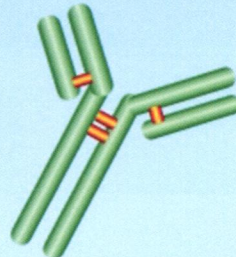
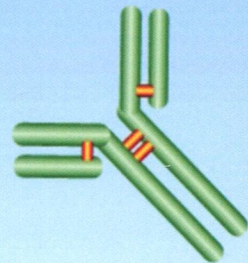
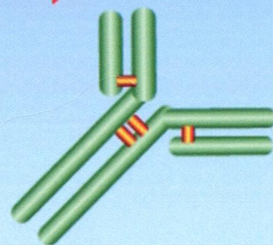
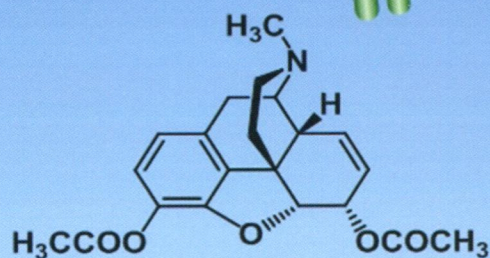
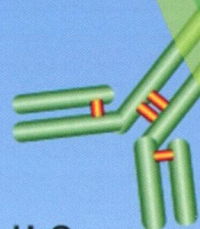
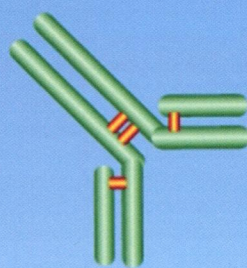
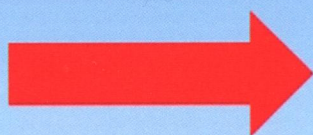
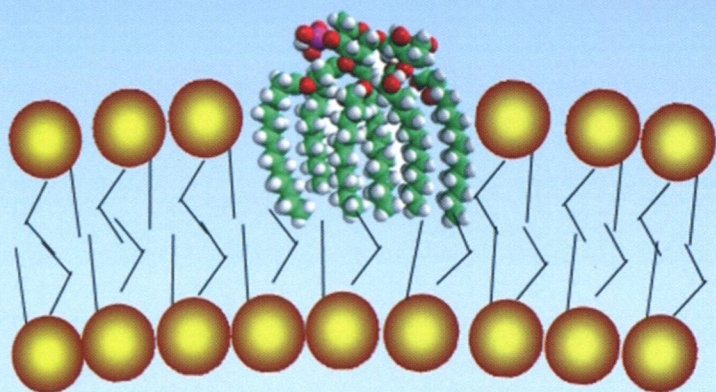
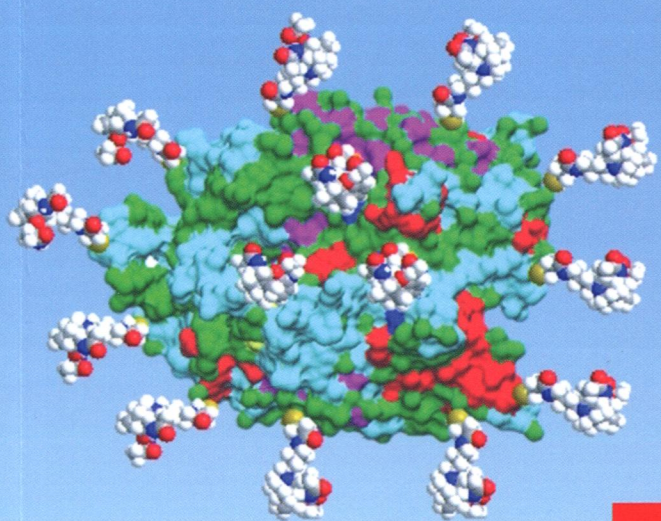
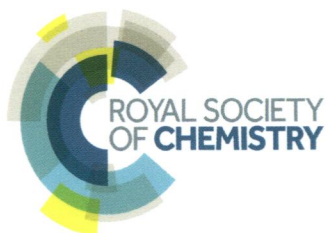


# Organic & Biomolecular Chemistry

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ISSN 1477-0520



PAPER  
Kenner C. Rice *et al.*  
Synthesis and immunological effects of heroin vaccines

