

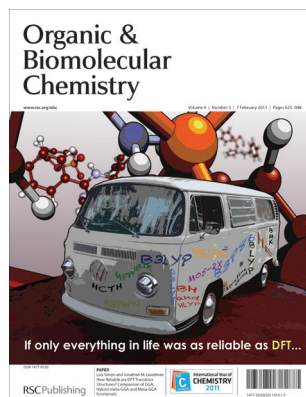
# Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry  
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## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 9(3) 625–984 (2011)



### Cover

See Luis Simón and Jonathan M. Goodman, pp. 689–700.

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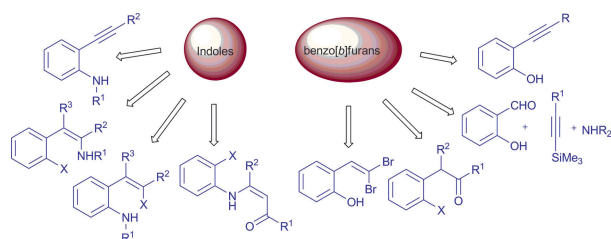
## PERSPECTIVE

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### Copper catalysis in the construction of indole and benzo[*b*]furan rings

Sandro Cacchi,\* Giancarlo Fabrizi and Antonella Goggiamani

This perspective reports on some of the main copper-catalyzed routes to the construction of the indole and benzo[*b*]furan systems.



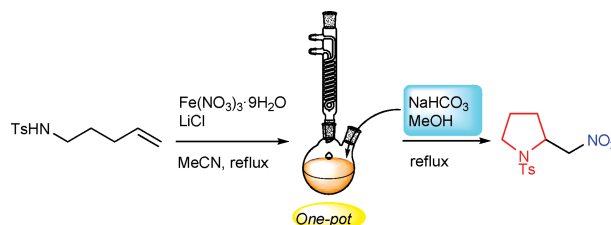
## COMMUNICATIONS

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### Iron-mediated one-pot formal nitrocyclization onto unactivated alkenes

Tsuyoshi Taniguchi,\* Tatsuya Fujii and Hiroyuki Ishibashi

One-pot synthesis of heterocycles having a nitromethyl group using iron(III) nitrate nonahydrate has been developed.



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# Organic & Biomolecular Chemistry

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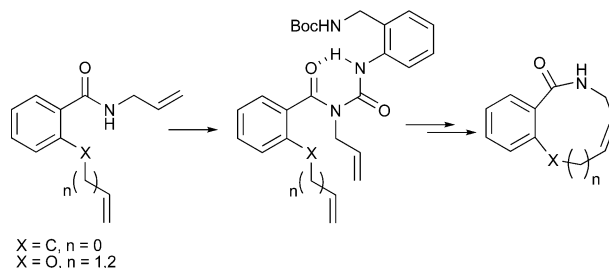
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### Benzoylureas as removable *cis* amide inducers: synthesis of cyclic amides *via* ring closing metathesis (RCM)

Ryan M. Brady, Yelena Khakham, Guillaume Lessene\* and Jonathan B. Baell\*

Through an intramolecular hydrogen bond, the benzoylurea motif induces a *cis*-amide conformation that allows rapid and high yielding synthesis of lactams.

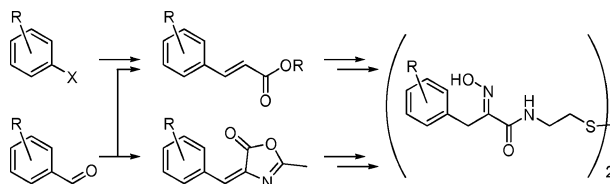


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### New synthetic strategies towards psammaphin A, access to natural product analogues for biological evaluation

Matthias G. J. Baud, Thomas Leiser, Franz-Josef Meyer-Almes and Matthew J. Fuchter\*

New synthetic routes to psammaphin A were developed, using commercially available starting materials and allowing access to analogues not accessible *via* reported methods. Preliminary studies revealed these compounds to be the most potent non peptidic inhibitors of histone deacetylase 1 (class I) discovered so far.

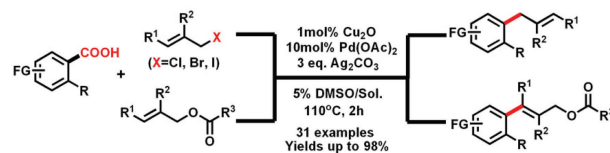


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### Pd(II)-catalyzed decarboxylative allylation and Heck-coupling of arene carboxylates with allylic halides and esters

Jiantao Wang, Zili Cui, Yuexia Zhang, Huajie Li, Long-Min Wu and Zhongquan Liu\*

This work demonstrates an alternative method to prepare allylated arenes and aryl-substituted allylic esters *via* catalytic decarboxylative C–C bond formation using aromatic carboxylic acids and allylic halides and esters.

