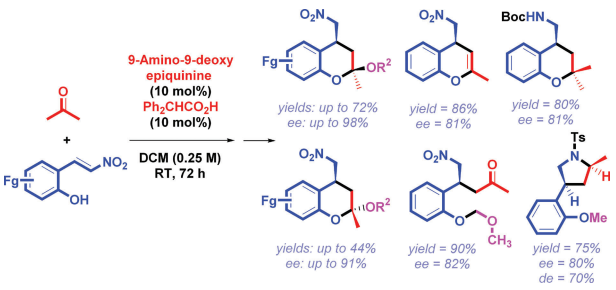


Diastereoselective hydrophosphonylation of imines using (*R*,*R*)-TADDOL phosphite. Asymmetric synthesis of α-aminophosphonic acid derivatives

Francisco Palacios,* Tomasz K. Olszewski and Javier Vicario

Efficient synthesis of α-aminophosphonic acids is achieved the key step being a diastereoselective hydrophosphonylation of *N*-diphenylphosphinyl imines using a chiral phosphonate derived from inexpensive natural tartaric acid.

4259



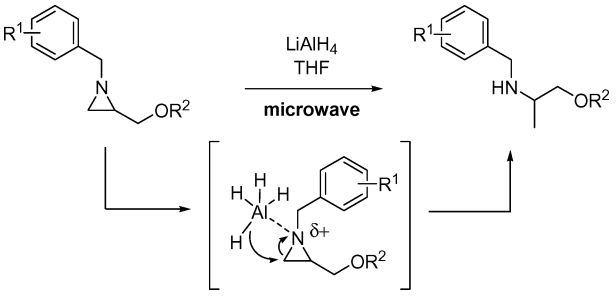
Sequential combination of Michael and acetalization reactions: direct catalytic asymmetric synthesis of functionalized 4-nitromethyl-chromans as drug intermediates

Dhevalapally B. Ramachary* and Rajasekar Sakthidevi

Functionalized chiral 4-nitromethyl-chromans as drug intermediates were achieved for the first time through sequential combination of Michael and acetalization reactions on 2-(2-nitro-vinyl)-phenols with acetone and alcohols under organocatalysis.

PAPERS

4266

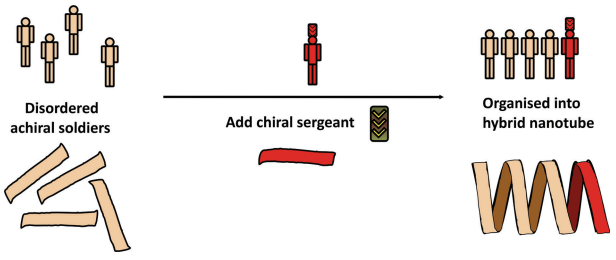


Microwave-assisted regioselective ring opening of non-activated aziridines by lithium aluminium hydride

Sonja Stanković, Matthias D'hooghe and Norbert De Kimpe*

A new protocol for the $LiAlH_4$-promoted regioselective ring opening of non-activated aziridines towards 2-aminopropanes under microwave irradiation was developed.

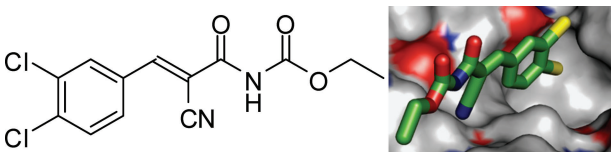
4274

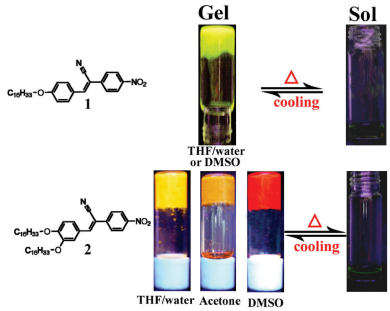


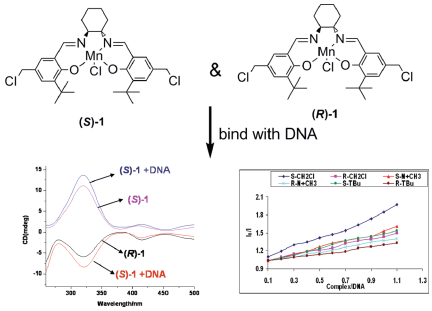
The sergeants-and-soldiers effect: chiral amplification in naphthalenediimide nanotubes

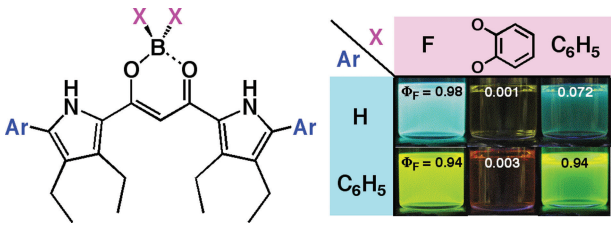
Tom W. Anderson, Jeremy K. M. Sanders and G. Dan Pantoş*

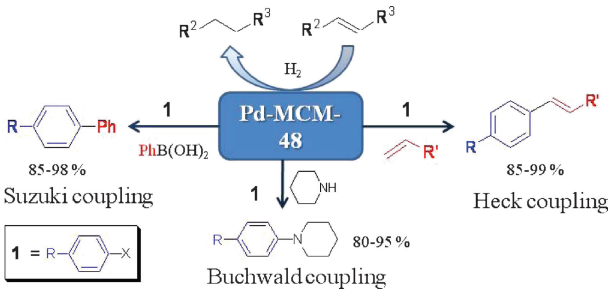
Self-assembling naphthalenediimide-based helical organic nanotubes display sergeants-and-soldiers behaviour, chiral monomers imposing a supramolecular structure upon achiral monomers. Nanotubes containing predominantly the most effective soldier are effective hosts for C_{60}.

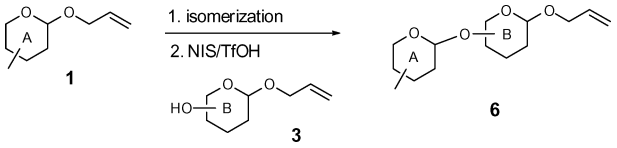


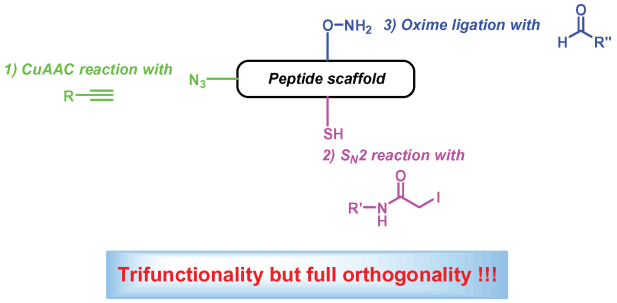


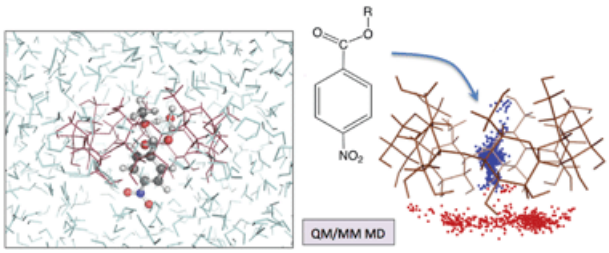


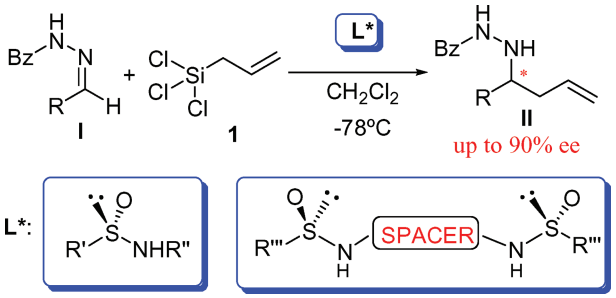


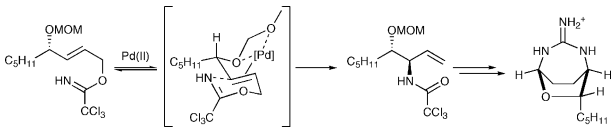


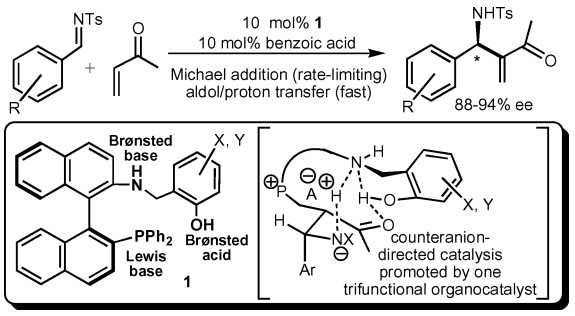


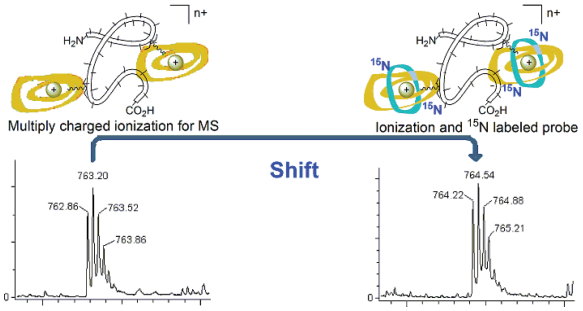


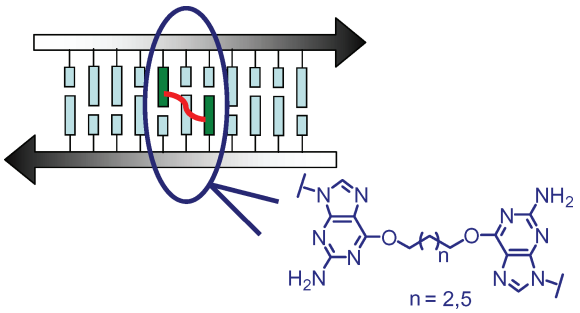


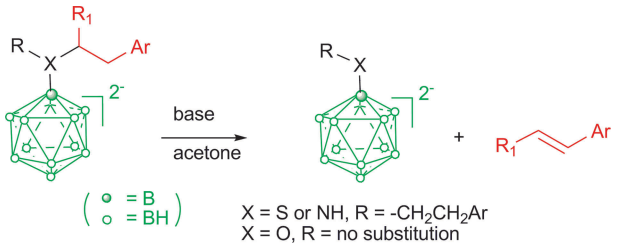


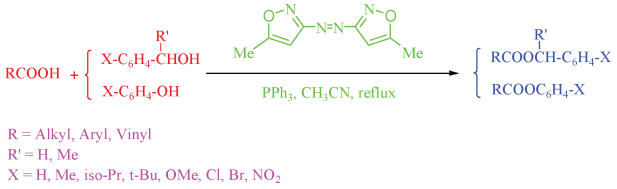


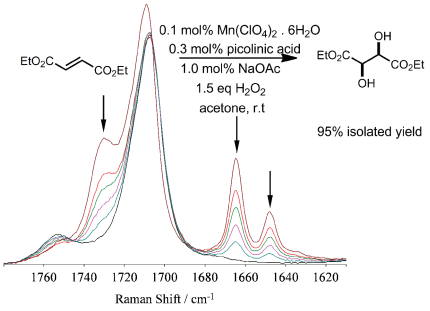




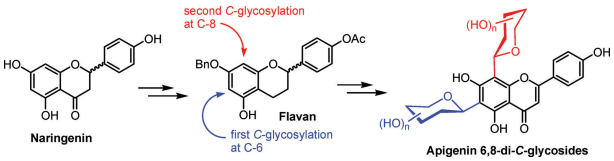








4451

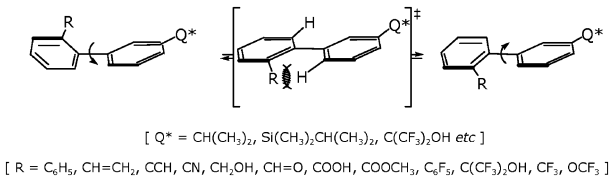


Regioselective synthesis of di-*C*-glycosylflavones possessing anti-inflammation activities

Jiun-Jie Shie, Chih-An Chen, Chih-Chien Lin, Angela Fay Ku, Ting-Jen R. Cheng, Jim-Min Fang* and Chi-Huey Wong*

A series of 6,8-di-*C*-glycosylflavones bearing identical or distinct glycosyl moieties are synthesized and shown to exhibit anti-inflammation activity.