# Organic & Biomolecular Chemistry

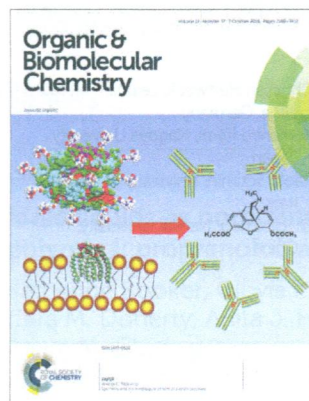
An international journal of synthetic, physical and biomolecular organic chemistry

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## IN THIS ISSUE

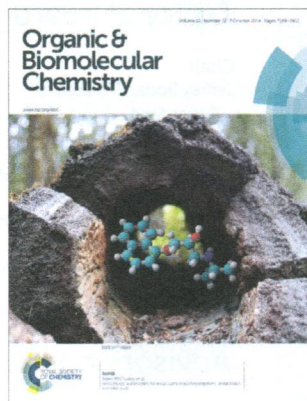
ISSN 1477-0520 CODEN OBCRAK 12(37) 7169–7412 (2014)



### Cover

See Kenner C. Rice *et al.*, pp. 7211–7232.

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### Inside cover

See Adam McCluskey *et al.*, pp. 7201–7210.

Image reproduced by permission of Adam McCluskey from *Org. Biomol. Chem.*, 2014, **12**, 7201.

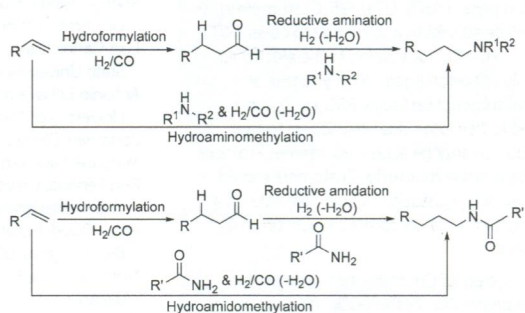
## REVIEW

7179

### Recent advances in catalytic C–N bond formation: a comparison of cascade hydroaminomethylation and reductive amination reactions with the corresponding hydroamidomethylation and reductive amidation reactions

Saeed Raoufmoghaddam

This review highlights and compares selected examples of hydroaminomethylation, reductive amination, hydroamidomethylation and reductive amidation reactions, and consequently reveals their potential applications.



## COMMUNICATIONS

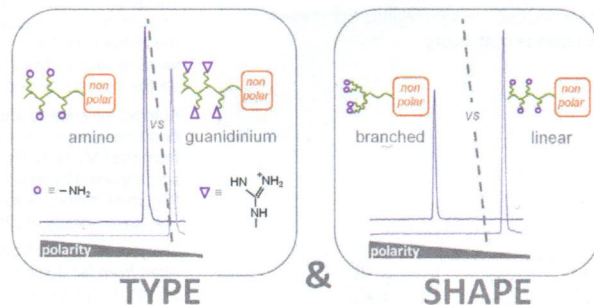
7194

### Linear versus branched poly-lysine/arginine as polarity enhancer tags

Marta Paradís-Bas, Maria Albert-Soriano, Judit Tulla-Puche\* and Fernando Albericio\*

The design and synthesis of Lys- and Arg-containing peptides as solubilizing tags were studied to evaluate their influence on polarity.

Федеральное государственное бюджетное учреждение науки  
Центральная научная библиотека  
Уральского отделения  
Российской академии наук (ЦНБ УрО РАН)

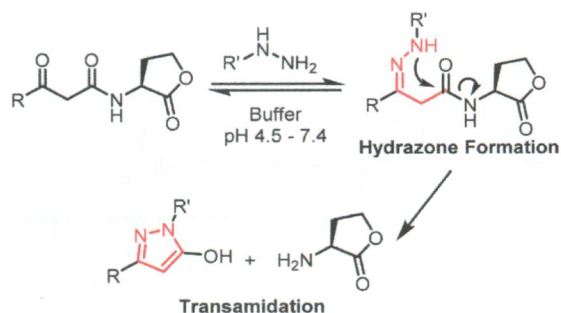


7197

### Selective transamidation of 3-oxo-*N*-acyl homoserine lactones by hydrazine derivatives

Michael A. Bertucci, Stephen J. Lee and Michel R. Gagné\*

Hydrazine derivatives are employed for selective amide cleavage of 3-oxo-*N*-acyl homoserine lactones under physiologically relevant conditions.