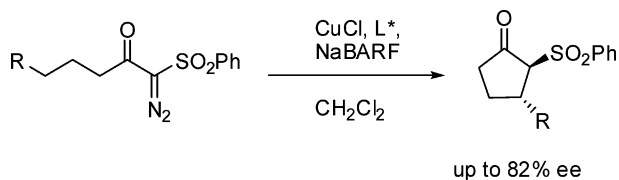


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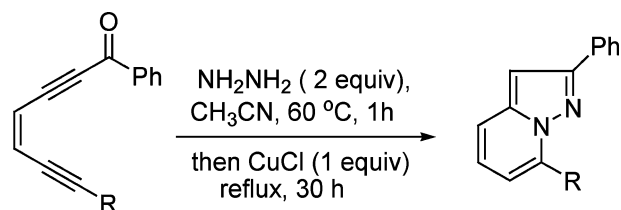
### Asymmetric copper-catalysed intramolecular C–H insertion reactions of $\alpha$ -diazo- $\beta$ -keto sulfones

Catherine N. Slattery and Anita R. Maguire\*

Asymmetric copper-catalysed intramolecular C–H insertion reactions of a series of  $\alpha$ -diazo- $\beta$ -keto sulfones are reported. Enantioselectivities of up to 82% ee were achieved in moderate to good yield. These results represent the highest level of enantiocontrol achieved to date for a copper-catalysed cyclopentanone synthesis *via* C–H insertion.



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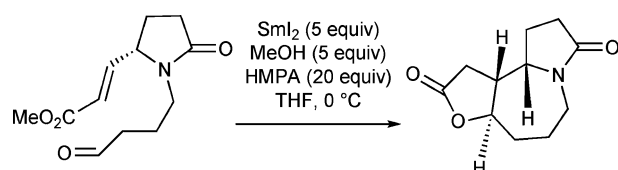


### A copper-mediated cyclization reaction of hydrazine with enediynes providing pyrazolo[1,5-*a*]pyridines

Hung-Chou Wu, Long-Chih Hwang and Ming-Jung Wu\*

This article describes a unique tandem cyclization of enediyne to give 2,7-disubstituted pyrazolo[1,5-*a*]pyridines by the reaction of hydrazine with enediynes mediated by copper chloride.

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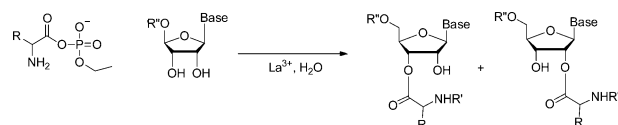


### Efficient total synthesis of (-)-stemoamide

Toshio Honda,\* Tomoha Matsukawa and Kazunori Takahashi

$\text{SmI}_2$ -promoted 7-*exo-trig* cyclization occurred stereoselectively to construct a basic skeleton of stemoamide.

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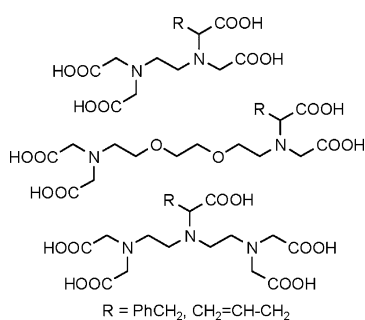


### Biomimetic protecting-group-free 2', 3'-selective aminoacylation of nucleosides and nucleotides

Sohyoung Her and Ronald Kluger\*

Efficient lanthanum-promoted aminoacylation of ribonucleosides and ribonucleotides can be achieved with an aminoacyl phosphate ester with a free amino group.

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### Stevens rearrangement as a tool for the structural modification of polyaminopolycarboxylic ligands

Giovanni B. Giovenzana,\* Daniela Imperio, Luciano Lattuada and Fulvio Uggeri

$\alpha$ -Substituted EDTA, EGTA, DTPA ligands are obtained through a one-step protocol involving *N*-alkylation and Stevens rearrangement.



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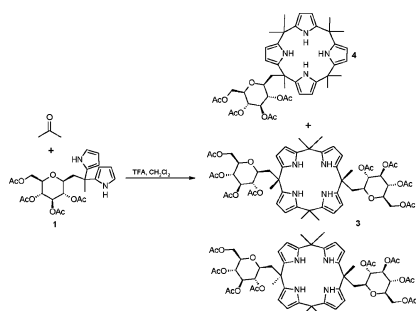
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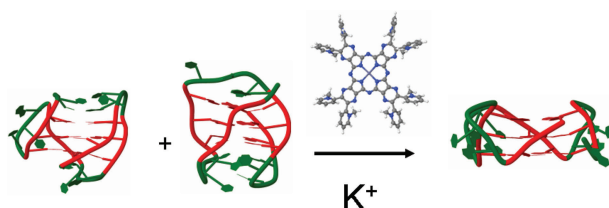


### Asymmetrically substituted calix[4]pyrrole with chiral substituents

Petr Štěpánek, Ondřej Šimák, Zdena Nováková,  
Zdeněk Wimmer and Pavel Drašar\*

There was prepared first calix[4]pyrrole containing unprotected carbohydrate moiety directly linked to *meso*-position of oligopyrrole by stable "C-glycosidic" bond. Basic examination of its superassembly capability is presented.

