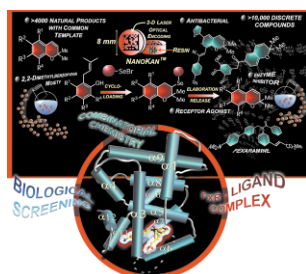


Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica

**Cover**See K. C. Nicolaou *et al.*, page 908

The cover shows combinatorial techniques used to synthesize a compound library from which potent ligands for the farnesoid X receptor (FXR) were discovered, and an X-ray crystallographic structure of a complex between one of these ligands and FXR.



Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*:
www.rsc.org/chembiol

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Profile: *Organic & Biomolecular Chemistry* profiles Professor K. C. Nicolaou

PERSPECTIVE

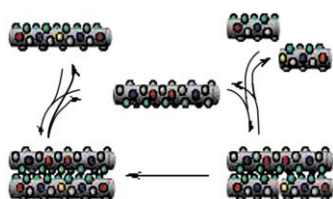
901

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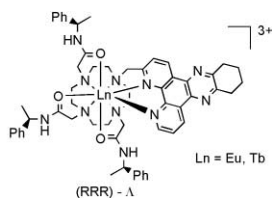
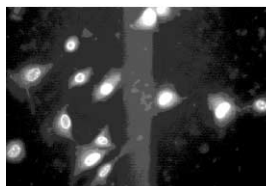
Challenges in the design of self replicating peptides

Xiangqun Li and Jean Chmielewski

Self replicating peptides hold much promise for use in biotechnology. Challenges facing their application are explored in this review.



905 907



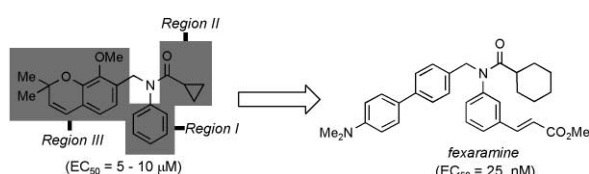
Luminescent nonacoordinate cationic lanthanide complexes as potential cellular imaging and reactive probes

Juan C. Frias, Gabriella Bobba, Martin J. Cann, Chris J. Hutchison and David Parker

Emissive lanthanide complexes are efficiently taken up by cells and localise in the cell nucleus; irradiation at 350 nm leads to cell death.

ARTICLES

908 920

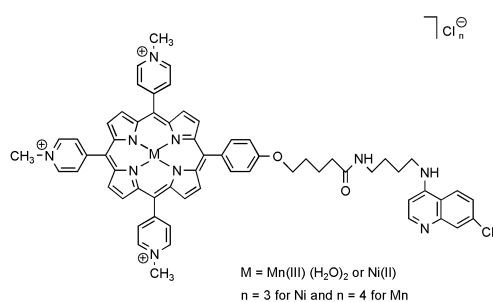


Discovery and optimization of non-steroidal FXR agonists from natural product-like libraries

K. C. Nicolaou, Ronald M. Evans, A. J. Roecker, Robert Hughes, Michael Downes and Jeffery A. Pfefferkorn

Four novel classes of FXR activators including the most potent agonists to date are reported.

921 927

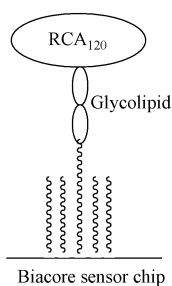


Porphyrin-aminopyridine conjugates as telomerase inhibitors

Alexandrine Maraval, Sonia Franco, Corine Vialas, Geneviève Pratviel, Maria A. Blasco and Bernard Meunier

Metalloporphyrin-aminopyridine hybrid molecules were prepared to target telomeric DNA as potential anticancer agents.

928 938

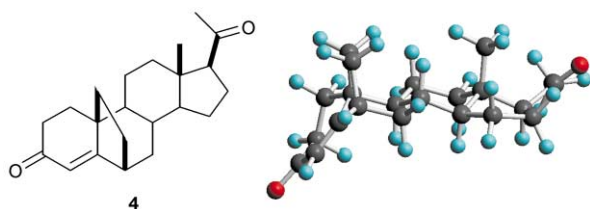


Carbohydrate-protein interactions at interfaces: synthesis of thiolactosyl glycolipids and design of a working model for surface plasmon resonance

Peter Critchley, M. Nicolas Willand, Atvinder K. Rullay and David H. G. Crout

Binding of RCA₁₂₀ lectin to lactose glycolipids is detected by surface plasmon resonance.