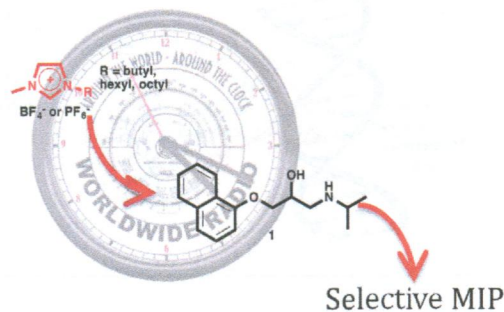
PAPERS

7201

### Ionic liquids as porogens for molecularly imprinted polymers: propranolol, a model study

Katherine Booker, Clovia I. Holdsworth, Cara M. Doherty, Anita J. Hill, Michael C. Bowyer and Adam McCluskey\*

The selectivity and rebinding capacity of molecularly imprinted polymers selective for propranolol (**1**) using the room temperature ionic liquids [BMIM][BF<sub>4</sub>], [BMIM][PF<sub>6</sub>], [HMIM][PF<sub>6</sub>] and [OMIM][PF<sub>6</sub>] and CHCl<sub>3</sub> were examined.

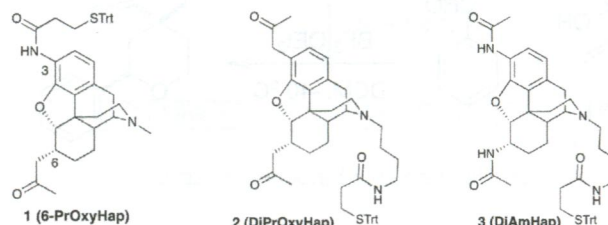


7211

### Synthesis and immunological effects of heroin vaccines

Fuying Li, Kejun Cheng, Joshua F. G. Antoline, Malliga R. Iyer, Gary R. Matyas, Oscar B. Torres, Rashmi Jalah, Zoltan Beck, Carl R. Alving, Damon A. Parrish, Jeffrey R. Deschamps, Arthur E. Jacobson and Kenner C. Rice\*

Multi-step syntheses provided three designed haptens for vaccines that were evaluated for their ability to block the effects of heroin and its metabolites.

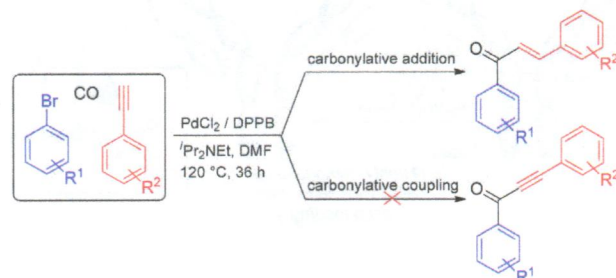


7233

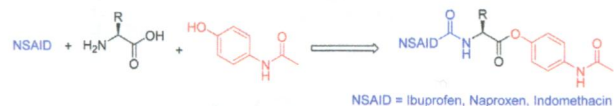
### Palladium-catalyzed carbonylative addition of aryl bromides to arylalkynes: a simple and efficient method for chalcone synthesis

Sheng Zhang, Lianguang Wang, Xiujuan Feng\* and Ming Bao\*

Chalcones can be prepared in satisfactory to excellent yields via palladium-catalyzed carbonylative addition of aryl bromides to terminal arylalkynes under mild conditions.



7238

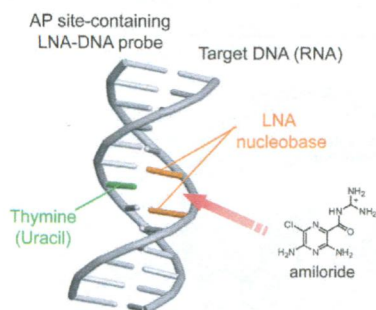


### Microwave assisted synthesis and QSAR study of novel NSAID acetaminophen conjugates with amino acid linkers

Anand D. Tiwari, Siva S. Panda,\* Adel S. Girgis, Sandhyamayee Sahu, Riham F. George, Aladdin M. Srour, Brian La Starza, Abdullah M. Asiri, C. Dennis Hall\* and Alan R. Katritzky

Twelve novel conjugates of NSAID linked by amino acid units to acetaminophen synthesized under microwave irradiation as potential anti-inflammatory agents.