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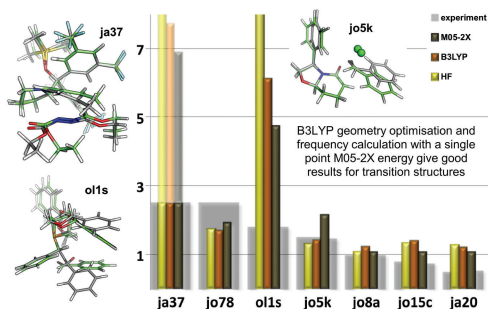
### A cationic Zn<sup>II</sup> porphyrazine induces a stable parallel G-quadruplex conformation in human telomeric DNA

Ilse Manet,\* Francesco Manoli, Maria Pia Donzello,\*  
Elisa Viola, Giuseppina Andreano, Annalisa Masi,  
Luciano Cellai and Sandra Monti\*

A *water soluble* octacationic Zn<sup>II</sup> porphyrazine macrocycle drives the conformational equilibrium of the G-quadruplex of a human telomeric sequence exclusively towards a parallel conformation upon complexation.

## PAPERS

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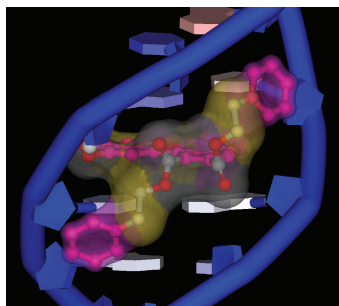


### How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals

Luis Simón\* and Jonathan M. Goodman\*

We present calculations of the geometries of nineteen covalent-bond forming transition states using HF and twelve different functionals. For the calculation of the TS geometries, we find that B3LYP is only slightly less accurate than newer methods, and conclude that M05-2X single point calculations on B3LYP optimised geometries is appropriate for many studies of organic reaction mechanisms.

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### Structural basis for the potential antitumour activity of DNA-interacting benzo[*k*]xanthene lignans

Simone Di Micco, Frédéric Mazué, Carmelo Daquino,  
Carmela Spatafora, Dominique Delmas, Norbert Latruffe,  
Corrado Tringali, Raffaele Riccio and Giuseppe Bifulco\*

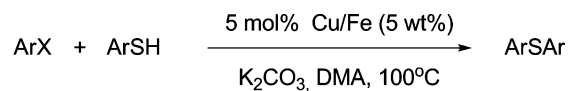
The investigation of benzo[*k*]xanthene as DNA ligands suggests they are suitable lead compounds for the design of new binders with potential antitumour properties.

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### Oxidoreductive coupling of thiols with aryl halides catalyzed by copper on iron

Szabolcs Kovács and Zoltán Novák\*

Synthesis and utilization of a simple copper on iron catalyst in the coupling of aryl halides with thiols through disulfide intermediate is reported. The iron support of copper catalyst ensures reductive media for the coupling, allows easy removal of the metals by outer magnetic field and enables the recycling of the catalyst.



**no inert atmosphere required**

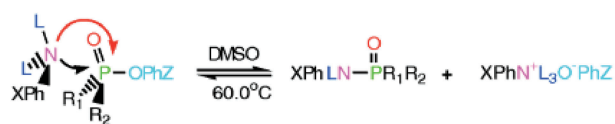
**27 examples  
43-97% yield**

717

### Kinetics and mechanism of the anilinolyses of aryl dimethyl, methyl phenyl and diphenyl phosphinates

Nilay Kumar Dey, Chan Kyung Kim\* and Hai Whang Lee\*

Mechanistic interpretation of anilinolyses of phosphinates is rationalized by deuterium kinetic isotope effects and cross-interaction constants.



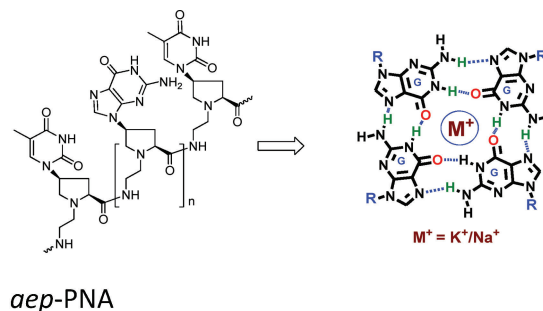
1: R<sub>1</sub> = R<sub>2</sub> = Me; 2: R<sub>1</sub> = Me, R<sub>2</sub> = Ph; 3: R<sub>1</sub> = R<sub>2</sub> = Ph  
L = H or D; k<sub>H</sub>/k<sub>D</sub> = 1.03 ~ 1.17 (1); 1.15 ~ 1.29 (2); 1.24 ~ 1.51 (3)  
1: Backside and Frontside attack; 2 and 3: Frontside attack

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### Enhanced stability of G-quadruplexes from conformationally constrained *aep*-PNA backbone

Nagendra K. Sharma\* and Krishna N. Ganesh

G-rich sequences of nucleic acids (DNA/RNA) are known to form G-quadruplex structures in the presence of monovalent metal ion. G-rich sequence of modified nucleic acid analogues, PNA and LNA, also form a G-quadruplex structure like DNA. In this report, we examine the ability of G-quadruplex formation in backbone modified *aep*-PNA by using UV, CD and mass spectroscopic techniques.