939 943

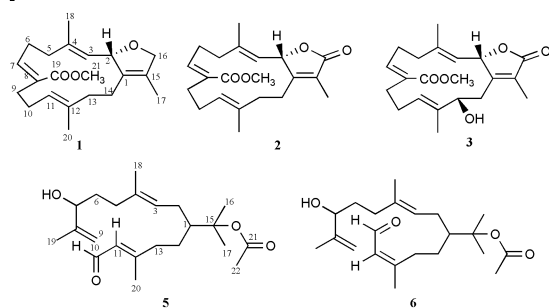


6,19-Carbon-bridged steroids. Synthesis of 6,19-methano-progesterone

María Joselevich, Alberto A. Ghini and Gerardo Burton

The methano-bridged progesterone analogue **4**, with a bent structure at the A/B ring junction, was synthesized in nine steps.

944 949

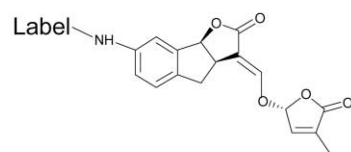


New cytotoxic cembrane based diterpenes from the soft corals *Sarcophyton cherbonnieri* and *Nephthea* sp.

Harald Gross, Stefan Kehraus, Markus Nett, Gabriele M. König, Winfried Beil and Anthony D. Wright

New furano-cembranoids (**1–3**) and seco-cembranoid acetates (**5, 6**) from *Nephthea* sp. and *Sarcophyton cherbonnieri*.

950 959

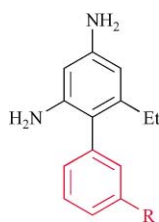


Synthesis and bioactivity of labelled germination stimulants for the isolation and identification of the strigolactone receptor

Anat Reizelman, Suzanne C. M. Wigchert, Cinzia del-Bianco and Binne Zwanenburg

Parasitic weeds belonging to the genera *Striga* and *Orobanche* severely reduce yields of economically important crops worldwide. This paper deals with the synthesis of labelled germination stimulants that might be used for the isolation of the strigolactone receptor.

960 964

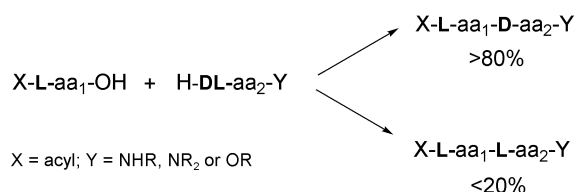


Pyrimethamine analogs as strong inhibitors of double and quadruple mutants of dihydrofolate reductase in human malaria parasites

Alireza Sardarian, Kenneth T. Douglas, Martin Read, Paul F. G. Sims, John E. Hyde, Penchit Chitnumsub, Rachada Sirawaraporn and Worachart Sirawaraporn

The best of these inhibitors was the *meta*-bromo analog, which is a strong inhibitor of the recombinant DHFR bearing the four mutations that cause clinical resistance to pyrimethamine, and also a strong inhibitor of the growth of parasite cultures carrying such a mutation pattern.

965 972

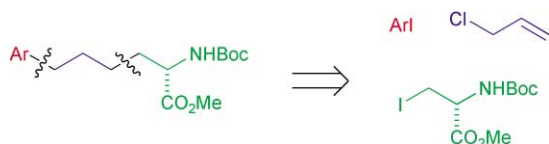


Enantioselection in peptide bond formation

Roger R. Hill, David Birch, Graham E. Jeffs and Michael North

N-Acylamino acids show a marked preference for heterochiral coupling when they form peptides with other amino acid amides or esters.

973 977

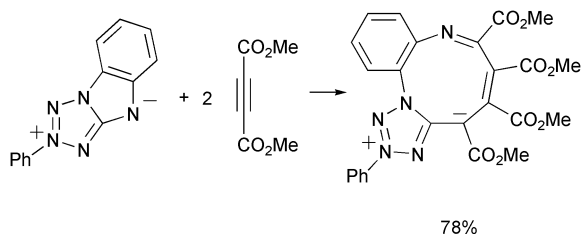


Combined application of organozinc chemistry and one-pot hydroboration–Suzuki coupling to the synthesis of amino acids

Arantxa Rodríguez, David D. Miller and Richard F. W. Jackson

A modular approach to the synthesis of phenylalanine homologues using a combination of metal-catalysed processes is described.