7250

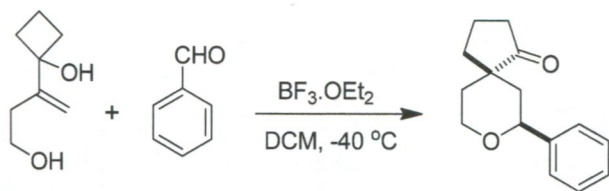


### The effect of LNA nucleobases as enhancers for the binding of amiloride to an abasic site in DNA/DNA and DNA/RNA duplexes

Yusuke Sato, Tetsushi Sato, Takaya Sato, Seiichi Nishizawa and Norio Teramae\*

We report on a significant effect of locked nucleic acid (LNA) nucleobases on the binding of amiloride for abasic site (AP)-containing DNA duplexes.

7257

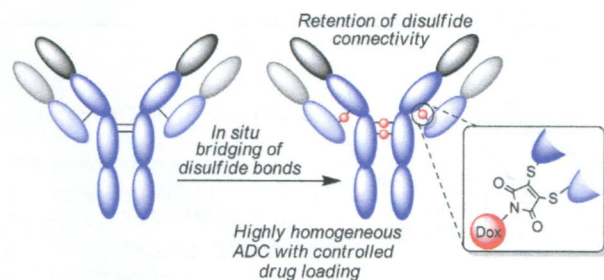


### Tandem Prins/pinacol reaction for the synthesis of oxaspiro[4.5]decan-1-one scaffolds

B. V. Subba Reddy,\* S. Gopal Reddy, M. Ramana Reddy, Manika Pal Bhadra and A. V. S. Sarma

A novel Lewis acid catalyzed Prins/pinacol cascade process has been developed for the synthesis of 7-substituted-8-oxaspiro[4.5]decan-1-ones in good yields with excellent selectivity. This is the first example of the synthesis of oxaspirocycles from aldehydes and 1-(4-hydroxybut-1-en-2-yl)cyclobutanol through a Prins/pinacol cascade.

7261



### Next generation maleimides enable the controlled assembly of antibody-drug conjugates via native disulfide bond bridging

Felix F. Schumacher, João P. M. Nunes, Antoine Maruani, Vijay Chudasama, Mark E. B. Smith, Kerry A. Chester, James R. Baker\* and Stephen Caddick\*

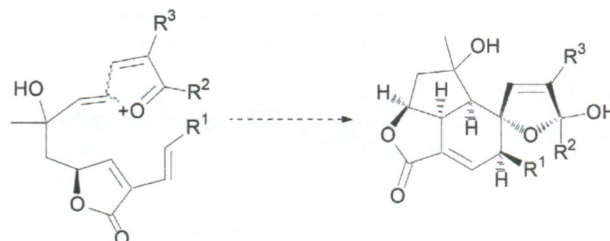
Highly homogeneous ADCs are generated by the efficient bridging of interchain disulfide bonds in trastuzumab, using next generation maleimides.

7270

### Investigation of transannular cycloaddition reactions involving furanoxonium ions using DFT calculations. Implications for the origin of plumarellide and rameswaralide and related polycyclic metabolites isolated from corals

B. Lygo,\* M. J. Palframan and G. Pattenden\*

DFT calculations probing potential cycloaddition pathways leading to the polycyclic ring systems found in the coral secondary metabolites plumarellide, mandapamate and rameswaralide are described.

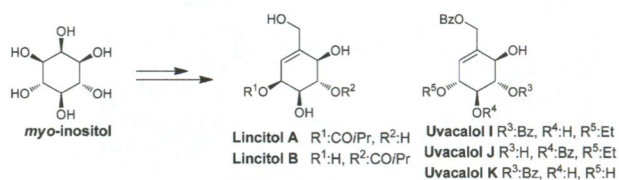


7279

### Total syntheses and structural validation of lincitol A, lincitol B, uvacalol I, uvacalol J, and uvacalol K

Soumik Mondal and Kana M. Sureshan\*

First total syntheses of lincitol A, lincitol B, uvacalol I, uvacalol J and uvacalol K were achieved in racemic form, validating their structure from a common intermediate, which was synthesized in six steps from low-cost and extensively available *myo*-inositol.

