

The cover shows the calculated changes in DNA when a thymidine base is exchanged for a spirocyclic nucleotide, as reviewed by Leo Paquette (p. 7).

# AUSTRALIAN JOURNAL OF CHEMISTRY

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## Editorial

### Editorial 2004

*Alison J. Green*

*Aust. J. Chem.* **2004**, *57*, 1–2.



A review of the Journal's achievements during 2003 and a preview of the exciting plans for 2004.

## Notice to Authors 2004

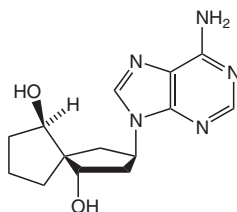
Pages 3–6.

## Review

### Spirocyclic Restriction of Nucleosides

*Leo A. Paquette*

*Aust. J. Chem.* **2004**, *57*, 7–17.



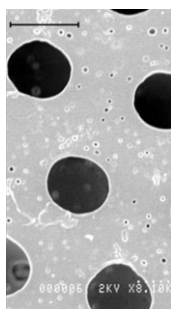
The synthesis of conformationally restricted nucleosides represents an exciting area of synthetic chemistry because select members of this class are amenable to the treatment of viral diseases. This overview describes concise routes towards spiro-fused nucleosides, including those featuring carbon (shown here) and sulfur at the apical position.

## Current Chemistry

### Complex Molecular Architecture Polymers via RAFT

*Leonie Barner, Christopher Barner-Kowollik, Thomas P. Davis, Martina H. Stenzel*

*Aust. J. Chem.* **2004**, *57*, 19–24.



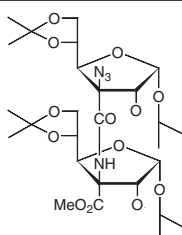
Hydrogels have attracted great attention owing to their potential biomedical application as contact lenses, wound dressings, and drug delivery vectors. This paper outlines the syntheses of such polymers via RAFT polymerization. The synthesis of polystyrene star polymers (an SEM image of which is shown here) using functionalized  $\beta$ -cyclodextrins is also discussed.

## Rapid Communications

### An Alternative Synthesis of Some Carbohydrate $\alpha$ -Amino Acids

*Grant S. Forman, Adrian Scaffidi, Robert V. Stick*

*Aust. J. Chem.* **2004**, *57*, 25–28.



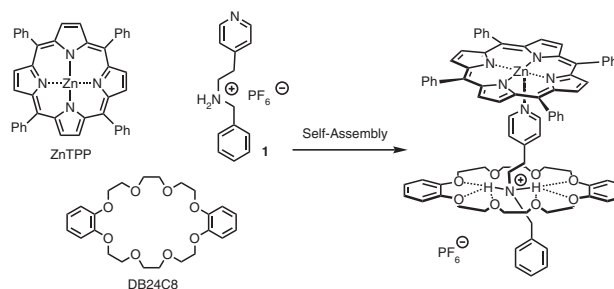
The Corey–Link reaction provides a ready access to  $\alpha$ -azido esters, direct precursors of  $\alpha$ -amino acids. Such a sequence has been applied to synthesize some carbohydrate  $\alpha$ -amino acids. Further, an amino ester and an azido acid have been coupled to form a dipeptide (shown).

### A Three Component Metalloporphyrin Assembly

Steven J. Langford, Vei-Lin Lau

*Aust. J. Chem.* **2004**, 57, 29–32.

The amount of molecular instruction programmed into **1**·PF<sub>6</sub> directs the two macrocyclic components, dibenzo-[24]crown-8 and zinc(II) tetraphenylporphyrin, into regiospecifically forming the [2]pseudorotaxane in a single step.



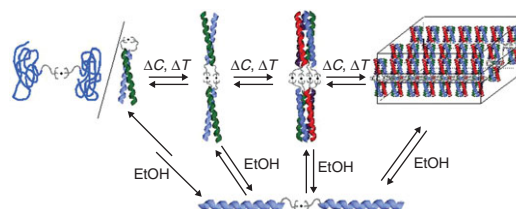
### Full Papers

#### Metal Ion Assisted Folding and Supramolecular Organization of a De Novo Designed Metalloprotein

Guido W. M. Vandermeulen,  
Christos Tziatzios, Dieter Schubert,  
Philip R. Andres, Alexander Alexeev,  
Ulrich S. Schubert, Harm-Anton Klok

*Aust. J. Chem.* **2004**, 57, 33–39.

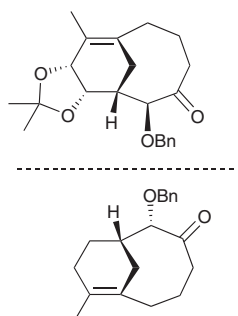
A detailed study of the folding and self-organization of a metalloprotein is presented. The metalloprotein's tertiary and quaternary structure was determined by the interplay of the combined processes of metal ion complexation and peptide folding. Folding and supramolecular organization could be manipulated by concentration, temperature, pH, and solvent.



#### Taxane Diterpene Synthesis Studies. Part 1: Chemoenzymatic and Enantiodivergent Routes to AB-ring Substructures of Taxoids and *ent*-Taxoids

Martin G. Banwell, Penny Damos,  
David C. R. Hockless

*Aust. J. Chem.* **2004**, 57, 41–52.



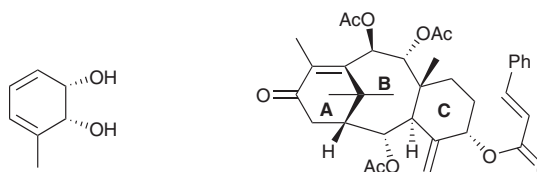
The illustrated and pseudo-enantiomeric AB-ring substructures of taxoids and *ent*-taxoids have been prepared from a common, readily available, and enantiomerically pure precursor.