978 983

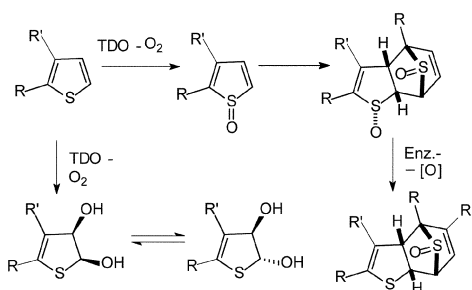


Reaction cascades initiated by nucleophilic attack of heteropentalene mesomeric betaine and nitrogen-rich mesoionic tetrazolium-5-amides on electron-deficient unsaturated compounds. Synthesis of novel heterocyclic systems

Shuki Araki, Masashi Kuzuya, Kenji Hamada, Masatoshi Nogura and Nayumi Ohata

Tetrazole mesomeric compounds show unique reaction behaviour towards electrophiles and are useful building blocks for the synthesis of new nitrogen heterocycles.

984 994

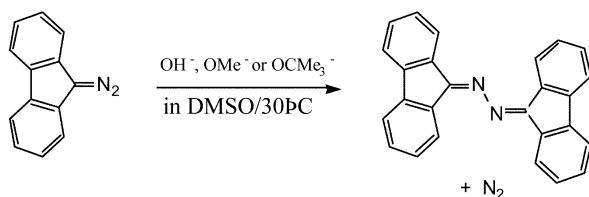


Dioxygenase-catalysed oxidation of monosubstituted thiophenes: sulfoxidation versus dihydrodiol formation

Derek R. Boyd, Narain D. Sharma, Nimal Gunaratne, Simon A. Haughey, Martina A. Kennedy, John F. Malone, Christopher C. R. Allen and Howard Dalton

A model is presented to allow prediction of when dioxygenase-catalysed thiophene sulfoxidation and *cis/trans* dihydroxylation will occur.

995 1003

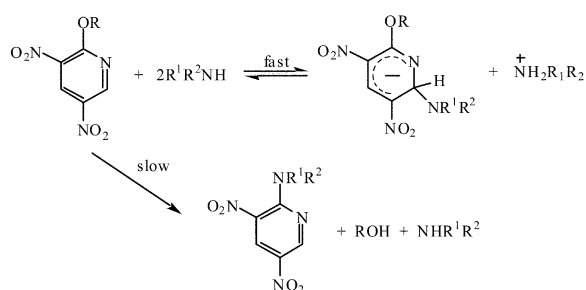


The decomposition of diazo-compounds induced by nucleophiles. The decomposition of 9-diazofluorene in the presence of hydroxide or alkoxide ions

Linda J. McDowell, M. Mehdi Khodaei and Donald Bethell

The rate equation, $v = k[\text{FIN}_2]^{3/2}[\text{Nu}^-]^{1/2}$, where Nu^- represents HO^- , RO^- or a fluorenyl anion, suggests an electron-transfer chain mechanism.

1004 1011

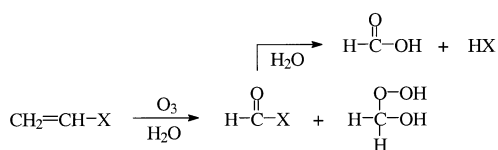


Kinetic and equilibrium studies of σ -adduct formation and nucleophilic substitution in the reactions of 2-phenoxy-3,5-dinitropyridine and 2-ethoxy-3,5-dinitropyridine with aliphatic amines in dipolar aprotic solvents

Michael R. Crampton, Thomas A. Emokpae, Judith A. K. Howard, Chukwuemeka Isanbor and Raju Mondal

Rate and equilibrium data, measured in DMSO, dimethylformamide and acetonitrile, are reported for the competitive nucleophilic attack by amines at the 2- and 6-positions of 2-substituted-3,5-dinitropyridines.

