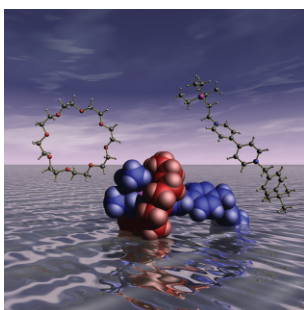


Organic & Biomolecular Chemistry

INDEXED IN MEDLINE

Incorporating Acta Chemica Scandinavica

**Cover**

See Norma Georges, Stephen J. Loeb, Jorge Tiburcio and James A. Wisner, pp. 2751–2756. Both phosphonium and pyridinium groups can be incorporated into the recognition element of a linear axle and together with 24-crown-8 ether wheels used to make [2]rotaxanes.

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contents

C73 C80

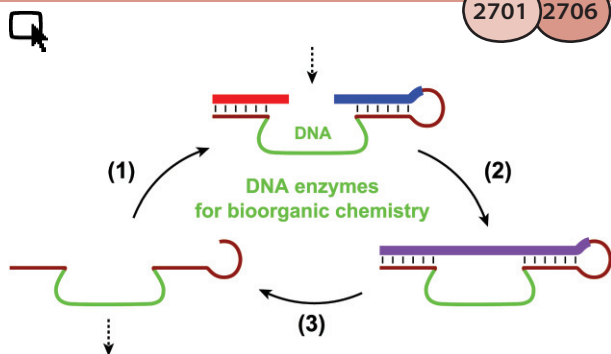
Chemical Science

October 2004/Volume 1/Issue 10

www.rsc.org/chemicalscience

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant advances.

2701 2706



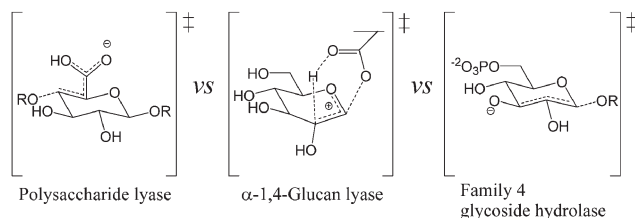
EMERGING AREA

Deoxyribozymes: DNA catalysts for bioorganic chemistry

Scott K. Silverman

Deoxyribozymes are DNA catalysts with significant promise for applications in bioorganic chemistry.

2707 2713

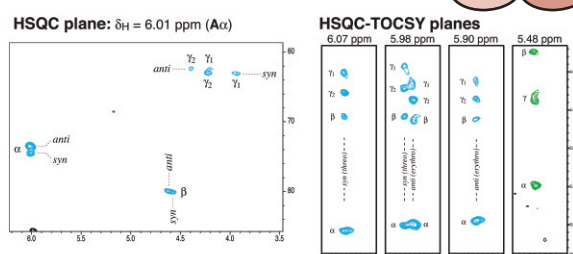


Nature's many mechanisms for the degradation of oligosaccharides

Vivian L. Y. Yip and Stephen G. Withers

In addition to classical oxocarbenium ion-like mechanisms, oligosaccharide cleavage can involve direct elimination or oxidation–elimination–addition–reduction sequences.

2714 2715



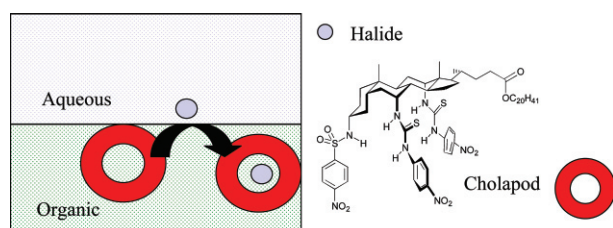
Clean 2D slices containing lignin sidechain data from a 3D TOCSY-HSQC NMR spectrum of unfractionated pine cell walls (following ball-milling/acetlylation).

Cryoprobe 3D NMR of acetylated ball-milled pine cell walls

John Ralph and Fachuang Lu

3D NMR of solubilized ball-milled pine cell walls reveals striking details of lignin units, right down to differentiating stereoisomers in the polymer.