4463

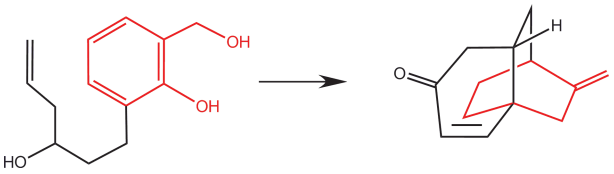


The biphenyl-monitored effective size of unsaturated functional or fluorinated *ortho* substituents

Renzo Ruzziconi,* Sara Spizzichino, Andrea Mazzanti,* Lodovico Lunazzi and Manfred Schlosser*

The effective size (*B* value) of a number of substituents has been probed by dynamic NMR measurements of the barriers to aryl–aryl rotation of the corresponding mono-*ortho* substituted biphenyls.

4472



Intramolecular cycloaddition in 6,6-spiroepoxycyclohexa-2,4-dienone: simple aromatics to (±)-Platencin

Vishwakarma Singh,* Bharat Chandra Sahu, Varsha Bansal and Shaikh M. Mobin

A formal synthesis of (±)-platencin from a simple aromatic precursor is reported. Oxidative dearomatization and intramolecular Diels–Alder reaction are the key features of the methodology.

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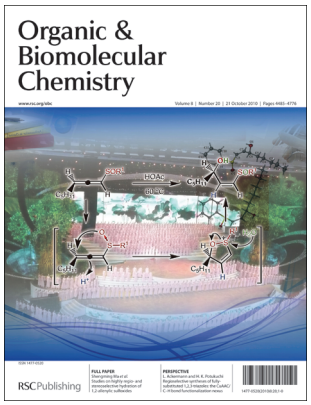
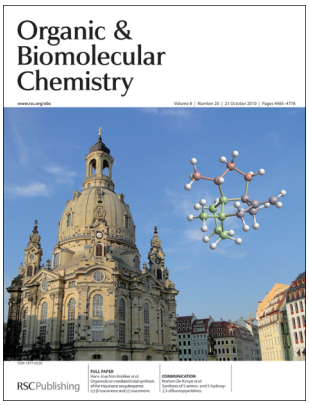
ISSN 1477-0520 CODEN OBCRAK 8(20) 4485–4776 (2010)



Cover
See Shengming Ma *et al.*, pp. 4554–4561.
1,2-Allenylic sulfoxides were hydrated *via* the five-membered intermediate with excellent regio- and stereoselectivity affording synthetically useful stereodefined 2-alkenols.

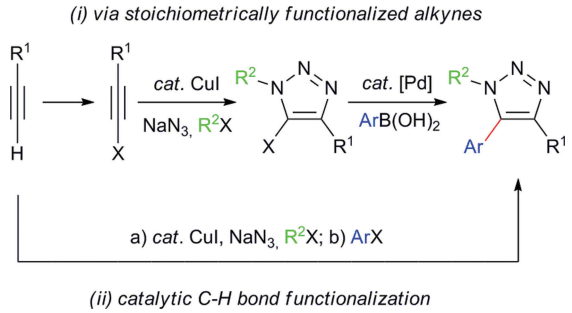
Image reproduced by permission of Shengming Ma from *Org. Biomol. Chem.*, 2010, **8**, 4554.



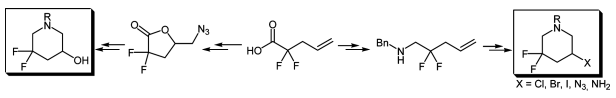
Inside cover
See Hans-Joachim Knölker *et al.*, pp. 4562–4568.
The element silicon is the connection between the Frauenkirche in Dresden, built of sandstone, and the triquinane framework of the natural product β-isocomene, constructed by a silicon-mediated cycloaddition.

Image reproduced by permission of Hans-Joachim Knölker from *Org. Biomol. Chem.*, 2010, **8**, 4562.

PERSPECTIVE



COMMUNICATIONS

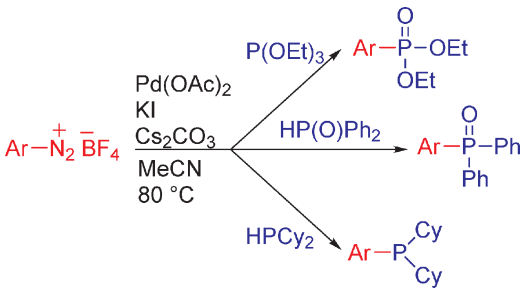


4518

Arenediazonium tetrafluoroborates in palladium-catalyzed C–P bond-forming reactions. Synthesis of arylphosphonates, -phosphine oxides, and -phosphines

Roberta Berrino, Sandro Cacchi,* Giancarlo Fabrizi, Antonella Goggiamani and Paolo Stabile

A palladium-catalyzed synthesis of aryl–P derivatives from arenediazonium tetrafluoroborates has been developed that can be performed as a one-pot process from anilines.

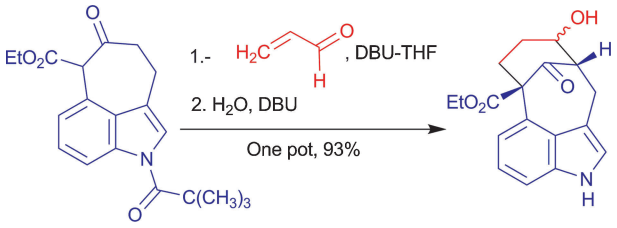


4521

Concise and very efficient synthesis of the *N*-methylwelwistatin tetracyclic core based on an anionic domino process

Miriam Ruiz, Pilar López-Alvarado and J. Carlos Menéndez*

An anionic domino reaction is used to create the tetracyclic core of the alkaloid *N*-methylwelwistatin from Kornfeld's ketone.

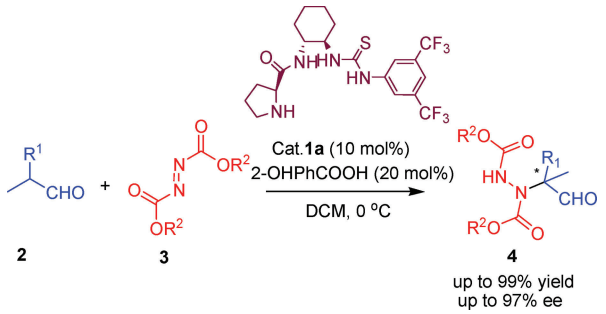


4524

Effective construction of quaternary stereocenters by highly enantioselective α-amination of branched aldehydes

Ji-Ya Fu, Xiao-Ying Xu, Yan-Chun Li, Qing-Chun Huang and Li-Xin Wang*

Chiral proline amide-thiourea bifunctional catalysts were successfully applied to the highly enantioselective amination of branched aldehydes with azadicarboxylates in excellent yields (up to 99%) and enantioselectivities (up to 97% ee).

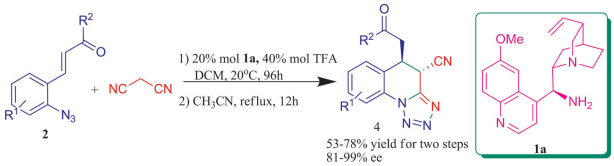


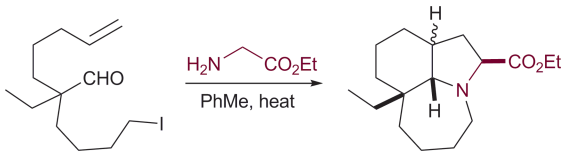
4527

The organocatalytic two-step synthesis of diversely functionalized tricyclic tetrazoles

Xiong Huang, Ping Li, Xin-Sheng Li, Dong-Cheng Xu and Jian-Wu Xie*

A simple method for the synthesis of diversely functionalized tricyclic tetrazoles from functionalized α,β-unsaturated ketones and malononitrile was described.

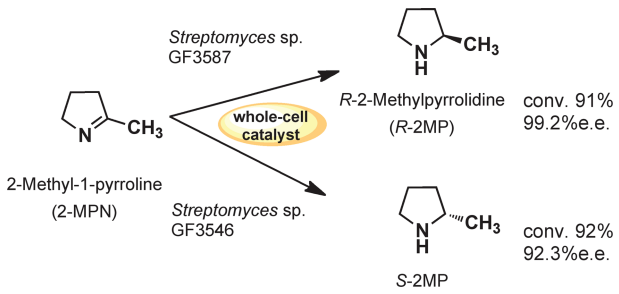




Synthesis of the core ring system of the stemona alkaloids by cascade condensation, cyclization, intramolecular cycloaddition

Adam. J. M. Burrell, Luke Watson, Nathaniel G. Martin, Niall Oram and Iain Coldham*

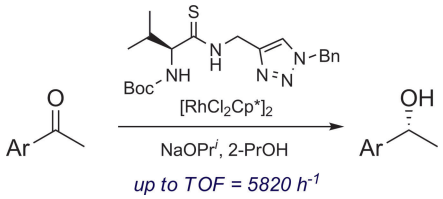
Heating amino-acids or amino-esters with 6-iodohexanals gives azomethine ylides that undergo intramolecular cycloaddition to the tricyclic core of stenine and neostenine



Asymmetric synthesis of chiral cyclic amine from cyclic imine by bacterial whole-cell catalyst of enantioselective imine reductase

Koichi Mitsukura,* Mai Suzuki, Kazuhiro Tada, Toyokazu Yoshida and Toru Nagasawa

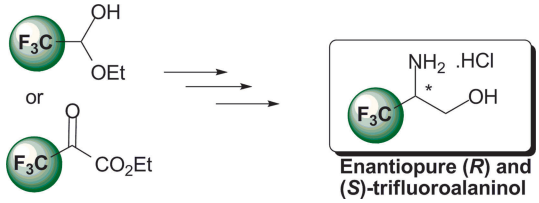
Streptomyces sp. GF3587 and 3546 were found to be imine-reducing strains with high *R*- and *S*-selectivity by screening using 2-methyl-1-pyrroline (2-MPN).



Asymmetric transfer hydrogenation of ketones catalyzed by rhodium complexes containing amino acid triazole ligands

Fredrik Tinnis and Hans Adolfsson*

Active and selective catalysts for the asymmetric reduction of ketones were obtained from $[RhCl_2Cp^*]_2$, and novel L-amino acid thioamide ligands functionalized with 1,2,3-triazoles.



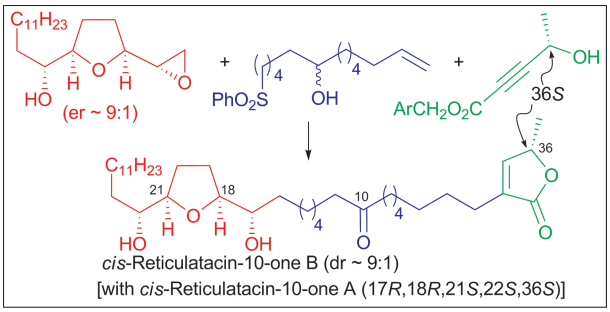
Straightforward synthesis of enantiopure (*R*)- and (*S*)-trifluoroalaninol

Julien Pytkowicz, Olivier Stéphany, Sinisa Marinkovic, Sébastien Inagaki and Thierry Brigaud*

Enantiopure (*R*)- and (*S*)-trifluoroalaninol were conveniently synthesized in a few steps from fluoral hemiacetal or ethyl trifluoropyruvate.

COMMUNICATIONS

4543



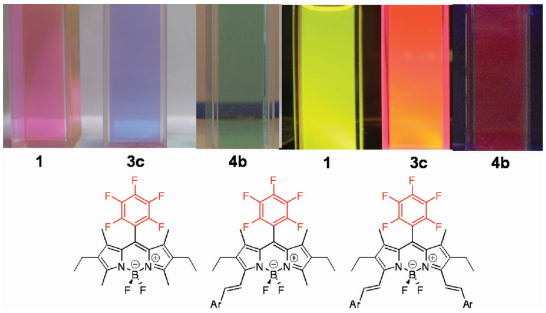
Total synthesis of *cis*-reticulatacin-10-ones A and B: absolute stereochemical assignment

Sherif B. Abdel Ghani, Lynda J. Brown, Bruno Figadère and Richard C. D. Brown*

The natural product *cis*-reticulaticin-10-one, isolated from *Annona muricata* L., was shown to be a mixture of A (17*R*,18*R*,21*S*,22*S*,36*S*) and B (17*S*,18*S*,21*R*,22*R*,36*S*) diastereoisomers by using chiral HPLC to compare the natural isolate with standards prepared by total synthesis.