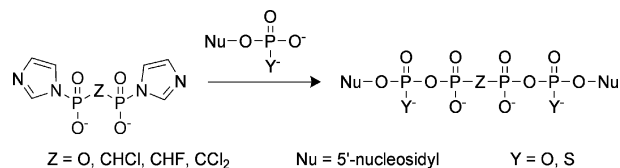


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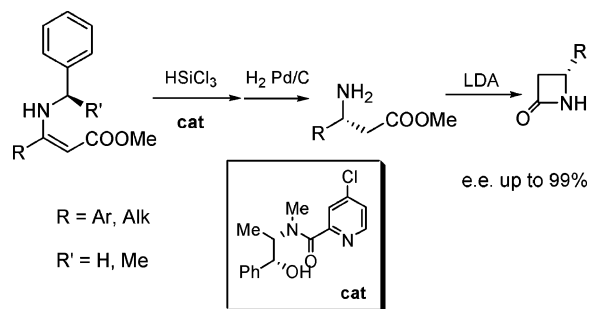
### P<sup>1</sup>,P<sup>2</sup>-Diimidazolyl derivatives of pyrophosphate and bis-phosphonates – synthesis, properties, and use in preparation of dinucleoside tetraphosphates and analogs

Ivan B. Yanachkov,\* Edward J. Dix, Milka I. Yanachkova and George E. Wright

P<sup>1</sup>,P<sup>2</sup>-Diimidazolides of pyrophosphate and its analogs were synthesized and used to prepare dinucleoside tetraphosphates and tetraphosphonates conveniently and in high yields.



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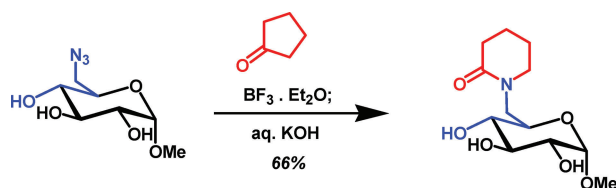


### Trichlorosilane-mediated stereoselective synthesis of $\beta$ -amino esters and their conversion to highly enantiomerically enriched $\beta$ -lactams

Stefania Guizzetti,\* Maurizio Benaglia,\*  
Martina Bonsignore and Laura Raimondi

A highly stereoselective trichlorosilane-mediated reduction of *N*-benzyl enamines was developed; easy deprotection by hydrogenolysis allowed to synthesize enantiomerically pure  $\beta$ -lactams.

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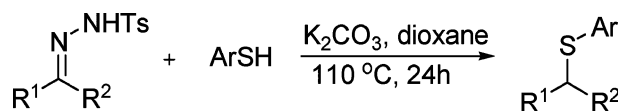


### Synthesis of novel sugar-lactam conjugates using the Aubé reaction

Suresh E. Kurhade, Tanaji Mengawade, Debnath Bhuniya,  
Venkata P. Palle and D. Srinivasa Reddy\*

The synthesis of novel sugar-lactam conjugates is reported starting from readily available sugar azides using the Aubé reaction. Cyclic azido alcohols are used in the Aubé reaction for the first time in a carbohydrate setting.

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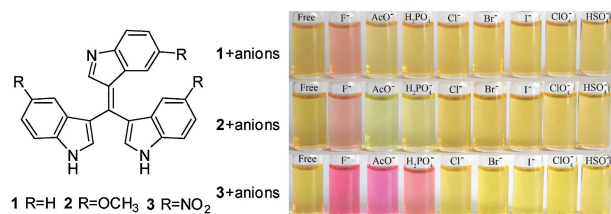


### Synthesis of thioethers *via* metal-free reductive coupling of tosylhydrazones with thiols

Qiuping Ding,\* Banpeng Cao, Jianjun Yuan, Xianjin Liu  
and Yiyuan Peng\*

An efficient, simple, inexpensive and metal-free procedure for the synthesis of thioethers is described *via* the base-promoted reductive coupling of tosylhydrazones with thiols through an insertion of a carbene into the S–H bond.

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### Tris(indolyl)methene molecule as an anion receptor and colorimetric chemosensor: tunable selectivity and sensitivity for anions

Litao Wang, Xiaoming He, Yong Guo, Jian Xu and  
Shijun Shao\*

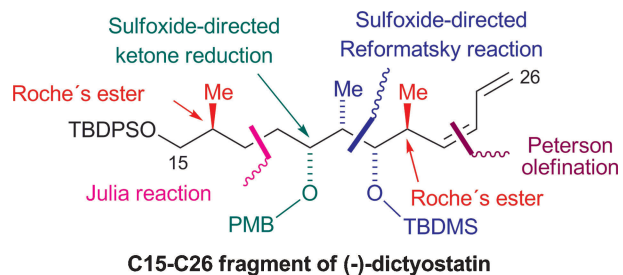
New anion receptors and colorimetric chemosensors based on tris(indolyl)methene skeleton were synthesized, which display tunable selectivity and sensitivity for anions.

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### Stereoselective synthesis of the C15–C26 fragment of the antitumor agent (–)-dictyostatin

Leticia Ferreiro-Mederos, Silvia Vila-Gisbert, Antonio Urbano,\* M. Carmen Carreño\* and Françoise Colobert\*

The synthesis of the C15–C26 fragment of (–)-dictyostatin is reported in 10 steps and 28% overall yield, the key steps being the two stereoselective sulfoxide-directed processes.