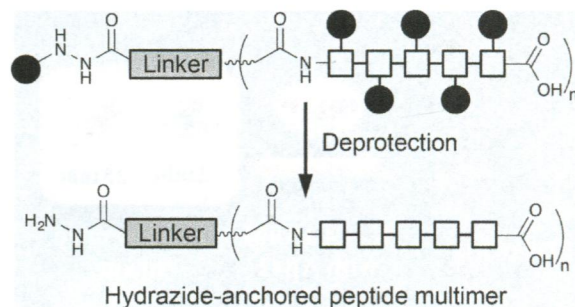


7290

### A hydrazide-anchored dendron scaffold for chemoselective ligation strategies

Liz O'Donovan and Paul A. De Bank\*

We report the design and synthesis of a dendron scaffold, enabling the chemoselective decoration of target molecules with multiple copies of functional species, such as peptides, *via* a hydrazone bond.

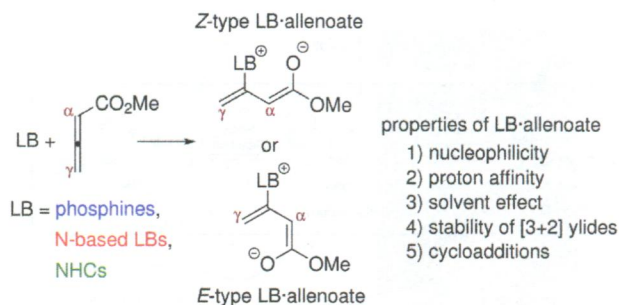


7297

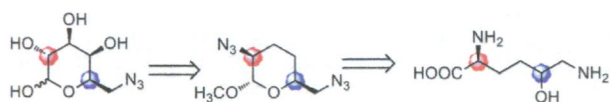
### A computational study of the activation of allenates by Lewis bases and the reactivity of intermediate adducts

Gou-Tao Huang, Timm Lankau and Chin-Hui Yu\*

Several chemical properties of Lewis base-allenolate adducts (LB-allenolate), such as solvent effect, basicity, nucleophilicity and cycloaddition, are studied to provide a detailed foundation for the analysis of LB-catalyzed reactions of allenates.



7310

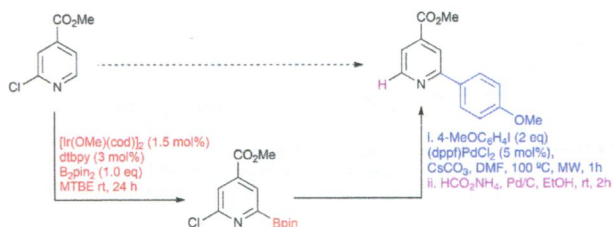


### Facile synthesis of 5-hydroxy-L-lysine from D-galactose as a chiral-precursor

Lina Guo, Taibao Liu, Kai Chen, Tianbang Song, Peng George Wang\* and Wei Zhao\*

A concise synthesis of (2*S*,5*R*) and (2*S*,5*S*)-5-hydroxy-lysine was achieved by utilizing D-galactose as a chiral-precursor with stereo retention. Using the diazido intermediate, the  $\beta$ -D-galactopyranosyl and  $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-galactosyl moieties were synthesized.

7318

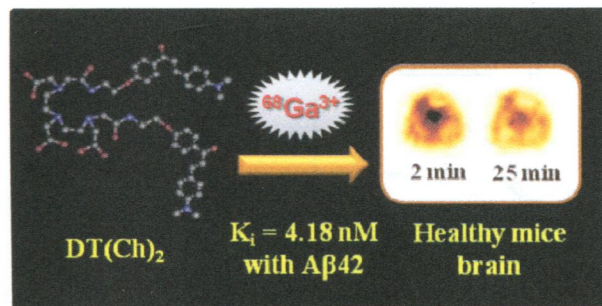


### Iridium-catalyzed C–H borylation of pyridines

Scott A. Sadler, Hazmi Tajuddin, Ibraheem A. I. Mkhaliid, Andrei S. Batsanov, David Albesa-Jove, Man Sing Cheung, Aoife C. Maxwell, Lena Shukla, Bryan Roberts, David C. Blakemore, Zhenyang Lin, Todd B. Marder\* and Patrick G. Steel\*

Iridium-catalysed C–H borylation is an efficient method for the preparation of pyridyl and related azinyl boronate esters.