PAPERS

4546

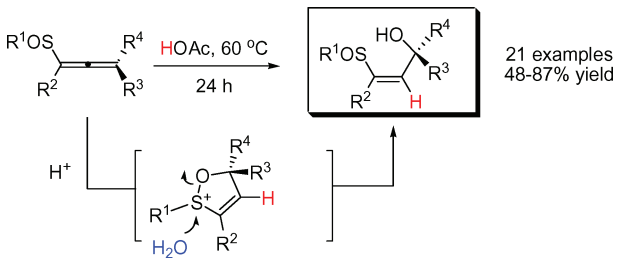


Rational design of visible and NIR distyryl-BODIPY dyes from a novel fluorinated platform

Olivier Galangau, Cécile Dumas-Verdes, Rachel Méallet-Renault and Gilles Clavier*

A new series of red emissive distyryl-BODIPY has been obtained from a novel fluorinated platform with various electron donor and, for the first time, electron acceptor aromatics.

4554

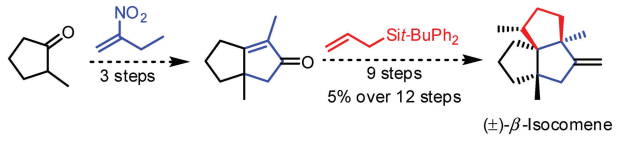


Studies on highly regio- and stereoselective hydration of 1,2-allenylic sulfoxides

Zhao Fang, Chao Zhou, Chunling Fu* and Shengming Ma*

A highly regio- and stereoselective hydration of 1,2-allenylic sulfoxides with proton as the electrophile affords 3-sulfoxyl-2(*Z*)-alkenols *via* a five-membered intermediate.

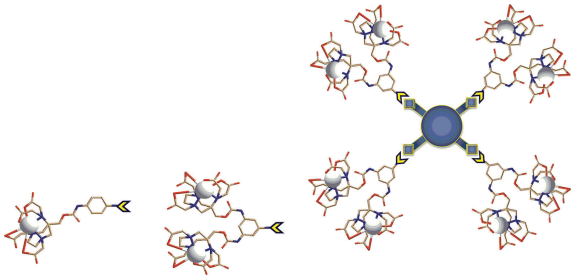
4562

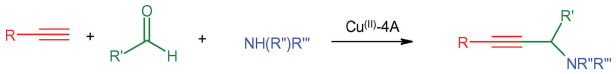


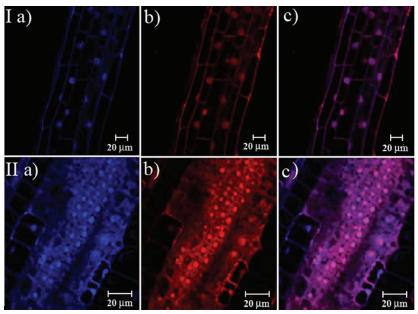
Organosilicon-mediated total synthesis of the triquinane sesquiterpenes (±)-*β*-isocomene and (±)-isocomene

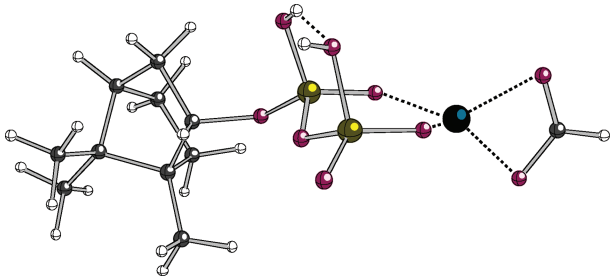
Arndt W. Schmidt, Thomas Olpp, Elke Baum, Tina Stiffel and Hans-Joachim Knölker*

We describe an efficient total synthesis of the sesquiterpenes (±)-*β*-isocomene and (±)-isocomene using a Lewis acid-promoted [3 + 2] cycloaddition of allyl-*tert*-butyldiphenylsilane as the key-step.







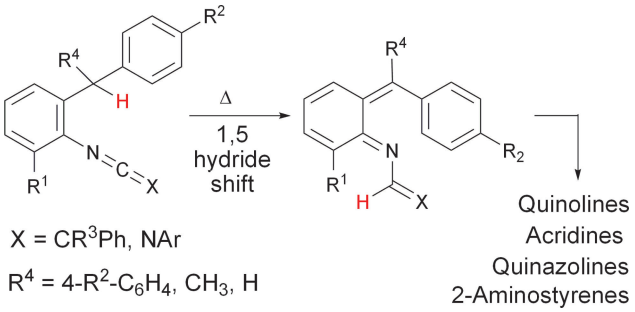


4690

Domino reactions initiated by intramolecular hydride transfers from tri(di)arylmethane fragments to ketenimine and carbodiimide functions

Mateo Alajarin,* Baltasar Bonillo, Maria-Mar Ortin, Pilar Sanchez-Andrada, Angel Vidal* and Raul-Angel Orenes

Ketenimines and carbodiimides bearing tri(di)arylmethane substructures experience tandem [1,5]-H (or Ar) shift/6π-ERC sequences. The H shifts are qualified as hydride transfers.

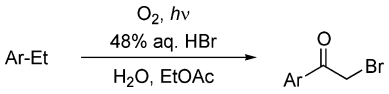


4701

Direct synthesis of α-bromoketones from alkylarenes by aerobic visible light photooxidation

Norihiro Tada, Kazunori Ban, Shin-ichi Hirashima, Tsuyoshi Miura and Akichika Itoh*

The direct synthesis of α-bromoketones from alkylarenes by aerobic photooxidation with hydrobromic acid is reported.

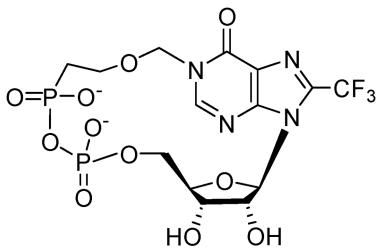


4705

Trifluoromethylated cyclic-ADP-ribose mimic: synthesis of 8-trifluoromethyl-N^1-[(5″-*O*-phosphorylethoxy)methyl]-5′-*O*-phosphorylinosine-5′,5″-cyclic pyrophosphate (8-CF_3-cIDPRE) and its calcium release activity in T cells

Min Dong, Tanja Kirchberger, Xiangchen Huang, Zhen Jun Yang, Liang Ren Zhang, Andreas H. Guse* and Li He Zhang*

A convenient reagent and protection strategy are reported for the synthesis of cell membrane-permeant trifluoromethylated cyclic-ADP-ribose agonist, 8-CF_3-cIDPRE **1**.



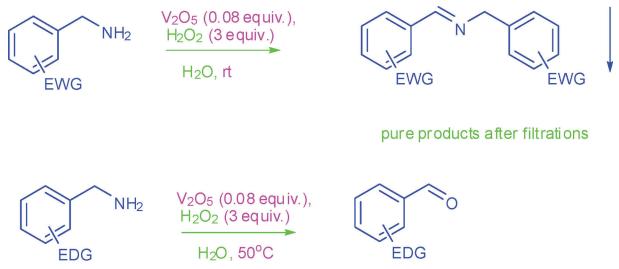
8-$CF_3$$^-$ cIDPRE 1

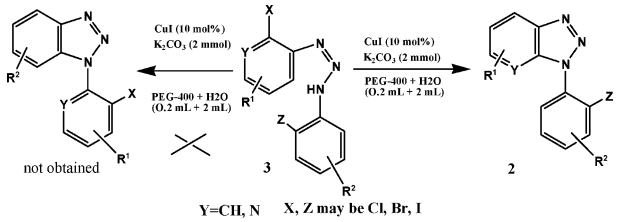
4716

Convenient and clean synthesis of imines from primary benzylamines

Guobiao Chu and Chunbao Li*

Clean oxidation of primary benzylamines has been successfully achieved, using H_2O_2 in water at room temperature catalyzed by V_2O_5. The products were obtained in good to quantitative yields.

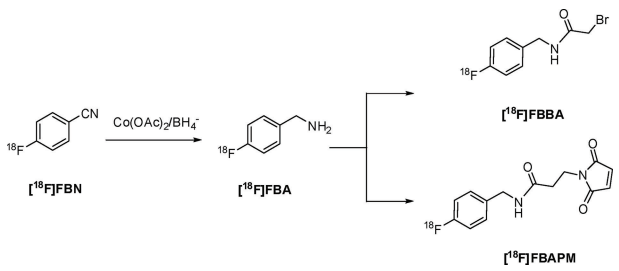




A ligand-free copper (1) catalysed intramolecular N-arylation of diazoaminobenzenes in PEG-water: an expeditious protocol towards regiospecific 1-aryl benzotriazoles

Chhanda Mukhopadhyay,* Pradip Kumar Tapaswi and Ray J. Butcher

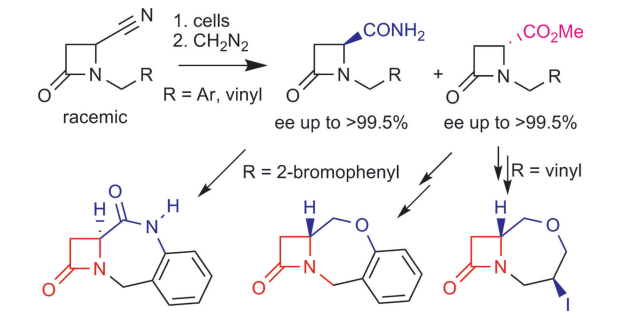
Regiospecific 1-aryl benzo and pyridotriazoles have been synthesized by the application of ligand-free copper(I) catalysed intramolecular N-arylation reaction.



Synthesis and application of 4-[^{18}F]fluorobenzylamine: A versatile building block for the preparation of PET radiotracers

Ingrid Koslowsky, John Mercer and Frank Wuest*

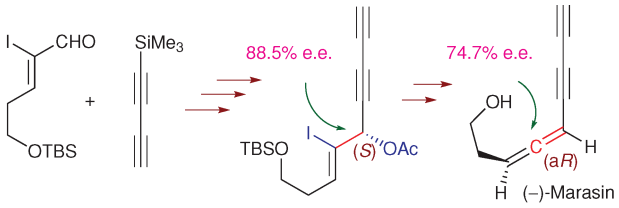
A novel synthesis of 4-[^{18}F]fluorobenzylamine ([^{18}F]FBA) by means of transition metal-assisted sodium borohydride reduction of 4-[^{18}F]fluorobenzonitrile ([^{18}F]FBN) is described.



Highly efficient and enantioselective biotransformations of β-lactam carbonitriles and carboxamides and their synthetic applications

Dong-Hui Leng, De-Xian Wang, Zhi-Tang Huang and Mei-Xiang Wang*

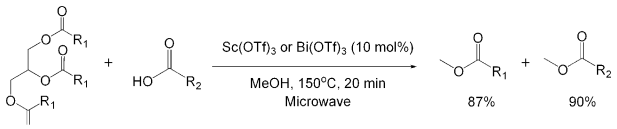
Biotransformations of nitriles and amides provide a highly efficient and enantioselective approach to enantioenriched β-lactam compounds, which are useful intermediates in the synthesis of fused heterocycles

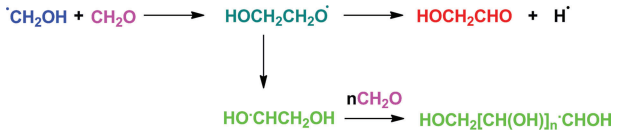


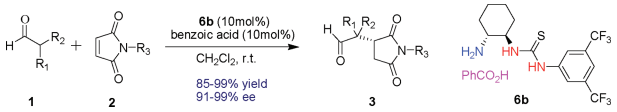
An enantioselective total synthesis of natural antibiotic marasin

Yan Zhang and Yikang Wu*

An enantioselective synthesis of the natural antibiotic marasin has been achieved, with the chiral allenic axis derived from a stereogenic center at the allylic position *via* an *i*-PrMgBr-mediated elimination reaction. Results of constructing the key chiral allene-diyne arrangement using different protocols are also reported.







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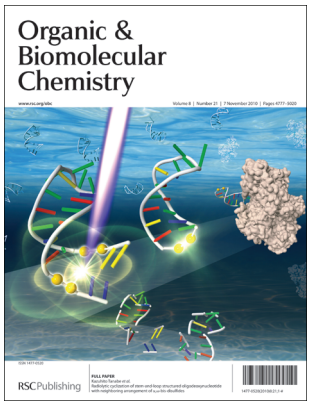

Cover
See Kazuhito Tanabe *et al.*, pp. 4837–4842.
X-Ray irradiation of an aqueous solution of modified oligodeoxynucleotides with a pair of disulfides at both ends causes efficient cyclization *via* an intramolecular exchange reaction.