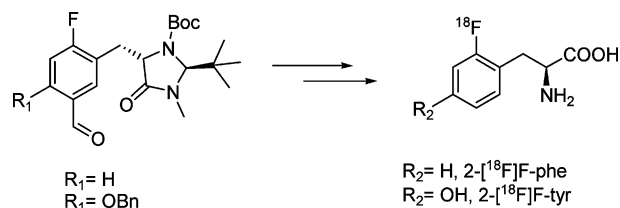


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### Enantiospecific synthesis of 2-[<sup>18</sup>F]fluoro-L-phenylalanine and 2-[<sup>18</sup>F]fluoro-L-tyrosine by isotopic exchange

Johnny Castillo Meleán, Johannes Ermer\* and Heinz H. Coenen

2-[<sup>18</sup>F]Fluoro-L-phenylalanine and 2-[<sup>18</sup>F]fluoro-L-tyrosine were synthesized by isotopic exchange on corresponding precursors, followed by removal of the formyl group with Rh(PPh<sub>3</sub>)<sub>3</sub>Cl and subsequent hydrolysis of the protecting groups.

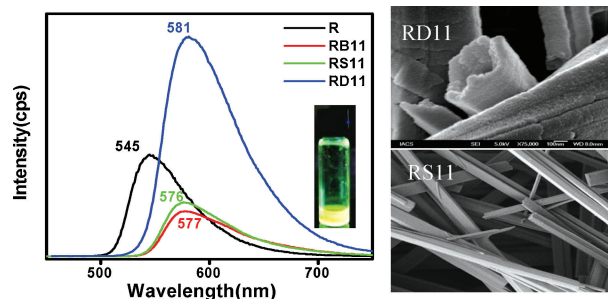


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### Effect of complementary small molecules on the properties of bicomponent hydrogel of riboflavin

Abhijit Saha, Bappaditya Roy, Aluri Esterrani and Arun K. Nandi\*

Molecules complementary to riboflavin producing bicomponent hydrogels have a pronounced effect on morphology, structure, stability and optical property of the gels.

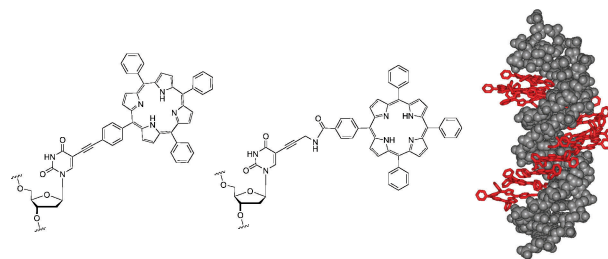


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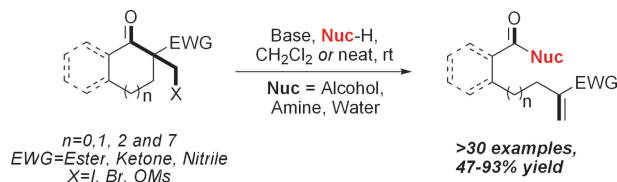
### Introducing structural flexibility into porphyrin–DNA zipper arrays

Ashley Brewer, Guiliano Siligardi, Cameron Neylon and Eugen Stulz\*

The synthesis of a novel tetraphenyl porphyrin modified nucleotide joined *via* a propargyl amide linker is presented. The spectroscopic data and molecular modelling reveal differences in structure and stability, depending on the linker (alkyne, amide) used. At higher concentrations, formation of bundles is observed.



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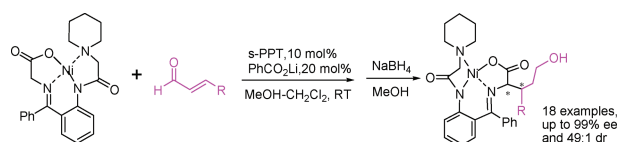


### The Grob/Eschenmoser fragmentation of cycloalkanones bearing $\beta$ -electron withdrawing groups: a general strategy to acyclic synthetic intermediates

Judith Hierold, Tina Hsia and David W. Lupton\*

Introduction of a  $\beta$ -electron withdrawing group to cycloalkanones allows broad ranging fragmentation to proceed with various nitrogen and oxygen nucleophiles.

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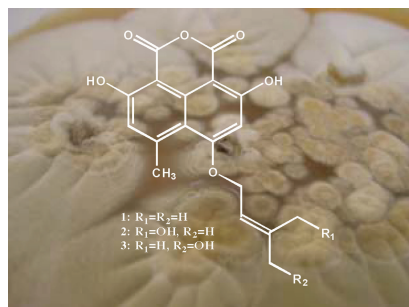


### Catalytic asymmetric Michael addition of $\alpha,\beta$ -unsaturated aldehydes to Ni(II) complexes of the Schiff base of glycine

Xiaoyan Luo, Zhichao Jin, Pengfei Li, Jiabin Gao, Weimin Yue, Xinmiao Liang and Jinxing Ye\*

The conjugate addition of Ni(II) complexes of the Schiff base of glycine to  $\alpha,\beta$ -unsaturated aldehydes catalyzed by (*S*)-2-(diphenyl(trimethylsilyloxy)methyl)pyrrolidine afforded adducts in excellent yields with up to 49 : 1 dr and 99% ee.

