



Virtual screening aims to identify classes of biologically active molecules for a given assay; the challenge is to provide better performance (faster, cheaper) than experimental methods. Learn more in the review by Branson and Smith (p. 1029).

AUSTRALIAN JOURNAL OF CHEMISTRY

AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

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Reviews

The Role of Virtual Screening in Computer Aided Structure-Based Drug Design

Kim M. Branson, Brian J. Smith

Aust. J. Chem. **2004**, 57, 1029–1037.

```
for r1 in 'cat R1';
do for r2 in 'cat R2';
do for r3 in 'cat R3';
do echo "c1c($r1)cc($r2)c($r3)c1" >>Combi_library;
done;
done;
done;
```

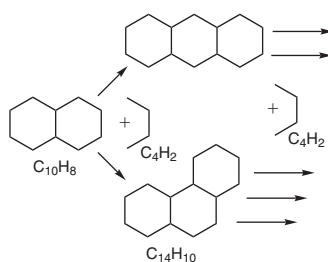
R1	R2	R3	Combi_library
H F Cl Br	C CC C(C)C	O C(O)O N	c1c(H)cc(C)c(O)c1 c1c(H)cc(C)c(C(O)O)c1 c1c(H)cc(C)c(N)c1 . . .

The pharmaceutical industry is under constant pressure to increase the production of new pharmaceuticals and reduce development costs (estimated to be upward of \$US 800 million for a new drug). This review examines the current status of in silico screening methods, an example of which is shown, with an emphasis on removing leads that are unlikely to produce the desired results.

A Periodic Table for Benzenoid Hydrocarbon Isomer Classes and Beyond

Jerry Ray Dias

Aust. J. Chem. **2004**, 57, 1039–1049.



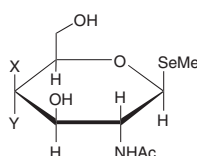
The concept of a periodic table set or a 'super spreadsheet' is demonstrated here for the benzenoid hydrocarbons. These compounds have been organized into a Periodic Table for Benzenoid Hydrocarbons, which allows the identification and understanding of property trends and demonstrates the use of such devices for helping study similar sets of compounds.

Rapid Communication

Synthesis of Methyl 2-Acetamido-2-deoxy-1-seleno-β-D-glucopyranoside: Selenium Metabolites in Human Urine

Pedro Traar, Ferdinand Belaj,
Kevin A. Francesconi

Aust. J. Chem. **2004**, 57, 1051–1053.



The metalloid selenium is of interest in human health because not only is it an essential trace element but also it can elicit toxic effects at modest intake levels. Here, a simple and efficient synthesis of two selenium metabolites (pictured; X,Y = H,OH or OH,H) found in human urine is reported, which will be used in further studies on the metabolism and toxicology of selenium.

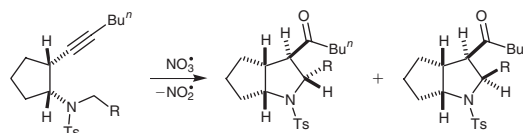
Full Papers

NO₃[•] Induced Self-Terminating Radical Oxygenations: Diastereoselective Synthesis of Anellated Pyrrolidines

Arne Stademann, Uta Wille

Aust. J. Chem. **2004**, 57, 1055–1066.

Nitrate radicals were used as oxidants to synthesize anellated pyrrolidines (pictured) through a diastereoselective self-terminating, oxidative radical cyclization cascade. The diastereoselectivity of this reaction sequence was found to be strongly influenced by the nature of the substituents at the nitrogen atom.

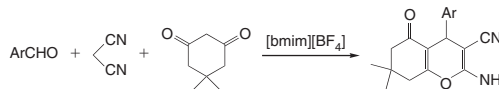


Ionic Liquid Promoted Knoevenagel and Michael Reactions

Xuesen Fan, Xueyuan Hu, Xinying Zhang,
Jianji Wang

Aust. J. Chem. **2004**, 57, 1067–1071.

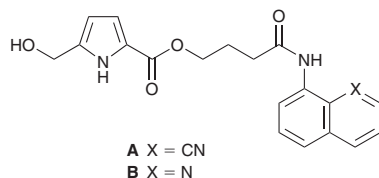
The utilization of the ionic liquid [bmim][BF₄] as both reaction medium and promoter for the title reactions is demonstrated here with the synthesis of some useful electrophilic alkenes and chromene derivatives in high yields (pictured). The discussed benefits include mild conditions, cleaner reactions, and easy and efficient recovery and recycling of the reaction medium.



The Synthesis and Testing of α -(Hydroxymethyl)pyrroles as DNA Binding Agents

Derek C. Martyn, Andrew D. Abell

Aust. J. Chem. **2004**, 57, 1073–1077.

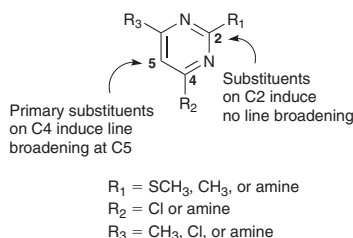


α -(Hydroxymethyl)pyrroles are an important class of π -excessive heterocycle that are particularly susceptible to nucleophilic substitution. The α -(hydroxymethyl)pyrroles **A** and **B** were prepared and shown to be cytotoxic against the P388 cancer cell line. Compound **B** was also shown to bind to DNA in a DNA binding assay.