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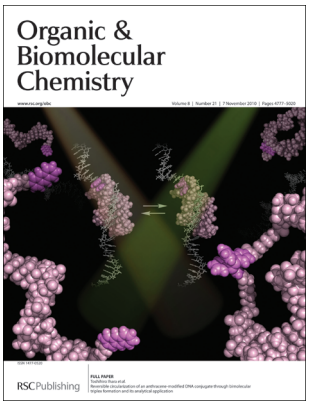

Inside cover
See Toshihiro Ihara *et al.*, pp. 4843–4848.
The oligonucleotide conjugate was reversibly circularized through photodimerization of the antracenes attached on both ends. This process would be potentially useful as a probe reaction with high specificity and sensitivity.

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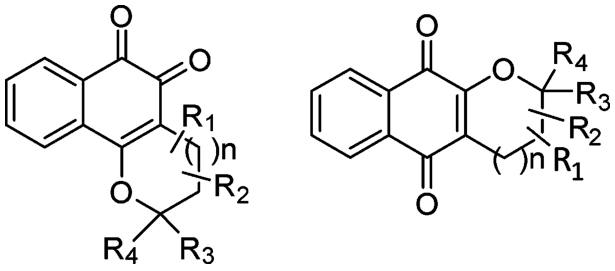
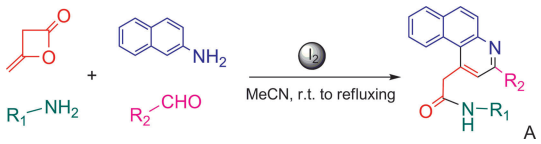
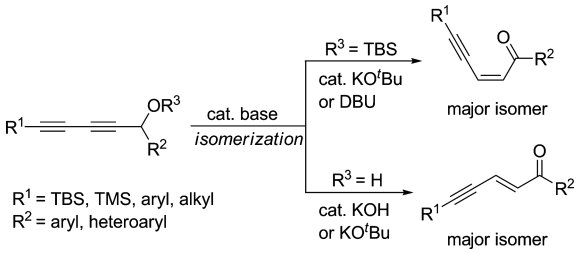
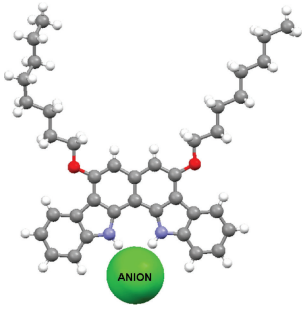
PERSPECTIVE

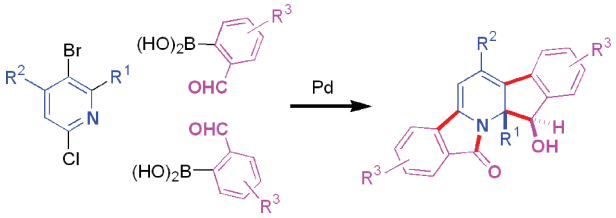


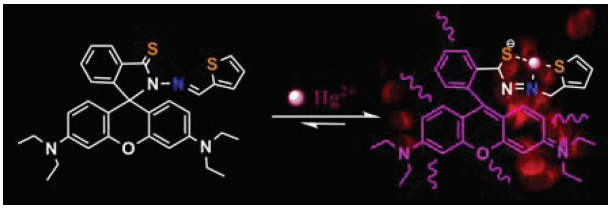
COMMUNICATIONS

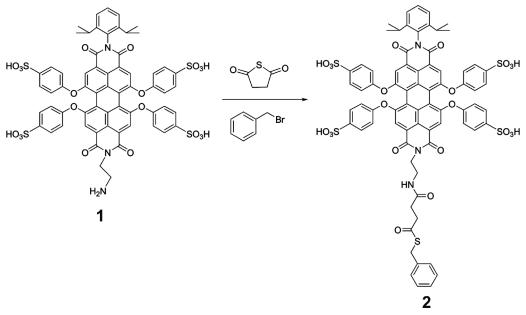








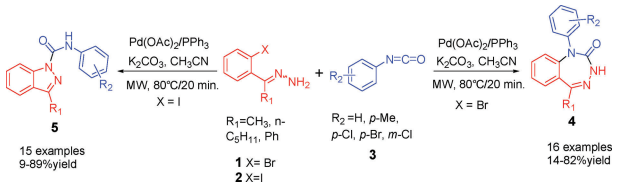




Site-specific incorporation of perylene into an N-terminally modified light-harvesting complex II

Kalina Peneva, Kristina Gundlach, Andreas Herrmann, Harald Paulsen and Klaus Müllen*

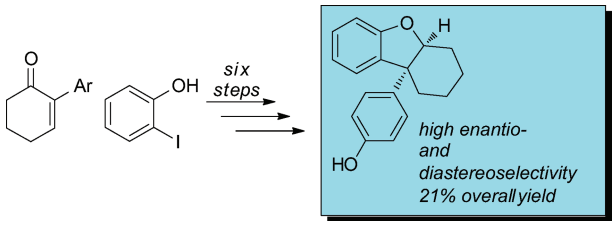
Employing the utility of the native chemical ligation, site-specific attachment of an ultrastable perylene dye to a derivative of the major light-harvesting complex (LHCII) was demonstrated.



Facile synthesis of 1,3,4-benzotriazepines and 1-arylamide-1*H*-indazoles *via* palladium-catalyzed cyclization of aryl isocyanates and aryl hydrazones under microwave irradiation

Chune Dong,* Lingli Xie, Xiaohong Mou, Yashan Zhong and Wei Su

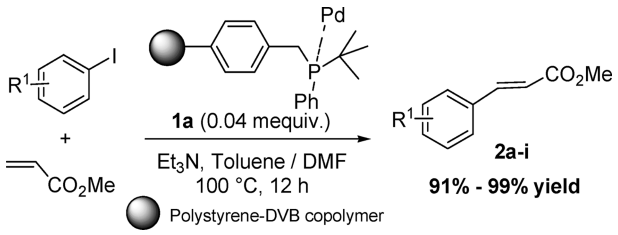
A strategy involving palladium-catalyzed cyclization of halophenyl hydrazones and aryl isocyanates provides convenient synthesis of 1,3,4-benzotriazepines (**4**) or 1-arylamide-1*H*-indazoles (**5**) in one step under microwave irradiation.



Asymmetric synthesis of a tricyclic benzofuran motif: a privileged core structure in biologically active molecules

Henrik Sundén and Roger Olsson*

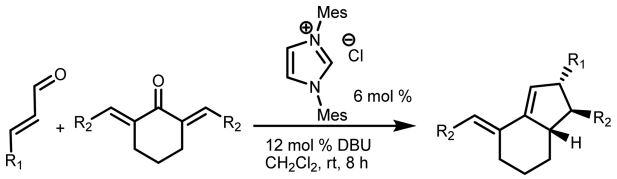
An efficient synthetic strategy for the asymmetric synthesis of a hexahydrodibenzofuran core structure, with a quaternary stereogenic center.

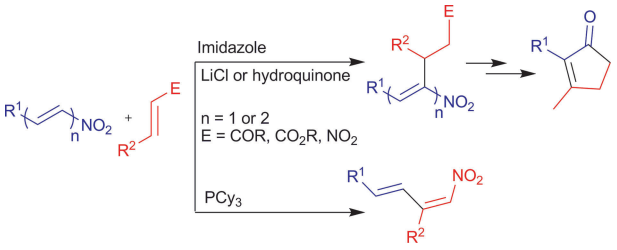


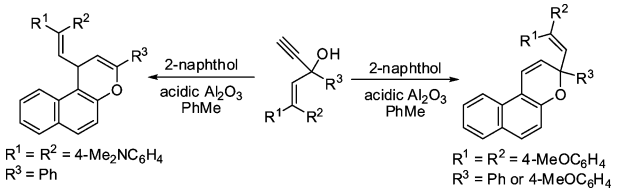
Reusable polystyrene-supported Pd catalyst for Mizoroki–Heck reactions with extremely low amounts of supported Pd

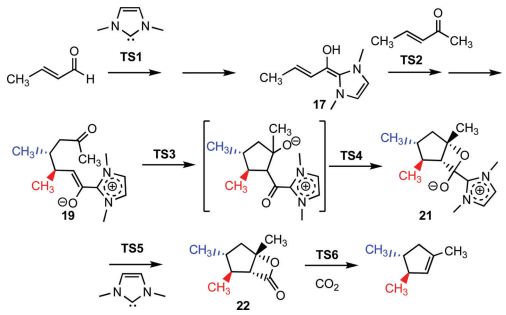
Carine Diebold, Stéphane Schweizer, Jean-Michel Becht* and Claude Le Drian*

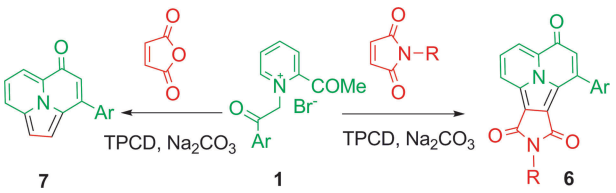
Heck reactions of aryl iodides using extremely low amounts of supported Pd (0.04 mequiv.) are reported. The catalyst can be reused successfully up to three times.







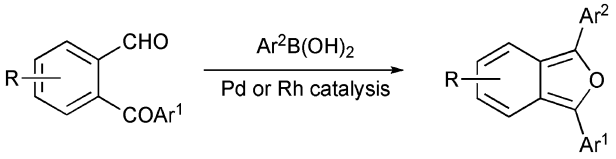




Synthesis of 1,2-annulated and 1,2-unsubstituted pyrrolo[2,1,5-*de*]quinolizin-5-ones (cycl[3.3.2]azin-5-ones) *via* [3+2] cycloadditions of 1-oxoquinolizinium ylides with cyclic alkenes

Yun Liu, Hua-You Hu, Yan Zhang, Hong-Wen Hu and Jian-Hua Xu*

1,2-Annulated and 1,2-unsubstituted pyrrolo[2,1,5-*de*]quinolizin-5-ones have been synthesized by one pot tandem reactions of 2-acetyl-*N*-phenacylpyridinium bromides with electron-deficient cyclic alkenes.



Regiospecific synthesis of functionalised 1,3-diarylisobenzofurans *via* palladium- and rhodium-catalysed reaction of boronic acids with *o*-acylbenzaldehydes under thermal or microwave activation

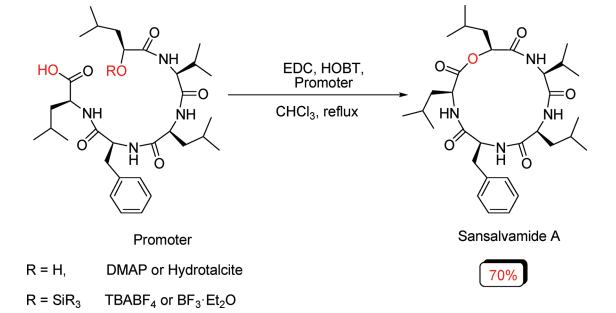
Jérôme Jacq, Bernard Bessières, Cathy Einhorn and Jacques Einhorn*

Variously substituted 1,3-diarylisobenzofurans have been regiospecifically prepared *via* palladium- and rhodium-catalysed reaction of functionalised boronic acids onto *o*-acylbenzaldehydes, using classical or microwave heating.