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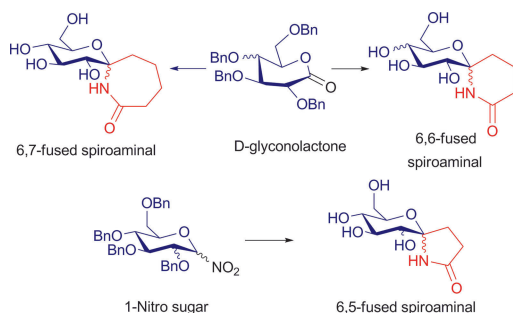


### Antimicrobial phenalenone derivatives from the marine-derived fungus *Coniothyrium cereale*

Mahmoud Fahmi Elsebai, Stefan Kehraus, Ulrike Lindequist, Florenz Sasse, Saad Shaaban, Michael Gütschow, Michael Josten, Hans-Georg Sahl and Gabriele M. König\*

The marine algae-derived fungus *Coniothyrium cereale* produces phenalenone derivatives with a variety of significant biological activities.

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### Synthesis of sugar-derived spiroaminals *via* lactamization and metathesis reactions

Adabala Pal John Pal, Parasuraman Kadigachalam, Asadulla Mallick, Venkata Ramana Doddi and Yashwant D. Vankar\*

The lactamization and metathesis pathways provided a significant route for the synthesis of novel oxa-aza spiro compounds in good yields.

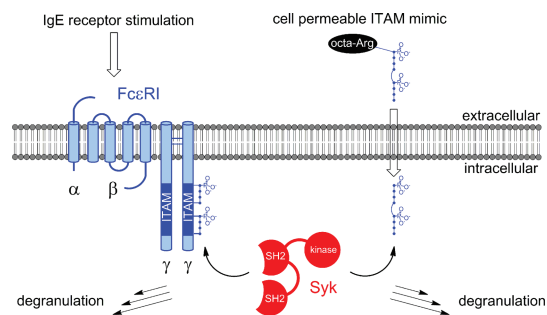


820

### Cell permeable ITAM constructs for the modulation of mediator release in mast cells

Joeri Kuil, Marcel J. E. Fischer, Nico J. de Mol and Rob M. J. Liskamp\*

A synthetic cell permeable ITAM construct can enhance mast cell degranulation up to 140%.

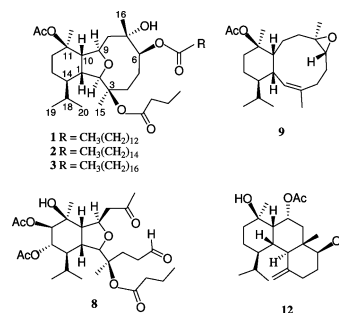


834

### Klysimplexins I–T, unicellin-based diterpenoids from the cultured soft coral *Klyxum simplex*

Bo-Wei Chen, Chih-Hua Chao, Jui-Hsin Su, Chung-Wei Tsai, Wei-Hsien Wang, Zhi-Hong Wen, Chiung-Yao Huang, Ping-Jyun Sung, Yang-Chang Wu and Jyh-Horng Sheu\*

New unicellin-base diterpenoids, klysimplexins I–T, were isolated from a cultured soft coral *Klyxum simplex*; their structures were elucidated by spectroscopic methods, particularly in 1D and 2D NMR experiments.

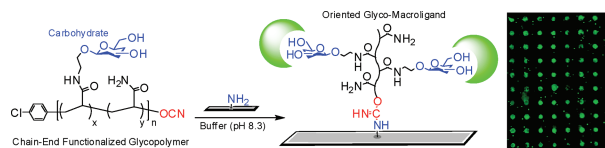


845

### Orientated glyco-macroligand formation based on site-specific immobilization of *O*-cyanate chain-end functionalized glycopolymer

Satya Nandana Narla and Xue-Long Sun\*

An orientated glyco-macroligand formation was demonstrated by immobilizing an *O*-cyanate chain-end functionalized glycopolymer onto amine-functionalized silica gel and glass slides *via* isourea bond formation.

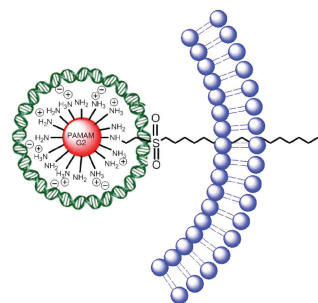


851

### Alkyl sulfonyl derivatized PAMAM-G2 dendrimers as nonviral gene delivery vectors with improved transfection efficiencies

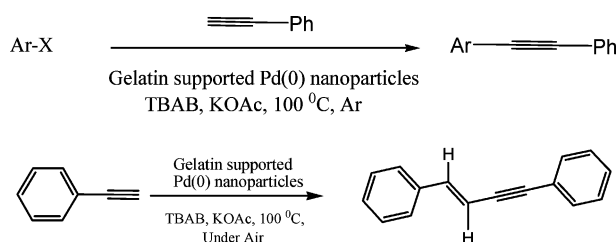
Julia Morales-Sanfrutos, Alicia Megia-Fernandez, Fernando Hernandez-Mateo, M<sup>a</sup> Dolores Giron-Gonzalez, Rafael Salto-Gonzalez and Francisco Santoyo-Gonzalez\*

Amphiphilic PAMAM-G2 derivatives engineered with peripheral alkyl chains are nonviral gene delivery vectors that exhibit high transfection efficiencies and low toxicity, particularly in the case of functionalization with C18 tails.