2716 2718

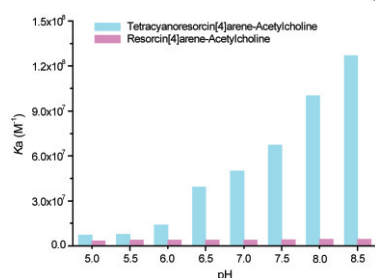


Electrochemical quantification of high-affinity halide binding by a steroid-based receptor

Robert A. W. Dryfe, Simon S. Hill, Anthony P. Davis, Jean-Baptiste Joos and Edward P. L. Roberts

Liquid/liquid voltammetry has been used to quantify the strength of binding of halides to cholapod ligands, showing that the affinities for halide ions are very high and peak at chloride.

2719 2721

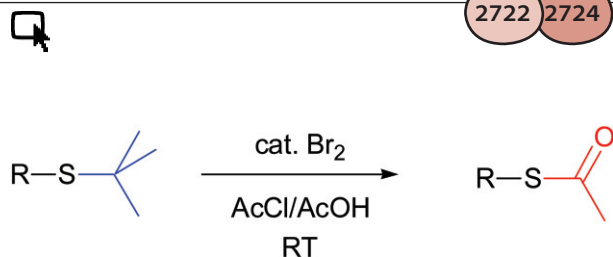


Tetracyanoresorcin[4]arene as a pH dependent artificial acetylcholine receptor

Song-De Tan, Wen-Hua Chen, Akiharu Satake, Bo Wang, Zun-Le Xu and Yoshiaki Kobuke

Tetracyanoresorcin[4]arene was synthesized to show highly pH dependent affinities for acetylcholine in the physiological pH region.

2722 2724



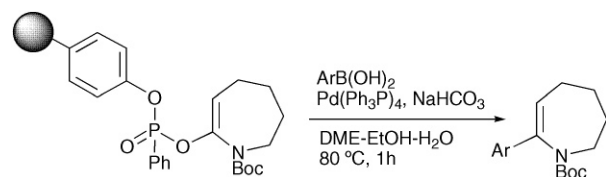
Bromine catalyzed conversion of *S*-*tert*-butyl groups into versatile and, for self-assembly processes accessible, acetyl-protected thiols

Alfred Błaszczyk, Mark Elbing and Marcel Mayor

Facile and efficient conversion of the robust and easy to introduce *tert*-butyl thiol group into a versatile *in situ* hydrolysable acetyl protected thiol.



2725 2727



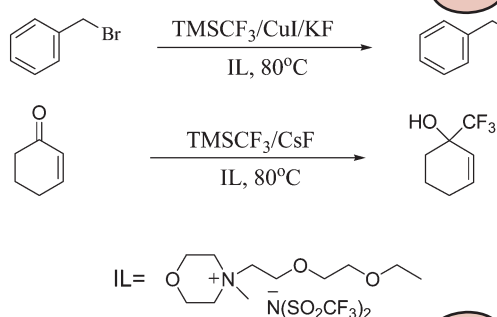
A simple solid phase diversity linker strategy using enol phosphonates

Ian B. Campbell, Jun Guo, Edward Jones and Patrick G. Steel

Solid supported enol phosphonates are easily prepared and provide a stable, storable, diversity linker cleavable by simple Suzuki cross coupling reactions

ARTICLES

2728 2734

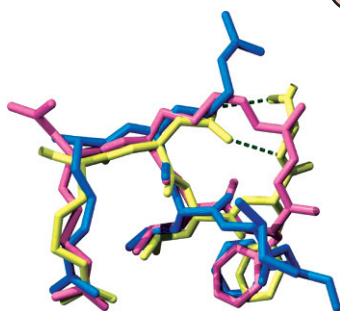


The first Cu(I)-mediated nucleophilic trifluoromethylation reactions using (trifluoromethyl)trimethylsilane in ionic liquids

Jinwi Kim and Jean'ne M. Shreeve

New thermally stable ionic liquids, including *N*-[2-(2-ethoxyethoxy)ethyl]-*N*-methylmorpholinium bis(trifluoromethanesulfonyl)amide (**6a**), are useful solvents for nucleophilic trifluoromethylation reactions.