Radical formation of amino acid precursors in interstellar regions? Ser, Cys and Asp

Daniel J. Knowles, Tianfang Wang and John H. Bowie*

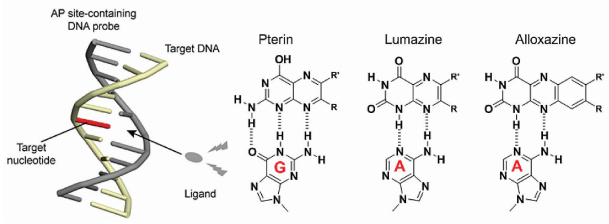
Theoretical calculations indicate that favourable reactions between $NH_2^{\bullet}CHCN$ and $R^{\bullet}$ (R = CH_2OH, CH_2SH and CH_2CN) should produce the Ser, Cys and Asp precursors $NH_2CH(R)CN$

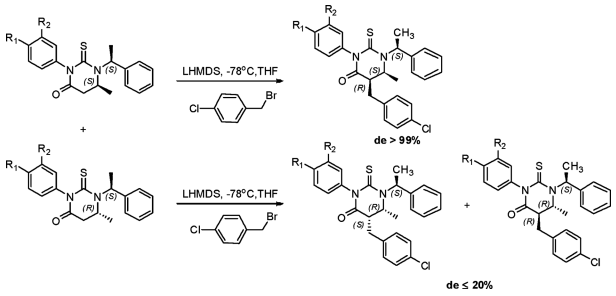


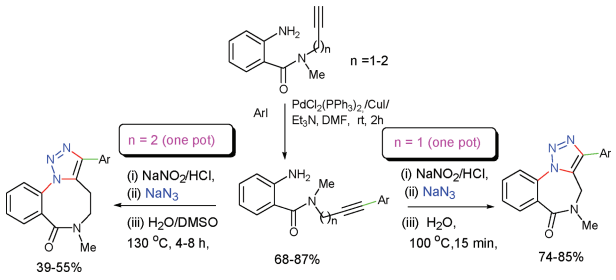
Highly efficient macrolactonization of ω-hydroxy acids using benzotriazole esters: synthesis of Sansalvamide A

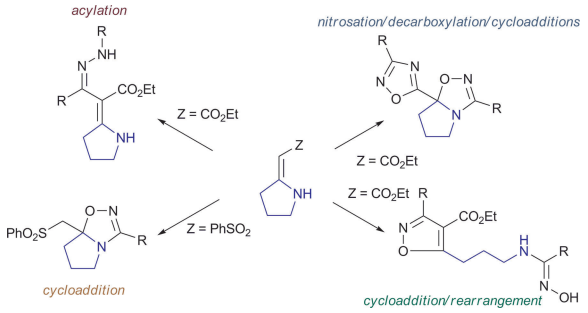
José Antonio Morales-Serna, Ericka Sánchez, Ricardo Velázquez, Jorge Bernal, Eréndira García-Ríos, Rubén Gaviño, Guillermo Negrón-Silva and Jorge Cárdenas*

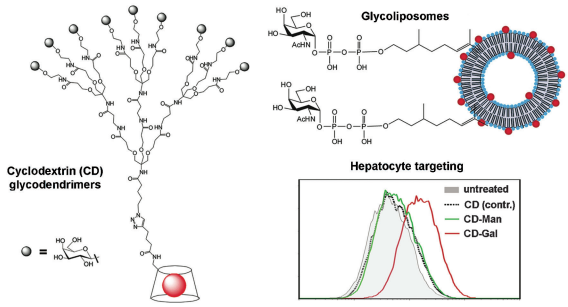
A facile and mild macrolactonization reaction of ω-hydroxy acids in the presence of EDC/HOBT was developed. The reactions were performed under basic, neutral and acidic conditions.

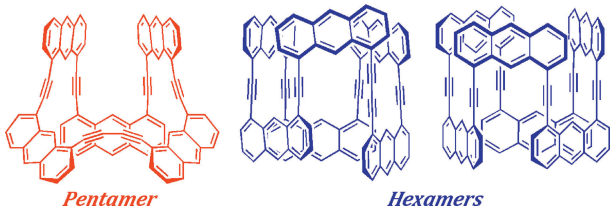


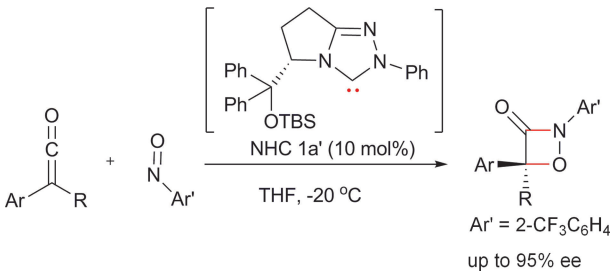


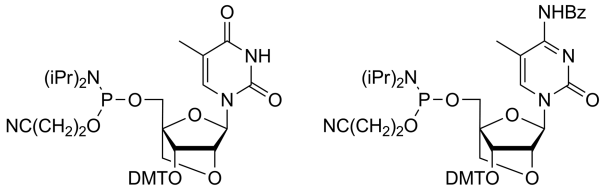












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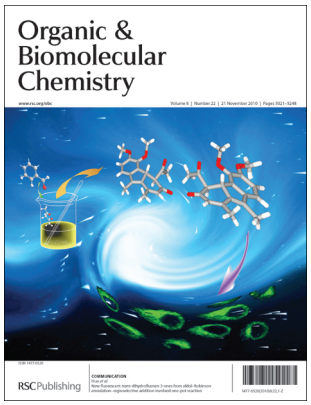

Cover

See Xianzhang Bu *et al.*, pp. 5048–5052.

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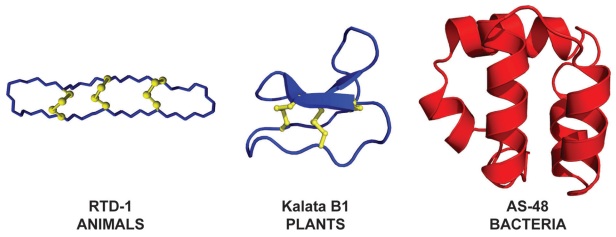
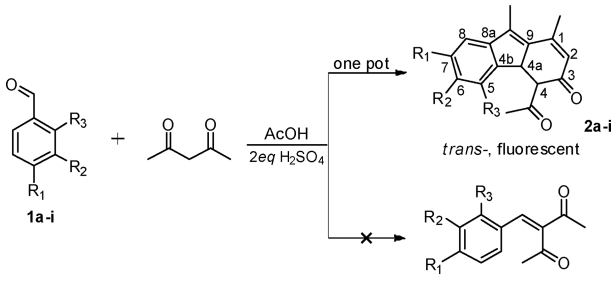
PERSPECTIVE



COMMUNICATIONS

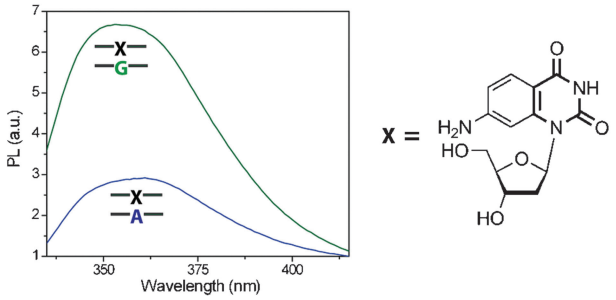


5053

Fluorescent nucleoside analogue displays enhanced emission upon pairing with guanine

Yun Xie, Tucker Maxson and Yitzhak Tor*

A fluorescent nucleobase analogue, 7-aminoquinazoline-2,4-(1*H*,3*H*)-dione, is incorporated into a DNA oligonucleotide and senses mismatched pairing by displaying G-specific fluorescence enhancement.

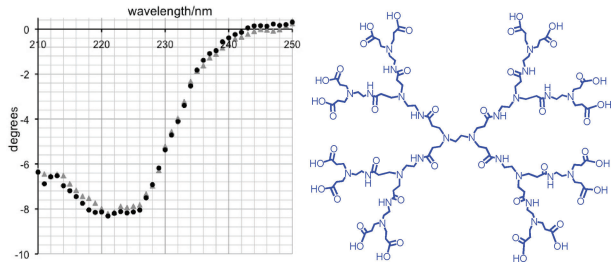


5056

Investigating possible changes in protein structure during dendrimer–protein binding

F. Chiba, G. Mann and L. J. Twyman*

The mechanism of dendrimer–protein binding is probed using CD spectroscopy. The results demonstrated that dendrimer/protein binding was *not* accompanied by changes in the protein's structure.

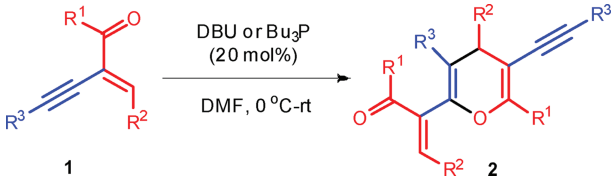


5059

Organocatalytic hetero [4+2] cycloaddition reactions of 2-(1-alkynyl)-2-alkene-1-ones: metal-free access to highly substituted 4*H*-pyrans

Xiuzhao Yu, Zhongyan Cao and Junliang Zhang*

Highly substituted 4*H*-pyrans can be smoothly synthesized from readily available 2-(1-alkynyl)-2-alkene-1-ones by an unexpected DBU or Bu_3P-catalyzed hetero-[4+2] cycloaddition reaction, in which the enone moieties act as the heterodienes and the electron-deficient alkyne moieties act as the heterodienophiles.

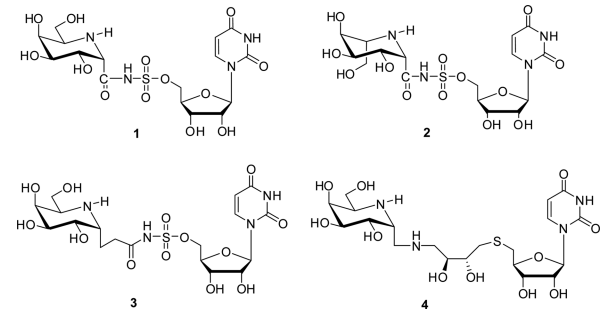


5062

Concise syntheses of selective inhibitors against α-1,3-galactosyltransferase

Guo-Liang Zhang, Li-He Zhang and Xin-Shan Ye*

Selective inhibitors of iminosugar-based UDP-Gal mimetics against α-1,3-galactosyltransferase were designed and synthesized.

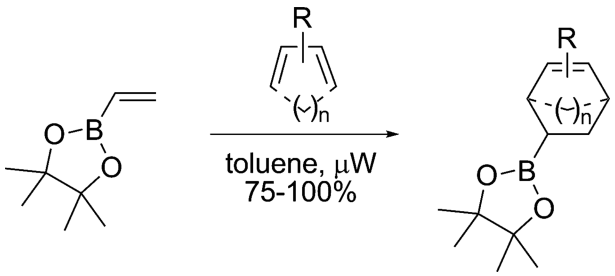


5069

A facile microwave-assisted Diels–Alder reaction of vinylboronates

Ariel M. Sarotti, Pablo L. Pisano and Silvina C. Pellegrinet*

This is the first example of microwave-assisted Diels–Alder reaction of boron-substituted dienophiles. Subsequent *in situ* oxidation of the cycloadducts with alkaline hydrogen peroxide afforded the alcohols efficiently.

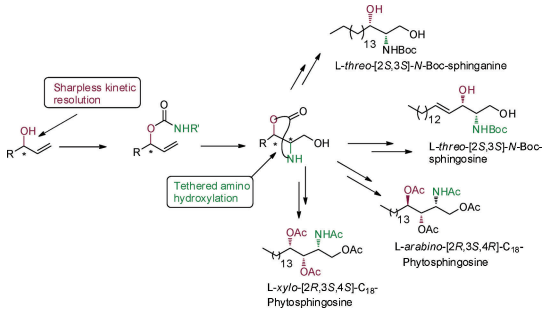


5074

A general and concise asymmetric synthesis of sphingosine, safingol and phytosphingosines *via* tethered aminohydroxylation

Pradeep Kumar,* Abhishek Dubey and Vedavati G. Puranik

A novel, practical and efficient enantioselective synthesis of sphingoid bases, L-*threo*-[2*S*,3*S*]-sphinganine (safingol), L-*threo*-[2*S*,3*S*]-sphingosine, L-*arabino*-[2*R*,3*S*,4*R*] and L-*xylo*-[2*R*,3*S*,4*S*]-C_{18}-phytosphingosine is described. The synthetic strategy features the Sharpless kinetic resolution and tethered aminohydroxylation as the key steps.

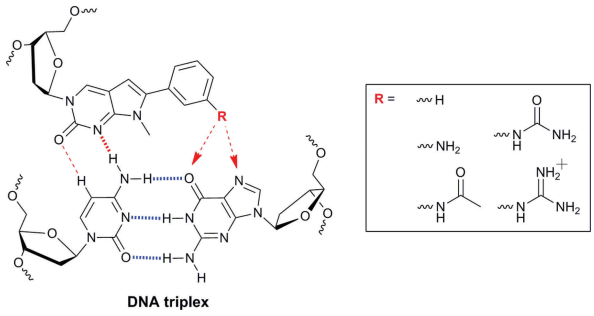


5087

CG base pair recognition within DNA triple helices by modified *N*-methylpyrrolo-dC nucleosides

Simon R. Gerrard, Mastoura M. Edrees, Imenne Bouamaied, Keith R. Fox and Tom Brown*

Enhanced triplex-mediated recognition of the CG base pair in DNA with new analogues of the non-natural bicyclic nucleoside, *N*-methylpyrrolo-dC.