1012 1019



Ozonolysis of vinyl compounds, $\text{CH}_2=\text{CH-X}$, in aqueous solution—the chemistries of the ensuing formyl compounds and hydroperoxides

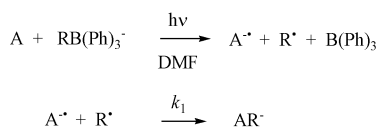
Achim Leitzke, Roman Flyunt, Jacob A. Theruvathu and Clemens von Sonntag

Reactions of ozone with $\text{CH}_2=\text{CH-X}$ give rise to formyl compounds which usually hydrolyse readily; there are interesting exceptions.

1020 1025

Direct determination of rate constants for coupling between aromatic radical anions and alkyl and benzyl radicals by laser-flash photolysis

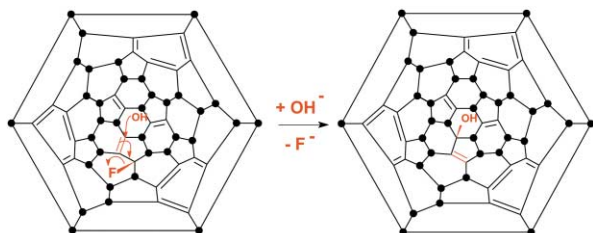
Torben Lund, Peter Christensen and Robert Wilbrandt

Coupling rates k_1 between radicals and aromatic radical anions have been obtained by a new laser-flash photolysis method.

1026 1033

In the first proven S_N2' fullerene reaction, both C_3 and C_1 $C_{60}F_{36}$ hydrolyse to C_1 isomers of $C_{60}F_{35}OH$ that eliminate HF to give epoxides $C_{60}F_{34}O$; $C_{60}F_{36}O$ oxides are shown to be ethers, and a fourth isomer of $C_{60}F_{36}$ exists

Anthony G. Avent, Ala'a K. Abdul-Sada, Brian W. Clare, David L. Kepert, Joan M. Street and Roger Taylor

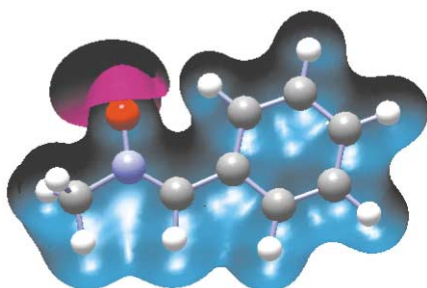
Two isomers of $C_{60}F_{35}OH$, produced by the first proven S_N2' reaction of a fullerene derivative, have been isolated and fully characterised.

1034 1040

Experimental and theoretical charge distribution in (*Z*)-*N*-methyl-*C*-phenylnitron

David E. Hibbs, Jane R. Hanrahan, Michael B. Hursthouse, David W. Knight, Jacob Overgaard, Peter Turner, Ross O. Piltz and Mark P. Waller

The molecular electrostatic potential derived from the electron density distribution indicates likely activity of the studied nitrones.

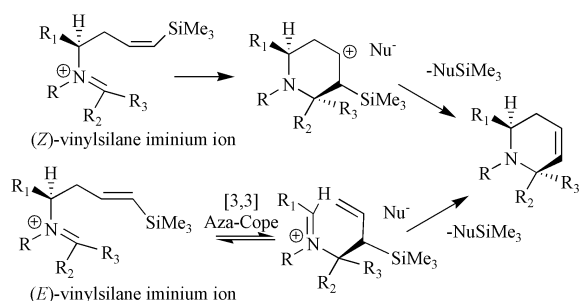


1041 1048

Experimental and quantum-mechanical investigation of the vinylsilane-iminium ion cyclization

Lisbet Kværnø, Per-Ola Norrby and David Tanner

Quantum-mechanical calculations rationalize observed reactivity/diastereoselectivity trends in the vinylsilane-iminium ion cyclization.

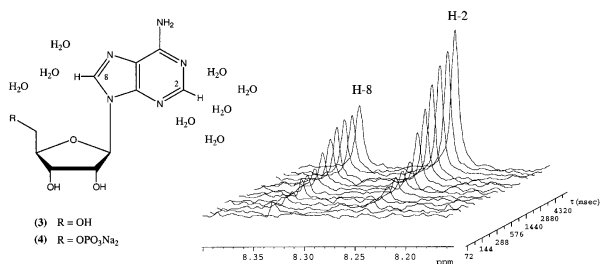


1049 1052

Site-specific solvation determined by intermolecular nuclear Overhauser effect—measurements and molecular dynamics

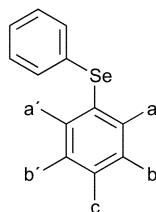
Manuel Angulo, Christoph Hawat, Hans-Jörg Hofmann and Stefan Berger

NOE transfer measurements are shown to provide information on the arrangement of solvent molecules in the vicinity of various structural parts of a solute, which could be important for the understanding of its behaviour in solution and contribute to a better understanding of solvation phenomena.