Identification of Aminopyrimidine Regioisomers via Line Broadening Effects in ¹H and ¹³C NMR Spectroscopy

James Garner, Tim Hill, Luke Odell,
Paul Keller, Jody Morgan,
Adam McCluskey

Aust. J. Chem. **2004**, 57, 1079–1083.



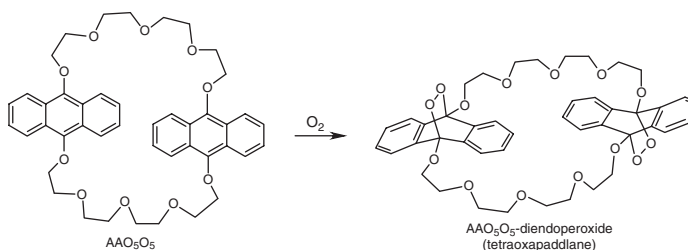
Substituted mono- and di-aminopyrimidines were synthesized as part of a medicinal chemistry programme. Primary amines substituted at the 4-position exhibited room-temperature line broadening effects in both ¹H and ¹³C NMR spectroscopy due to the presence of rotamers, but such effects were not observed for substituents in the 2-position. This provided a simple diagnostic tool for the identification of regioisomers, a determination which would otherwise have required two-dimensional experiments.

Molecular and Crystal Structure of a Bisanthracene-9,10-diyl Macrocyclic Coronand AAO₅O₅ and of its Bis-1,4-endoperoxide, a Bistetraoxapaddlane

Pierre Marsau, Gérard Guinand,
Jean Hirschberger, Jean-Pierre Desvergne,
Henri Bouas-Laurent

Aust. J. Chem. **2004**, 57, 1085–1089.

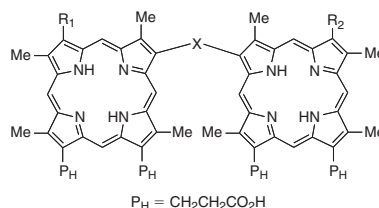
The successful determination of the crystal structure of AAO₅O₅, a bisanthracene macrocyclic cyclophane capable of acting as an Na⁺ fluorosensor, is reported here. The bisendoperoxide of AAO₅O₅ (shown), also isolated in its crystalline state, represents the first tetraoxa[2.2.2.*n*] paddlane, analogues of which should prove a strong synthetic challenge.



The Photodynamic Therapy (PDT) Anticancer Activity of a Range of Porphyrin Dimers and Related Compounds Derived from Hematoporphyrin

Christopher J. Byrne, Mathew A. Cooper,
Prudence A. Cowled,
Robert A. W. Johnstone,
Lorraine Mackenzie, Lorely V. Marshallsay,
Ian K. Morris, Craig A. Muldoon,
Mark J. Raftery, Sek Sau Yin, A. David Ward

Aust. J. Chem. **2004**, 57, 1091–1102.

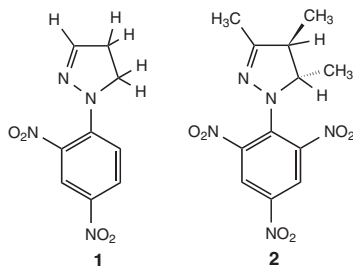


The photoactive fraction of hematoporphyrin derivative (HPD), known as Photofrin II and produced from hematoporphyrin IX, is a complex mixture of porphyrin dimers and oligomers. A series of diporphyrins and analogous compounds were synthesized and their photodynamic activity assessed to help identify factors that influence their anticancer activity (such as the presence of hydrophobic side chains).

The Structure of Two 1-(Nitrophenyl)- Δ^2 -pyrazolines: a Crystallographic and Theoretical Study

Glenn P. A. Yap, Ibon Alkorta,
Nadine Jagerovic, José Elguero

Aust. J. Chem. **2004**, 57, 1103–1108.



The crystal and molecular structures of two pyrazolines, 1-(2',4'-dinitrophenyl)-2-pyrazoline **1** and *trans*-1-(2',4',6'-trinitrophenyl)-3,4,5-trimethyl- Δ^2 -pyrazoline **2**, are reported. A theoretical analysis revealed that the *ortho*-nitro group interacts with the lone pair of electrons of the pyrazoline –N= atom, thus explaining the preferred conformation.

Bandshape Parameters' Dependence on Solvent in Raman Excitation Profiles, and Absorption Spectra of Violaxanthin and Lutein

Gia G. Maisuradze

Aust. J. Chem. **2004**, 57, 1109–1115.

Experimentally determined Raman excitation profiles (REPs) and absorption spectra for two example carotenoids in a variety of solvents have been interpreted in terms of an improved vibronic interaction theory to study solute–solvent interaction. The major mechanistic contributions to band broadening are shown to be solvent-dependent.

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