865

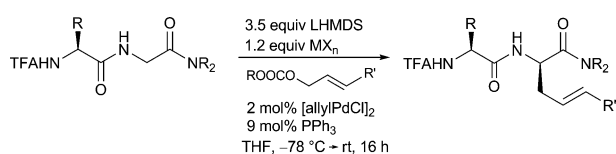


### Gelatin as a bioorganic reductant, ligand and support for palladium nanoparticles. Application as a catalyst for ligand- and amine-free Sonogashira–Hagihara reaction

Habib Firouzabadi,\* Nasser Iranpoor\* and Arash Ghaderi

Herein, a novel method using palladium nanoparticles supported on gelatin to catalyze Sonogashira–Hagihara reaction is presented.

872

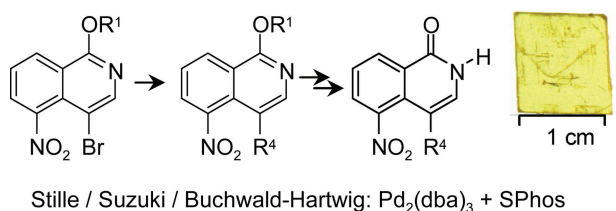


### Stereoselective palladium-catalyzed allylic alkylations of peptide amide enolates

Swarup Datta and Uli Kazmaier\*

Pd-catalyzed allylations are an excellent tool for stereoselective peptide modifications, being clearly superior to normal alkylations. The reactions proceed not only in high yield, but also high regio- and diastereoselectivities, and *trans*-products are formed exclusively. Therefore, this is a powerful synthetic tool for natural product and drug synthesis.

881

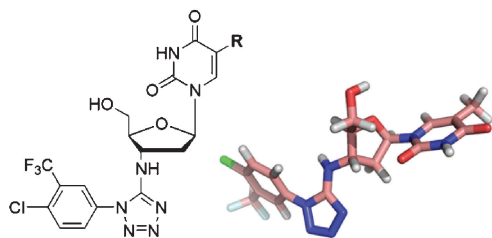


### Synthesis of 4-alkyl-, 4-aryl- and 4-arylamino-5-aminoisoquinolin-1-ones and identification of a new PARP-2 selective inhibitor

Peter T. Sunderland, Archana Dhama, Mary F. Mahon, Louise A. Jones, Sophie R. Tully, Matthew D. Lloyd, Andrew S. Thompson, Hashim Javaid, Niall M. B. Martin and Michael D. Threadgill\*

4-Substituted 5-nitro and 5-amino-isoquinolin-1-ones are accessible in good yields through Stille, Suzuki and Buchwald–Hartwig couplings to 1-alkoxy-4-bromo-5-nitro-isoquinolines.

892



R = CH<sub>3</sub>; IC<sub>50</sub> (TK2) = 0.035 nM  
R = CH=CH<sub>2</sub>Br; IC<sub>50</sub> (TK2) = 0.014 nM

### Synthesis, modeling and evaluation of 3'-(1-aryl-1H-tetrazol-5-ylamino)-substituted 3'-deoxythymidine derivatives as potent and selective human mitochondrial thymidine kinase inhibitors

Sara Van Poecke,\* Ana Negri, Jolien Janssens, Nicola Solaroli, Anna Karlsson, Federico Gago, Jan Balzarini and Serge Van Calenbergh

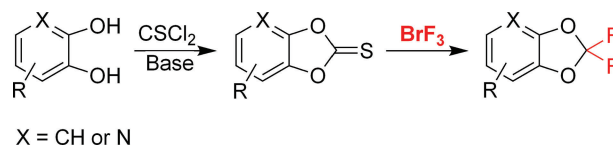
Replacement of the 3'-OH group of thymidine with a 3'-N-(1-aryltetrazol-5-yl)amino substituent was found to result in potent and selective inhibitors of thymidine kinase 2.

902

**Synthesis of difluoroaryldioxoles using BrF<sub>3</sub>**

Youlia Hagooly, Michael J. Welch and Shlomo Rozen\*

The general pathway for a new synthesis of difluoroaryldioxoles.

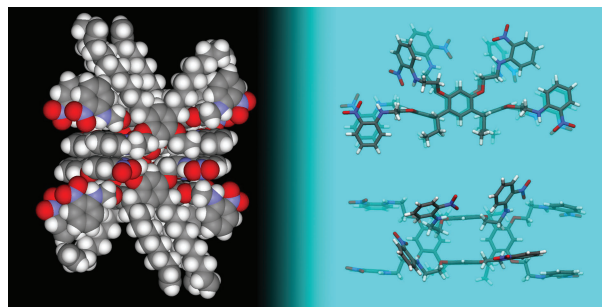


906

**Conformational polymorphism and amphiphilic properties of resorcinarene octapodands**

Kaisa Helttunen, Elisa Nauha, Anni Kurronen, Patrick Shahgaldian and Maija Nissinen\*

Amphiphilic self-assembling resorcinarene octapodands with conformational flexibility induced polymorphism could lead to temperature responsive binding properties.