1053 1060

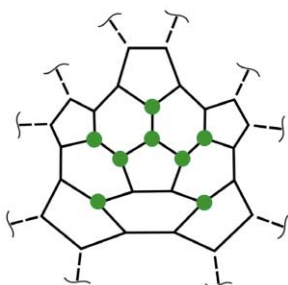


Relations between ^{77}Se NMR chemical shifts of (phenylseleno)-benzenes and their molecular structures derived from nine X-ray crystal structures

Jette Oddershede, Lars Henriksen and Sine Larsen

Through-space interactions between selenium and the *o*-substituents in the solid state are also likely to be present in solution.

1061 1066

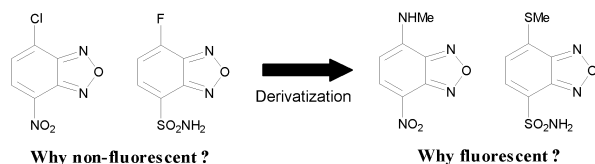


The energies of some isomers of C_{60}F_8 : the use of experimental and theoretical considerations to limit candidate structures

John P. B. Sandall and Patrick W. Fowler

Energy and NMR compatibility factors allow assignment of C_{60}F_8 as a low-energy isomer containing an isolated cyclopentene unit.

1067 1072



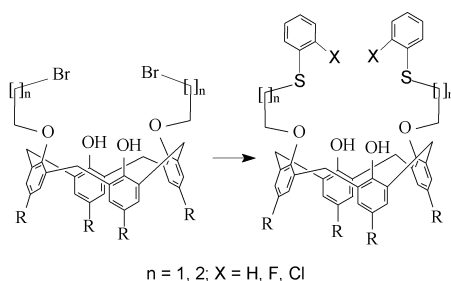
Fluorescence on–off switching mechanism of benzofurazans

Seiichi Uchiyama, Kazuyuki Takehira, Shigeru Kohtani, Kazuhiro Imai, Ryoichi Nakagaki, Seiji Tobita and Tomofumi Santa

The fluorescence on–off switching mechanism of the well-known fluorogenic reagents having a benzofurazan skeleton has been elucidated by the measurements of fluorescence, phosphorescence, photolysis, and time-resolved thermal lensing signals.



1073 1079



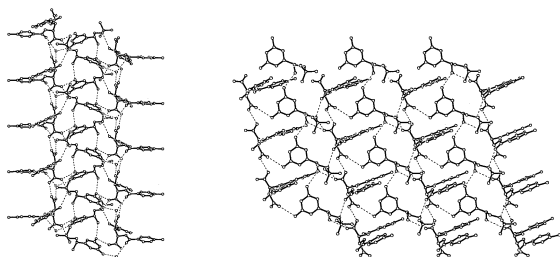
Synthesis of a tweezer-like bis(arythiaalkoxy)calix[4]arene as a cation sensor for ion-selective electrodes: an investigation of the influence of neighboring halogen atoms on cation selectivity

Xianshun Zeng, Hao Sun, Langxing Chen, Xuebing Leng, Fengbo Xu, Qinshan Li, Xiwen He, Wenqin Zhang and Zheng-Zhi Zhang

Some new tweezer-like substituted calix[4]arenes were synthesized and their properties as ion-selective electrodes investigated.



1080 1085



Facile resolution of racemic terbutaline and a study of molecular recognition through chiral supramolecules based on enantiodifferentiating self-assembly

Jian Liao, Xiaohua Peng, Juhua Zhang, Kaibei Yu, Xin Cui, Jin Zhu and Jingen Deng

An effective resolution of the chiral drug, (*R*)-terbutaline (**1**) was achieved and the different supramolecular structures of the less- (column) and more- (sheet) soluble salts (based on the enantiodifferentiating self-assembly between (2*S*,3*S*)-di-*O*-(*p*-toluoyl) tartaric acid (D-DTTA) and two enantiomers of *rac*-**1**, respectively) contribute to chiral discrimination.



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