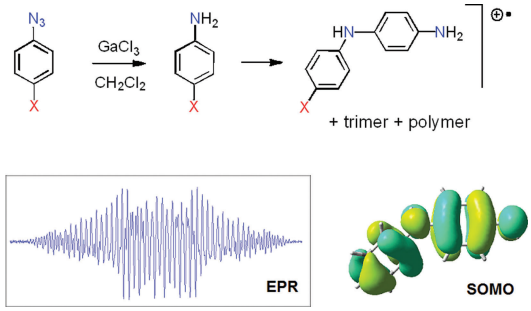


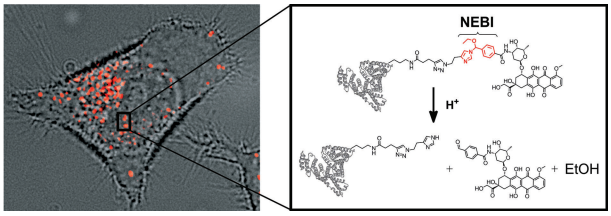
5097

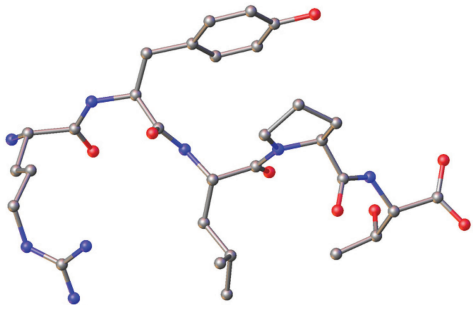
EPR and ENDOR spectroscopic study of the reactions of aromatic azides with gallium trichloride

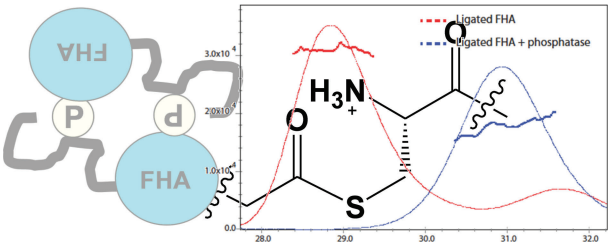
Giorgio Bencivenni, Riccardo Cesari, Daniele Nanni, Hassane El Mkami and John C. Walton*

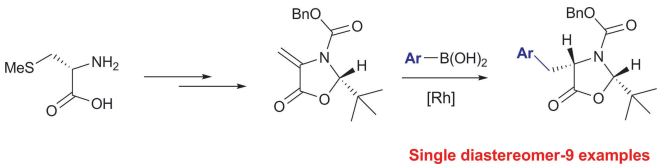
Brilliant blue-green species from $GaCl_3$ promoted reactions of aromatic azides were studied by product analysis, EPR and ENDOR spectroscopy.

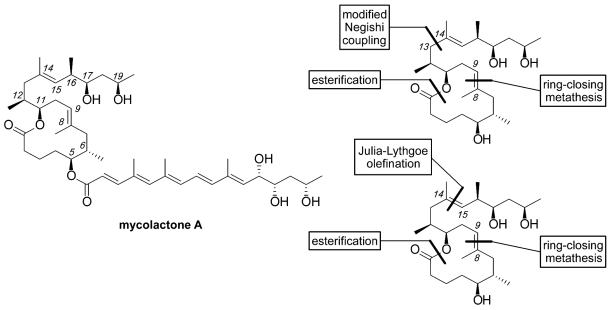


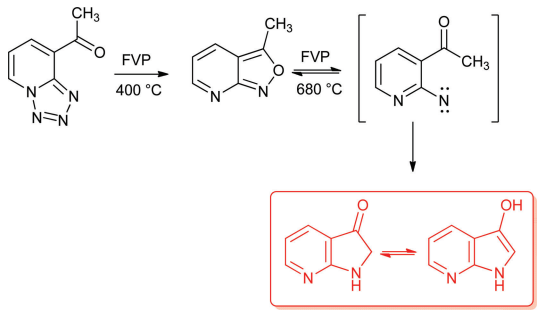


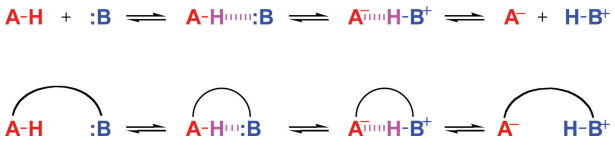


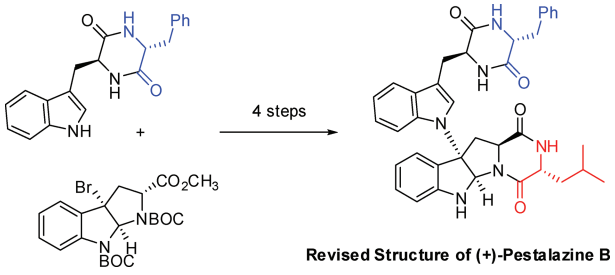




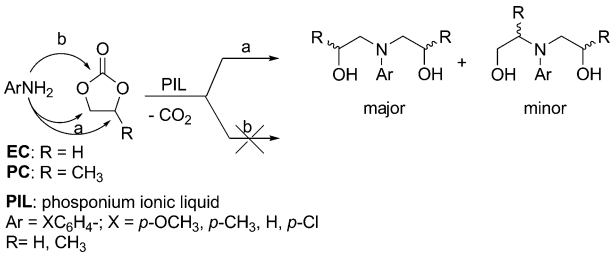








5187

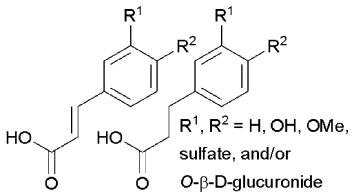


The reaction of primary aromatic amines with alkylene carbonates for the selective synthesis of bis-*N*-(2-hydroxy)alkylanilines: the catalytic effect of phosphonium-based ionic liquids

Maurizio Selva,* Massimo Fabris, Vittorio Lucchini, Alvise Perosa and Marco Noè

Phosphonium-based Ionic Liquids (PILs) efficiently catalyzed the reaction of primary aromatic amines with alkylene carbonates to produce bis-*N*-(2-hydroxy)alkylanilines.

5199



First synthesis, characterization, and evidence for the presence of hydroxycinnamic acid sulfate and glucuronide conjugates in human biological fluids as a result of coffee consumption

R. Fumeaux, C. Menozzi-Smarrito, A. Stalmach, C. Munari, K. Kraehenbuehl, H. Steiling, A. Crozier, G. Williamson and D. Barron*

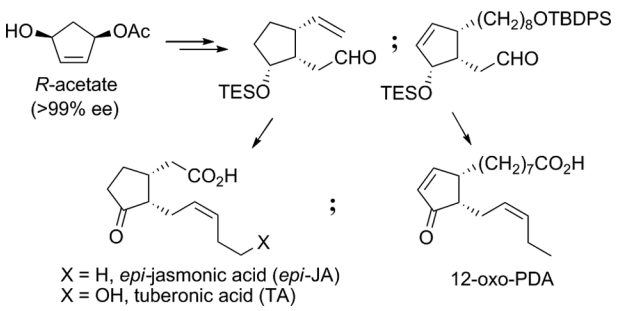
A set of 24 potential human metabolites of coffee polyphenols has been chemically prepared and used as analytical standards for unequivocal identifications in human biological fluids. The analytical standards included glucuronide conjugates and sulfate esters of caffeic, ferulic, isoferulic, *m*-coumaric and *p*-coumaric acids as well as their dihydro derivatives.

5212

Stereoselective synthesis of *epi*-jasmonic acid, tuberonic acid, and 12-oxo-PDA

Hisato Nonaka, Narihito Ogawa, Noriaki Maeda, Yong-Gang Wang and Yuichi Kobayashi*

The above aldehydes were designed as non-enolizable key intermediates for stereoselective synthesis of the title compounds.

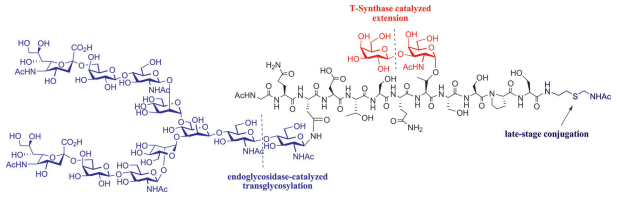


5224

Expeditious chemoenzymatic synthesis of CD52 glycopeptide antigens

Wei Huang, Xinyu Zhang, Tongzhong Ju, Richard D. Cummings and Lai-Xi Wang*

Facile synthesis of CD52 glycoforms carrying both N- and O-glycans was achieved by a convergent chemoenzymatic approach.

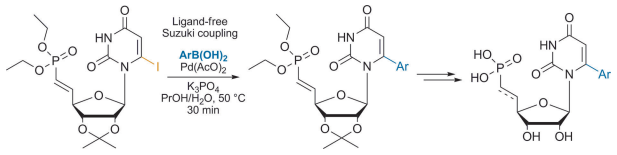


5234

Synthesis of C-6-substituted uridine phosphonates through aerobic ligand-free Suzuki–Miyaura cross-coupling

Radim Nencka, Davy Sinnaeve, Izet Karalic, José C. Martins and Serge Van Calenbergh*

We present an efficient protocol for the construction of C-6-(hetero)aryl-substituted uridine phosphonate analogues utilizing an aerobic, ligand-free Suzuki–Miyaura cross-coupling.



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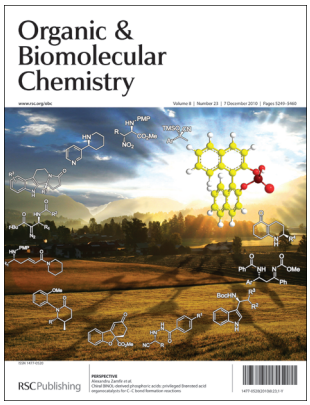
ISSN 1477-0520 CODEN OBCRAK 8(23) 5249–5460 (2010)



Cover

See Alexandru Zamfir *et al.*, pp. 5262–5276.

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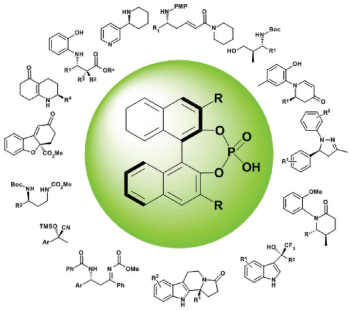
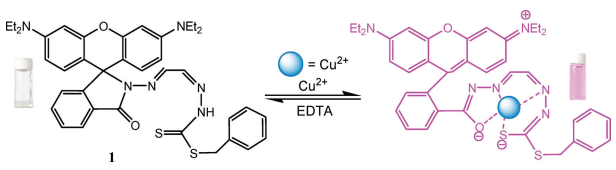
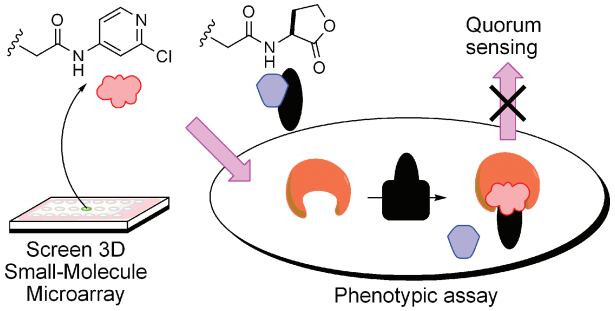
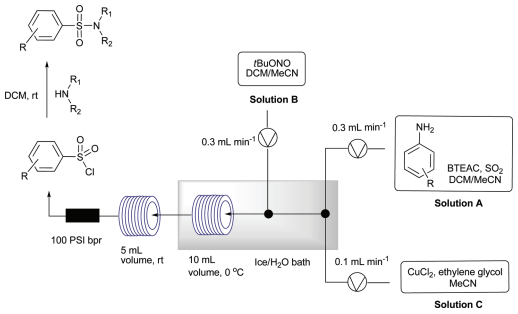
PERSPECTIVE