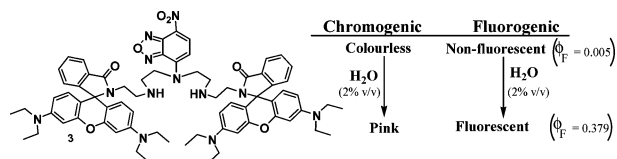


915

**Water induced chromogenic and fluorogenic signal modulation in a bi-fluorophore appended acyclic amino-receptor system**

Bamaprasad Bag\* and Ajoy Pal

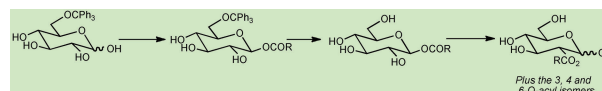
A bi-fluorophoric signaling system exhibits enhancement in absorption for naked eye detection as well as fluorescence enhancement in the presence of water in organic solvents at submicromolar level.



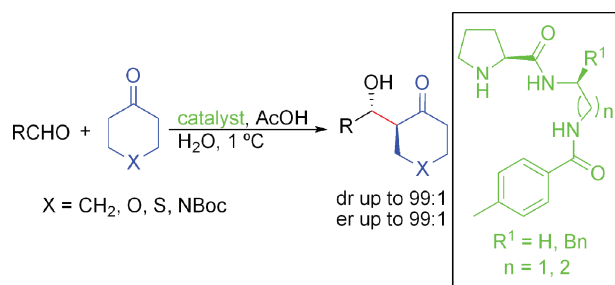
926

**Synthesis of a series of phenylacetic acid 1- $\beta$ -O-acyl glucosides and comparison of their acyl migration and hydrolysis kinetics with the corresponding acyl glucuronides**

Lisa Iddon, Selena E. Richards, Caroline H. Johnson, John R. Harding, Ian D. Wilson, Jeremy K. Nicholson, John C. Lindon and Andrew V. Stachulski\*

A set of 1- $\beta$ -O-acyl glucosides derived from phenylacetic acids with varying  $\alpha$ -substitution have been prepared and their acyl migration kinetics measured by NMR spectroscopy. Full kinetic analysis of the NMR data shows convincingly by comparison that the ionized carboxylate plays a part in acyl glucuronide migration behaviour.

935

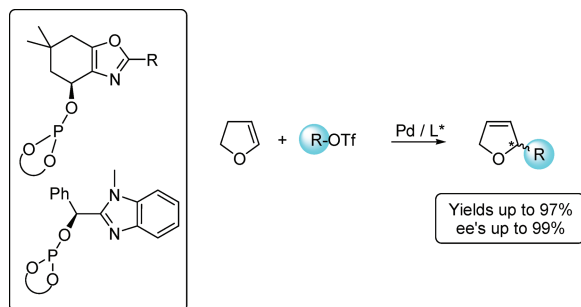


### Highly diastereo- and enantioselective direct Barbas–List aldol reactions promoted by novel benzamidoethyl and benzamidopropyl prolinamides in water

Rafael Pedrosa,\* José M. Andrés,\* Rubén Manzano, David Román and Silvia Téllez

Excellent results in terms of yield and diastereo- and enantiocontrol have been obtained by using novel prolinamides, prepared from ethylene- and propylene diamines, in the Barbas–List aldol reaction.

941



### Phosphite-oxazole/imidazole ligands in asymmetric intermolecular Heck reaction

Javier Mazuela, Paivi Tolstoy, Oscar Pàmies,\* Pher G. Andersson\* and Montserrat Diéguez\*

We describe the first application of phosphite-oxazole/imidazole ligands in asymmetric intermolecular Pd-catalyzed Heck reactions under thermal and microwave conditions.

# 16<sup>th</sup>

IUPAC International Symposium on Organometallic Chemistry  
Directed Towards Organic Synthesis (OMCOS 16)

July 24–28, 2011, Shanghai, China

- Organic synthesis with organometallic reagents
- Metal-mediated or -catalyzed reactions
- Asymmetric synthesis and catalysis
- Structural and mechanistic aspects of organometallics
- Environmentally benign processes using metals

#### > Confirmed Plenary Speakers

Matthias Beller (Leibniz Institute for Catalysis)  
Chi-Ming Che (The University of Hong Kong)  
Antonio M Echavarren (Institut Català d'Investigació Química, ICIQ)  
Alois Fürstner (Max-Planck-Institut für Kohlenforschung)  
Michael J. Krische (The University of Texas at Austin)  
Chao-Jun Li (McGill University)  
Rai-Shung Liu (National Tsing-Hua University)  
Eiichi Nakamura (The University of Tokyo)  
Andreas Pfaltz (University of Basel)  
Yoshinori Yamamoto (Tohoku University)

#### > Confirmed Invited Speakers

Marco Bandini (Università di Bologna)  
Gerhard Erker (University of Münster)  
Zhaomin Hou (Advanced Science Institute, RIKEN)  
Robert J. M. Klein Gebbink (Utrecht University)  
E. Peter Kündig (University of Geneva)  
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