7328

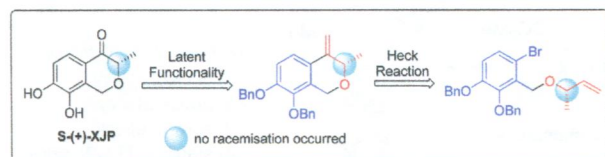


### <sup>68</sup>Ga based probe for Alzheimer's disease: synthesis and preclinical evaluation of homodimeric chalcone in $\beta$ -amyloid imaging

Kanchan Chauhan, Anupama Datta,\* Anupriya Adhikari, Krishna Chuttani, Ajai Kumar Singh and Anil K. Mishra\*

<sup>68</sup>Ga complex of chalcone-based bivalent ligand as a potential candidate for cost-effective PET imaging of Alzheimer's disease: a new perspective.

7338



### First total synthesis of antihypertensive natural products *S*-(+)-XJP and *R*-(-)-XJP

Chaolei Wang, Guoxiang Wei, Xue Yang, Hequan Yao, Jieyun Jiang, Jie Liu,\* Mingqin Shen, Xiaoming Wu and Jinyi Xu\*

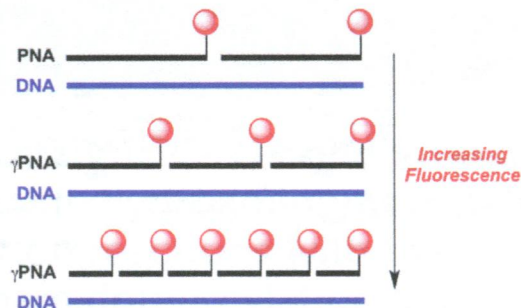
The first total synthesis of *S*-(+)-XJP and *R*-(-)-XJP has been achieved via intramolecular Heck reaction. A latent functionality strategy was implemented to circumvent the racemization in this endeavor.

7345

### Cooperative hybridization of $\gamma$ PNA miniprobcs to a repeating sequence motif and application to telomere analysis

Ha H. Pham, Connor T. Murphy, Gopalsamy Sureshkumar, Danith H. Ly, Patricia L. Opresko and Bruce A. Armitage\*

High affinity  $\gamma$ PNA oligomers hybridize cooperatively on telomeric DNA and provide bright fluorescent signals.

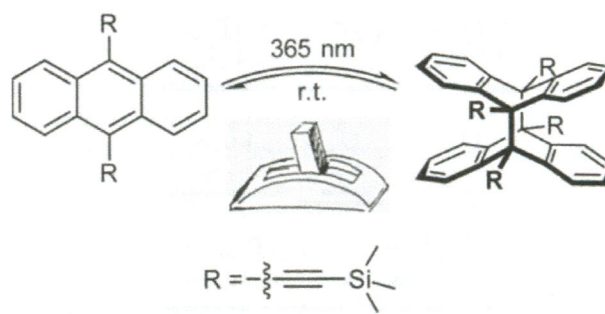


7355

### Polyalkynylanthracenes – syntheses, structures and their behaviour towards UV irradiation

Jan-Hendrik Lamm, Johanna Glatthor, Jan-Henrik Weddelling, Andreas Mix, Jasmin Chmiel, Beate Neumann, Hans-Georg Stammer and Norbert W. Mitzel\*

A series of 1,5-, 1,8-, 9,10- and 1,8,10-alkynyl-substituted anthracenes have been synthesised. Amongst others, 9,10-bis(trimethylsilyl)ethynylanthracene was photo-dimerised. The photodimer is thermally unstable as was investigated by VT NMR spectroscopy.



7366

### Nitroxide-labeled pyrimidines for non-covalent spin-labeling of abasic sites in DNA and RNA duplexes

Sandip A. Shelke, Gunnar B. Sandholt and Snorri Th. Sigurdsson\*

Of ten new pyrimidine-derived nitroxide spin labels, an N1-ethylamino triazole-linked uracil derivative binds fully to both DNA and RNA duplexes containing an abasic site, as determined by CW-EPR.