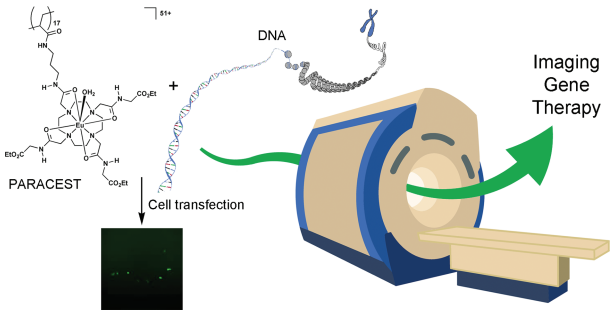


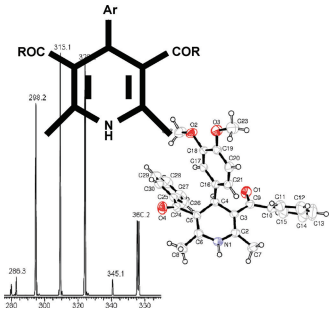
COMMUNICATIONS

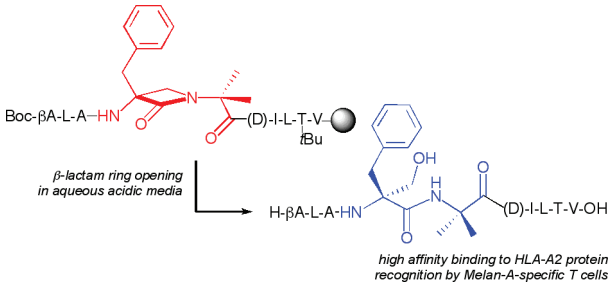








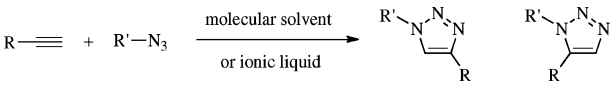




Design, synthesis and evaluation of β-lactam antigenic peptide hybrids; unusual opening of the β-lactam ring in acidic media

M. Tarbe, I. Azcune, E. Balentová, J. J. Miles, E. E. Edwards, K. M. Miles, P. Do, B. M. Baker, A. K. Sewell, J. M. Aizpurua, C. Douat-Casassus* and S. Quideau*

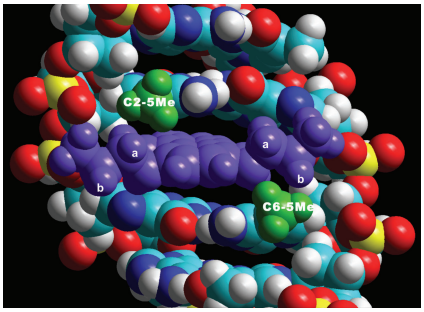
An unusual β-lactam ring opening occurred during aqueous TFA-mediated release of β-lactam–peptide hybrids from solid support, leading to the formation of a pseudopeptide that expresses a high HLA-A2 binding affinity and stimulates Melan-A-specific T cells.



The effects of ionic liquids on azide-alkyne cycloaddition reactions

Stephen R. D. George, Gavin L. Edwards and Jason B. Harper*

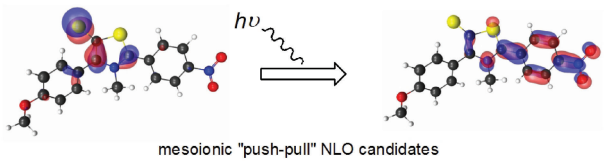
Ionic liquids increase the regioselectivity whilst effects on activation parameters are intermediate between coordinating and non-coordinating salts. The presence of small amounts of water grossly affects activation parameters.



DNA binding by pixantrone

Najia Adnan, Damian P. Buck, Benny J. Evison, Suzanne M. Cutts,* Don R. Phillips and J. Grant Collins*

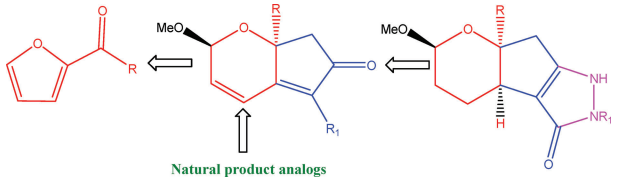
The anticancer drug pixantrone intercalates at the 5′-^{5Me}CpG sites of the octanucleotide d(A^{5Me}CGAT^{5Me}CGT)$_2$ from the major groove, with the methyl groups not presenting a steric barrier to intercalation.

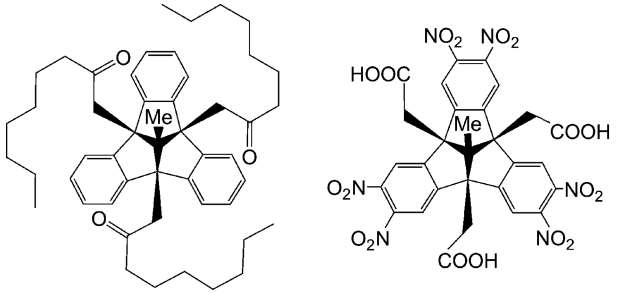


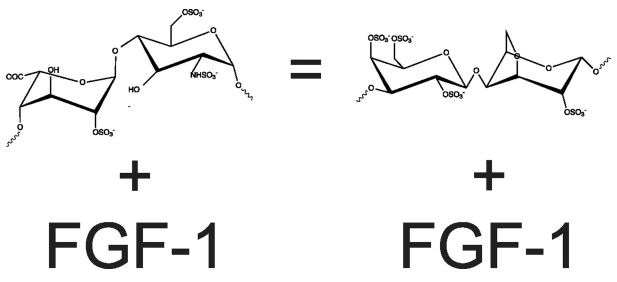
Push-pull 1,3-thiazolium-5-thiolates. Formation *via* concerted and stepwise pathways, and theoretical evaluation of NLO properties

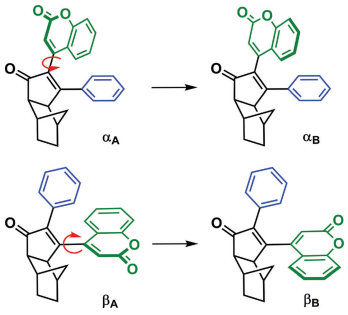
David Cantillo,* Martín Ávalos, Reyes Babiano, Pedro Cintas, José L. Jiménez, Mark E. Light, Juan C. Palacios and Valentín Rodríguez

Mesoionic rings possessing a 1,3-thiazolium-5-thiolate unit show promising perspectives in non-linear optics. Full synthetic studies combined with DFT calculations also provide a plausible mechanistic picture.







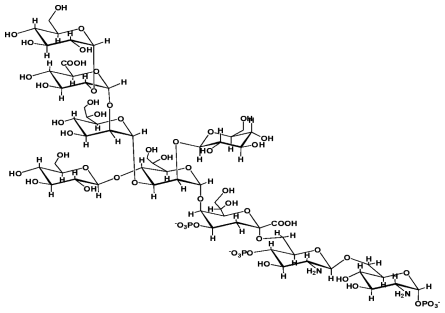


5404

Structural characterization of the core region from the lipopolysaccharide of the haloalkaliphilic bacterium *Halomonas alkaliantarctica* strain CRSS

Giuseppina Pieretti, Sara Carillo, Barbara Nicolaus, Annarita Poli, Rosa Lanzetta, Michelangelo Parrilli and Maria Michela Corsaro*

We described the core oligosaccharide structure from the LPS of the haloalkaliphile *Halomonas alkaliantarctica*, obtained after alkaline hydrolysis of the LPS, HPAEC purification, NMR spectroscopy and mass spectrometry analysis.

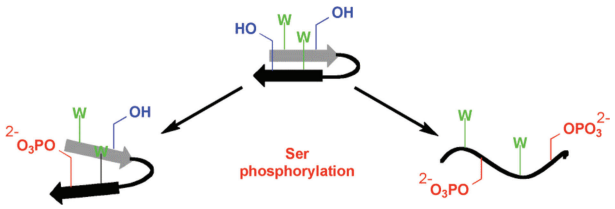


5411

Positional effects of phosphoserine on β-hairpin stability

Alexander J. Riemen and Marcey L. Waters*

Phosphorylation of a β-hairpin demonstrates the ability of this covalent modification to alter structure in a position-dependent manner, providing insight potential mechanisms by which protein phosphorylation influences structure and function.

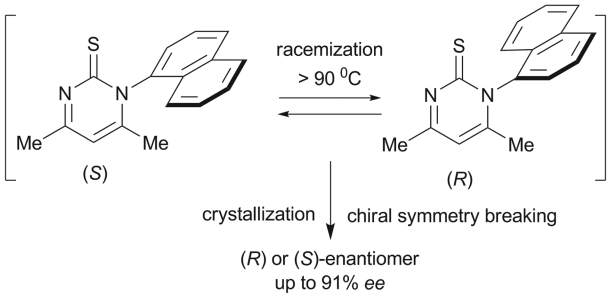


5418

Generation and amplification of optical activity of axially chiral *N*-(1-naphthyl)-2(*1H*)-pyrimidinethione by crystallization

Masami Sakamoto,* Fumitoshi Yagishita, Masaru Ando, Yuich Sasahara, Norifumi Kamataki, Mai Ohta, Takashi Mino, Yoshio Kasashima and Tsutomu Fujita

The crystallization of racemic axially chiral pyrimidinethione at high temperature led to the chiral breaking of symmetry up to 91% ee.

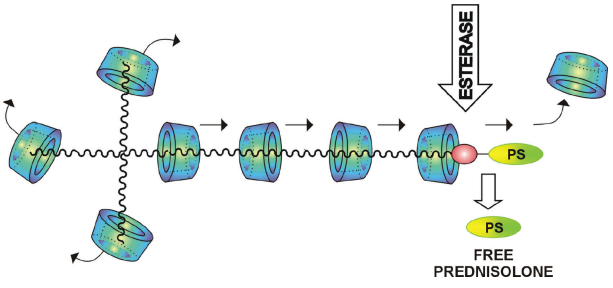


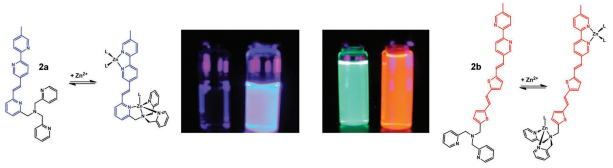
5423

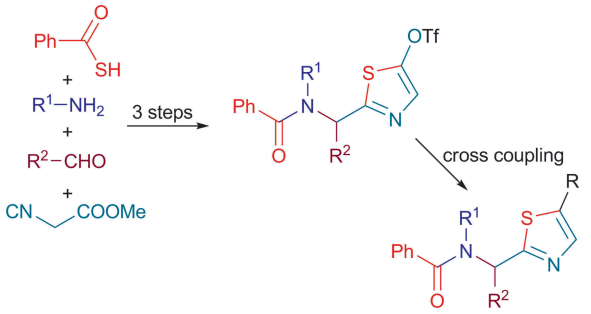
Prednisolone-α-cyclodextrin-star PEG polypseudorotaxanes with controlled drug delivery properties

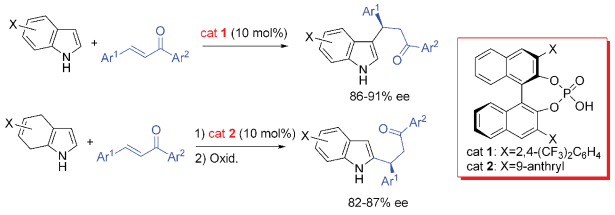
Eliška Bílková, Miloš Sedlák,* Bohuslav Dvořák, Karel Ventura, Petr Knotek and Ludvík Beneš

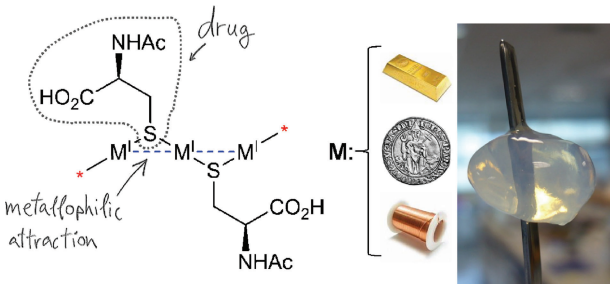
The synthesized polypseudorotaxanes were characterized by 2D NOESY NMR spectra, powder X-ray diffraction patterns, and STM. The rate of release of prednisolone from the carrier can be controlled by: character of the linker between polymeric carrier and prednisolone, molecular mass of PEG, and the kinetics of the dethreading of α-CD units.