2735 2741

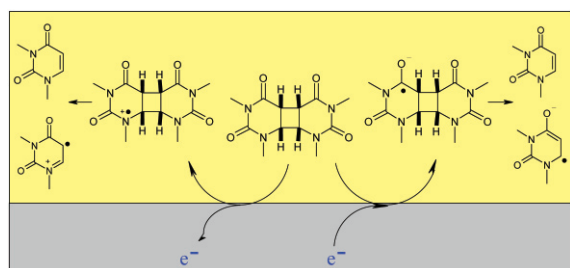


Design, synthesis, biological activity and structural analysis of cyclic peptide inhibitors targeting the substrate recruitment site of cyclin-dependent kinase complexes

Martin J. I. Andrews, Campbell McInnes, George Kontopidis, Lorraine Innes, Angela Cowan, Andy Plater and Peter M. Fischer

The design, synthesis and structural characterisation of a series of protein-protein interaction inhibitors are reported.

2742 2750



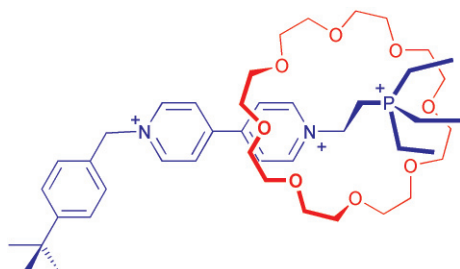
Dissociative electron transfer to and from pyrimidine cyclobutane dimers: An electrochemical study

Fabien Boussicault, Oliver Krüger, Marc Robert and Uta Wille

A mechanistic study of electrochemically induced splitting of pyrimidine cyclobutane dimers gives new insights in the enzymatic repair mechanism of DNA lesions.



2751 2756

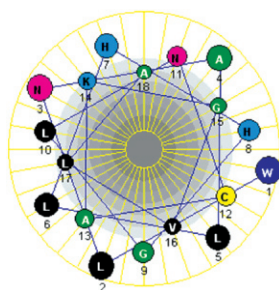


[2]Rotaxanes containing pyridinium-phosphonium axles and 24-crown-8 ether wheels

Norma Georges, Stephen J. Loeb, Jorge Tiburcio and James A. Wisner

A triethylphosphonium group attached to a pyridinium ethane moiety is used as an axle for the self-assembly of [2]pseudorotaxanes and [2]rotaxanes utilising 24-crown-8 ether, benzo-24-crown-8 ether and naphtho-24-crown-8 ether.

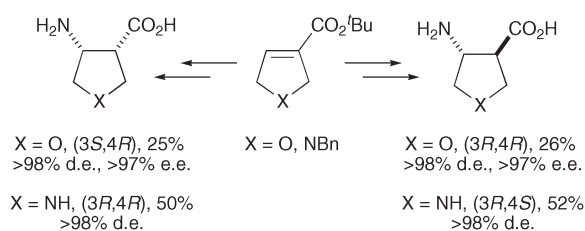
2757 2762

**Monomeric analogues of halocidin**

Xavier Doisy, Dan Ifrah and Paul R. Hansen

Synthesis, antibacterial and haemolytic activities of monomeric analogues of halocidin, an antimicrobial peptide isolated from *Halocynthia aurantium*, are described.

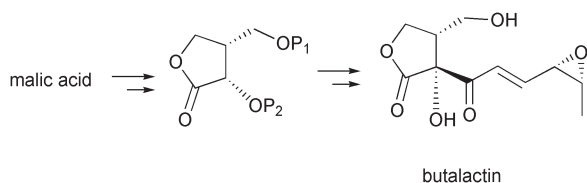
2763 2776

**Asymmetric synthesis of the *cis*- and *trans*-stereoisomers of 4-aminopyrrolidine-3-carboxylic acid and 4-aminotetrahydrofuran-3-carboxylic acid**

Mark E. Bunnage, Stephen G. Davies, Paul M. Roberts, Andrew D. Smith and Jonathan M. Withey

Diastereoselective conjugate addition of lithium (*S*)-*N*-benzyl-*N*- α -methylbenzylamide allows the efficient asymmetric synthesis of *cis*- and *trans*-4-aminopyrrolidine- and 4-aminotetrahydrofuran-3-carboxylic acids, giving the 4-aza and 4-oxa derivatives of cispentacin and transpentacin in >98% d.e. and >97% e.e.

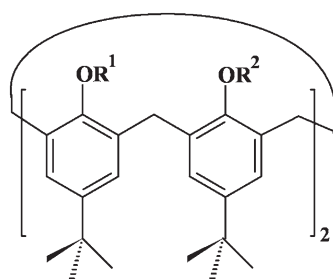
2777 2785

**Stereoselective synthesis and structure of butalactin and lactone II isolated from *Streptomyces* species**

Toshihiko Ueki and Takamasa Kinoshita

The stereoselective synthesis of butalactin and lactone II, two autoregulators with a wide range of biological activity, is described.