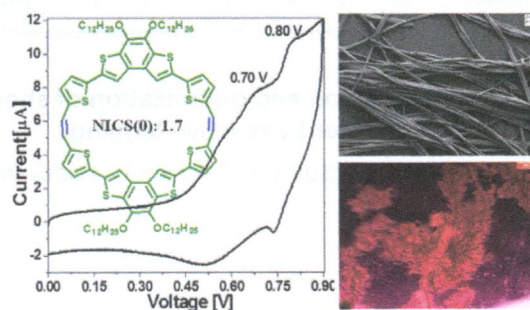


7375

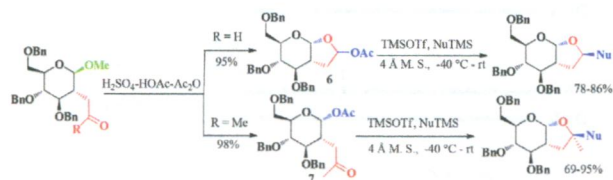
### Benzodithiophene based $\pi$ -conjugated macrocycles: synthesis, morphology and electrochemical characterization

Anjan Bedi\* and Sanjio S. Zade\*

A 7,8-didodecyloxybenzo[1,2-*b*:4,3-*b'*]dithiophene (BdT-Dod) containing a macrocycle was constructed from a thiophene capped BdT-Dod comonomer through a Ti(IV) mediated McMurry reaction. The macrocycle exhibited self-aggregation in the solid state to form microfibers of a thickness of  $\sim$ 400 nm.



7381

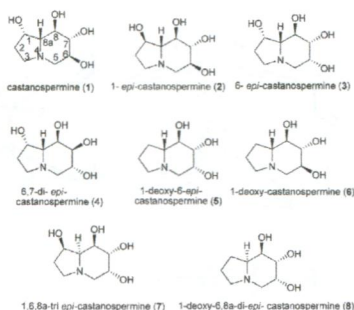


### A neighboring group participation strategy: direct and highly diastereoselective synthesis of 2-substituted and 2,2-bisubstituted perhydrofuro-[2,3-*b*]pyran derivatives

Xiaofeng Ma, Qin Tang, Jun Ke, Jichao Zhang, Xinglong Yang, Xudong Shen and Huawu Shao\*

A highly diastereoselective synthesis method for 2-substituted and 2,2-bisubstituted perhydrofuro[2,3-*b*]pyran derivatives from 2-*C*-branched sugars via a neighboring group participation strategy was developed.

7389

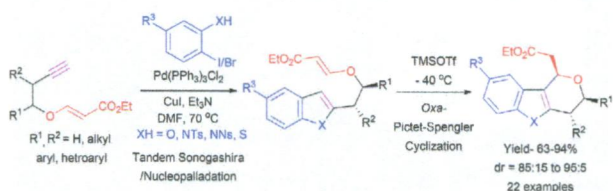


### Divergent total synthesis of 1,6,8a-tri-*epi*-castanospermine and 1-deoxy-6,8a-di-*epi*-castanospermine from substituted azetidin-2-one ( $\beta$ -lactam), involving a cascade sequence of reactions as a key step

Dipak Kumar Tiwari, Kishor Chandra Bharadwaj, Vedavati G. Puranik and Dharmendra Kumar Tiwari\*

A divergent, short, and novel total synthesis of 1,6,8a-tri-*epi*-castanospermine (**7**) and 1-deoxy-6,8a-di-*epi*-castanospermine (**8**) has been developed.

7397



### Stereoselective synthesis of *C*-fused pyranoindoles, pyranobenzofurans and pyranobenzothiophene scaffolds using oxa-Pictet–Spengler type reaction of vinyllogous carbonates

Santosh J. Gharpure\* and V. Prasath

*C*-fused pyranoheterocycles can be assembled in a highly diastereoselective manner using an intramolecular oxa-Pictet–Spengler type reaction of vinyllogous carbonates.

## CORRECTION

7410

### Correction: Identification and optimization of short helical peptides with novel reactive functionality as catalysts for acyl transfer by reactive tagging

Silvia Bezer, Masaomi Matsumoto, Michael W. Lodewyk, Stephen J. Lee, Dean J. Tantillo, Michel R. Gagné\* and Marcey L. Waters\*