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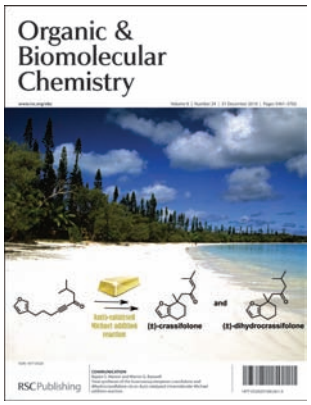

Cover
See Rajeev S. Menon and Martin G. Banwell, pp. 5483–5485.

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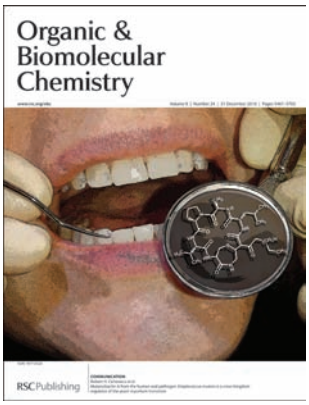

Inside cover
See Robert H. Cichewicz *et al.*, pp. 5486–5489.

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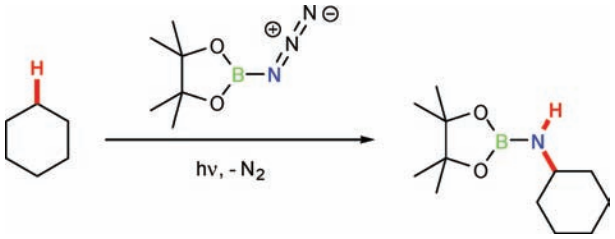
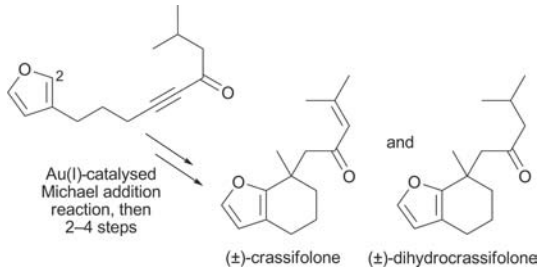
EMERGING AREA



COMMUNICATIONS



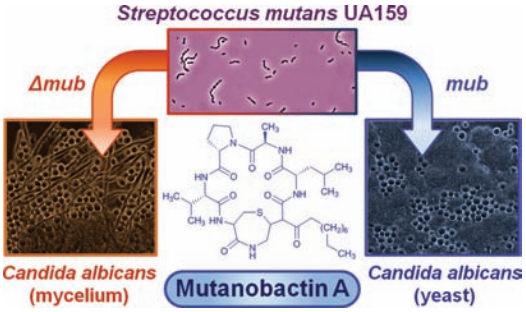
COMMUNICATIONS

5486

Mutanobactin A from the human oral pathogen *Streptococcus mutans* is a cross-kingdom regulator of the yeast-mycelium transition

P. Matthew Joyner, Jinman Liu, Zhijun Zhang, Justin Merritt, Fengxia Qi and Robert H. Cichewicz*

Mutanobactin A from *Streptococcus mutans* enables intracellular stress response pathways, as well as directs inter-kingdom interactions with eukaryotic microbes.

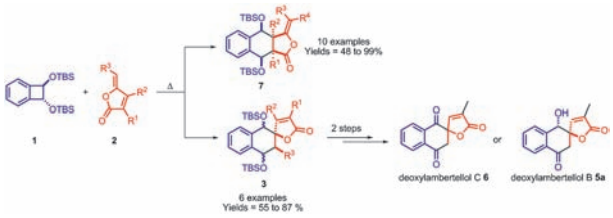


5490

Diels–Alder cycloaddition of *o*-quinonedimethides and alkylidene-5*H*-furan-2-ones: new and rapid access to lambertellol cores and arthrinone derivatives

Romain Blanc, Virginie Héran, Raphaël Rahmani, Laurent Commeiras* and Jean-Luc Parrain*

An efficient synthesis of deoxy-lambertellols was reported through a highly chemo- and diastereoselective DA cycloaddition. Such transformation with δ-substituted γ-alkylidenebutenolides, to prepare new analogues of these tricyclic spirolactones, was also studied.



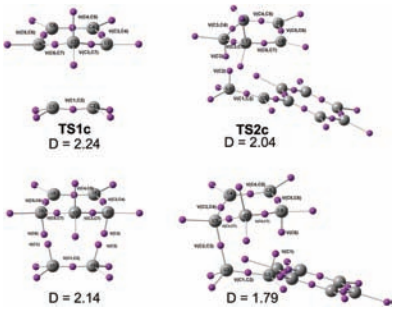
PAPERS

5495

Understanding the mechanism of non-polar Diels–Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms

Luis R. Domingo,* Eduardo Chamorro and Patricia Pérez

ELF analysis for the one-step pathways of the non-polar Diels–Alder reaction between Cp and ethylene or styrene suggests that these reactions take place through *pseudo-diradical* species.

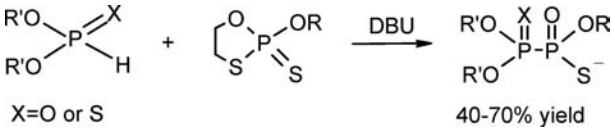


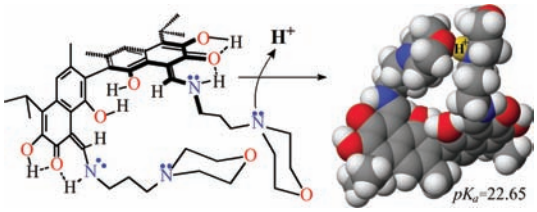
5505

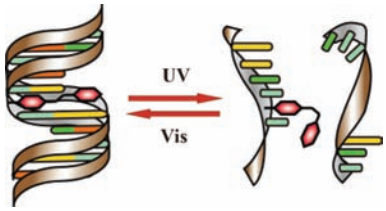
Stereoselective formation of a P–P bond in the reaction of 2-alkoxy-2-thio-1,3,2-oxathiaphospholanes with *O*,*O*-dialkyl *H*-phosphonates and *H*-thiophosphonates

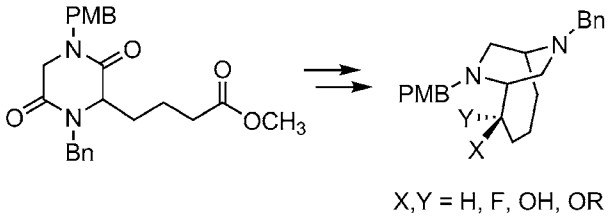
Damian Błaziak, Piotr Guga, Agata Jagiełło, Dariusz Korczyński, Anna Maciaszek, Anna Nowicka, Aleksandra Pietkiewicz and Wojciech J. Stec*

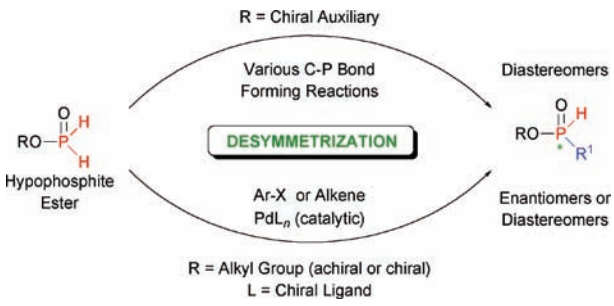
Organohypophosphates containing a P–P bond are obtained under mild conditions in a highly stereoselective reaction of 2-alkoxy-2-thio-1,3,2-oxathiaphospholanes with *O*,*O*-dialkyl *H*-phosphonates or *H*-thiophosphonates (R' = Me or Et).

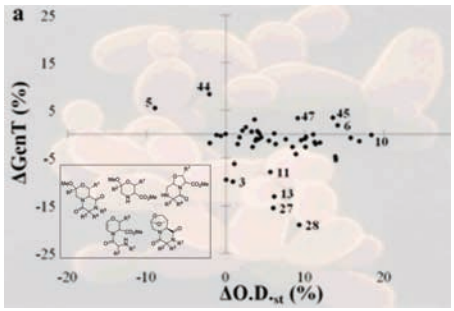


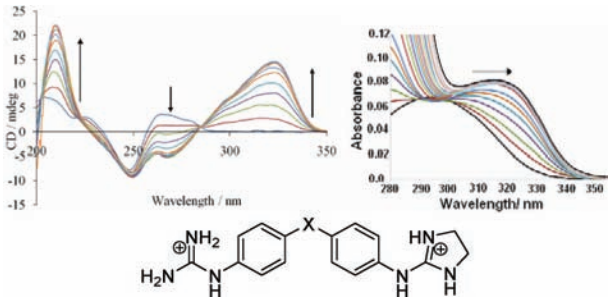


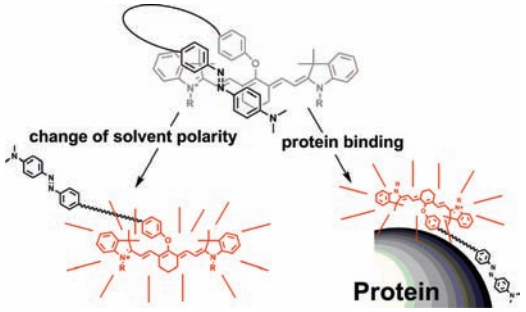










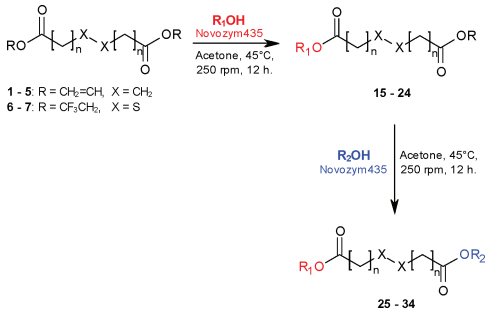


5583

Exploiting enzymatic regioselectivity: a facile methodology for the synthesis of polyhydroxylated hybrid compounds

Pietro Magrone, Francesco Cavallo, Walter Panzeri, Daniele Passarella and Sergio Riva*

A general two-step access to polyhydroxylated conjugated compounds based on enzymatic regioselective acylations is described.

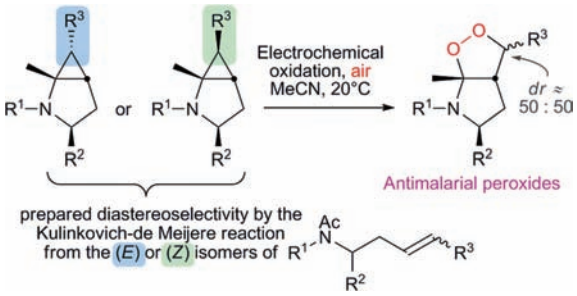


5591

Aminocyclopropanes as precursors of endoperoxides with antimalarial activity

Claire Madelaine, Olivier Buriez,* Benoît Crousse, Isabelle Florent, Philippe Grellier, Pascal Retailleau and Yvan Six*

Several bicyclic aminocyclopropanes were synthesised diastereoselectively using the Kulinkovich–de Meijere reaction, and then converted into novel moderately active antimalarial α-amino endoperoxides.

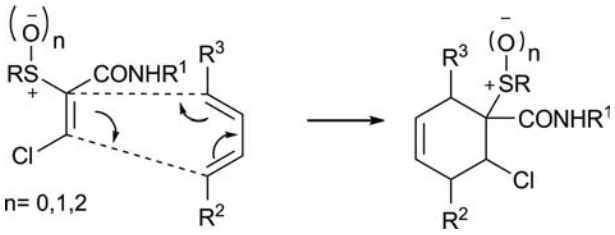


5602

The influence of reaction conditions on the Diels–Alder cycloadditions of 2-thio-3-chloroacrylamides; investigation of thermal, catalytic and microwave conditions

Marie Kissane, Denis Lynch, Jay Chopra, Simon E. Lawrence and Anita R. Maguire*

The Diels–Alder cycloadditions of cyclopentadiene and 2,3-dimethyl-1,3-butadiene to a range of 2-thio-3-chloroacrylamides under thermal, catalytic and microwave conditions is described.



5614

Synthesis of oxygen heterocycles by regioselective Heck reaction

Matthew McConville, Jiwu Ruan, John Blacker and Jianliang Xiao*

Regioselective Heck arylation of unsaturated alcohols followed by acid-mediated cyclisation affords 2,2-disubstituted tetrahydrofurans and tetrahydropyrans in a convenient one-pot fashion.