#### Taxane Diterpene Synthesis Studies. Part 2: Towards Taxinine—Enantiospecific Construction of an AB-ring Substructure Incorporating both Quaternary Carbon Centres and Attempts to Annulate the C-ring

Martin G. Banwell,  
Malcolm D. McLeod, Andrew G. Riches

*Aust. J. Chem.* **2004**, 57, 53–66.

The enantiomerically pure *cis*-1,2-dihydrocatechol (left structure) has been converted into a bicyclic product incorporating many of the structural features associated with the AB-ring substructure of the enantiomer of the illustrated diterpene taxinine (right structure).

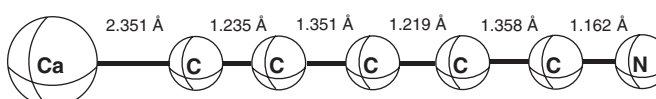


#### Circumstellar Calcium Chemistry

Simon Petrie

*Aust. J. Chem.* **2004**, 57, 67–76.

The feasibility of generating calcium-containing molecules as large as CaC<sub>5</sub>N within outflowing circumstellar envelopes, by a mechanism analogous to that held to account for similar magnesium-containing molecules, is explored through high-level quantum chemical calculations. Prospects for detecting these species are also discussed.

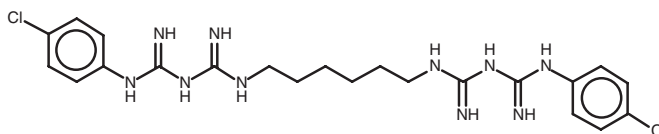


### Synthesis, Biological Activity, and QSAR Studies of Antimicrobial Agents Containing Biguanide Isosteres

Gregory T. Wernert, David A. Winkler,  
George Holan, Gina Nicoletti

*Aust. J. Chem.* **2004**, 57, 77–85.

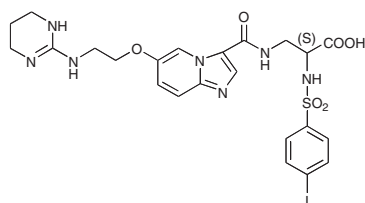
The antimicrobial properties of analogues of chlorhexidine (shown) are reported. Their activity showed a parabolic dependence on the lipophilicity of compounds and it was essential that compounds be charged at a physiological pH. The activity of this class of agents was also compared with other QSAR studies of a wide range of antimicrobial agents.



### Molecular Modelling and Design of Radiolabelled Complexes for Melanoma Diagnosis

C. T. Tell Tuttle, Shane A. Seabrook,  
Lauren E. Wise, Andrew Katsifis,  
Robert B. Knott, Brian F. Yates

*Aust. J. Chem.* **2004**, 57, 87–96.

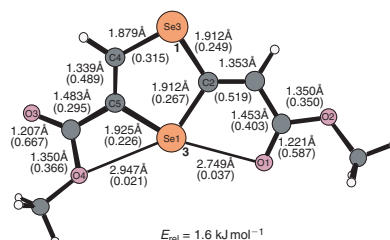


Molecular modelling has identified a novel radiolabelled antagonist which is predicted to be highly active at the  $\alpha_V\beta_3$  integrin receptor and to have a high degree of selectivity compared to the  $\alpha_{IIb}\beta_3$  receptor. These results are guiding the design of radiolabelled complexes for melanoma diagnosis.

### Ethyl 2-(2-Ethoxy-2-oxoethylidene)-1,3-diselenole-4-carboxylate—an Example of Unconventional Bonding in Organic Selenides

Michael W. Carland, Carl H. Schiesser,  
Jonathan M. White

*Aust. J. Chem.* **2004**, 57, 97–100.



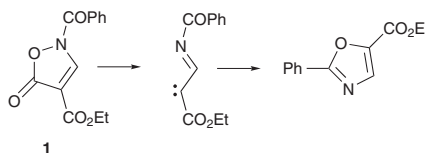
The title diselenole was isolated as a mixture of geometric isomers. These interesting crystalline compounds were found to exhibit unconventional bonding involving the oxoethylidene oxygen and the proximate selenium atom. Interestingly, the *Z*-isomer (pictured) was found to contain the shortest ‘non-bonded’ selenium–oxygen contact yet recorded.

### Triplet Lifetimes, Solvent, and Intramolecular Capture of Isoxazolones

Kiah H. Ang, Matthew Cox,  
Warren D. Lawrance, Rolf Prager,  
Jason A. Smith, Warren Staker

*Aust. J. Chem.* **2004**, 57, 101–105.

Isoxazolones, such as **1**, are a reliable source of singlet carbenes for synthesis purposes upon decarboxylation. The process of photochemical decarboxylation presumably proceeds from a triplet isoxazolone; this paper presents the first evidence for such a triplet state.

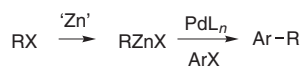


## Focus

### Advances in the Negishi Coupling

Guillaume Lessene

*Aust. J. Chem.* **2004**, 57, 107.



Negishi coupling reactions provide a mild and extremely effective way to create carbon–carbon bonds from highly functionalized precursors. This paper outlines recent developments in the two steps involved in this reaction, namely the preparation of organozinc reagents, with several now being commercially available, and the use of new palladium catalyst/ligand combinations.

## Book Reviews

Pages 109–110.

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