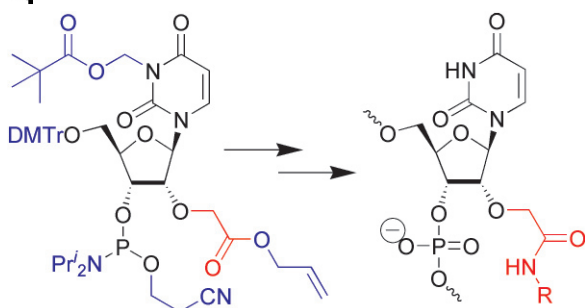
2786 2792

**Synthesis and binding properties of calix[4]arenes with [2 + 2'] mixed ligating functional groups**

Lassaad Baklouti, Jamila Cherif, Rym Abidi, Françoise Arnaud-Neu, Jack Harrowfield and Jacques Vicens

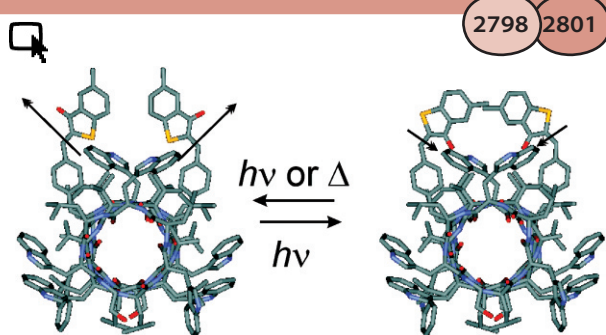
The formation of ML and/or ML₂ species depends on the ligand and the cation; the enthalpic and entropic factors have been assessed.

2793 2797

**Oligonucleotides with 2'-*O*-carboxymethyl group: synthesis and 2'-conjugation *via* amide bond formation on solid phase**

Anna Kachalova, Eugeny Zubin, Dmitry Stetsenko, Michael Gait and Tatiana Oretskaya

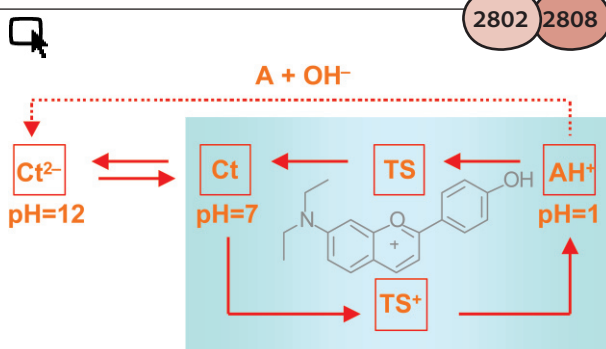
2'-*O*-Carboxymethyloligonucleotides synthesized by use of modified uridine phosphoramidite were conjugated on solid phase to a range of amines and peptides.



Photomodulation of ionic current through hemithioindigo-modified gramicidin channels

Tyler Lougheed, Vitali Borisenko, Thomas Hennig, Karola Rück-Braun and G. Andrew Woolley

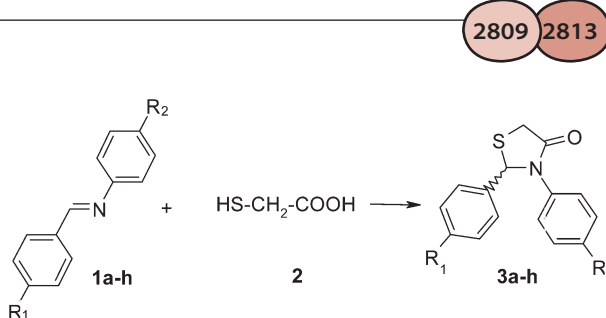
The hemithioindigo amino acid described can act as a functional switch in a biochemical context and can be used to produce predictable effects on function in a system for which the structure/function relationships are well understood.



Multistate properties of 7-(*N,N*-diethylamino)-4'-hydroxyflavylium. An example of an unidirectional reaction cycle driven by pH

Margarida C. Moncada, Damián Fernández, João C. Lima, A. Jorge Parola, Carlos Lodeiro, Filipe Folgosa, M. João Melo and Fernando Pina

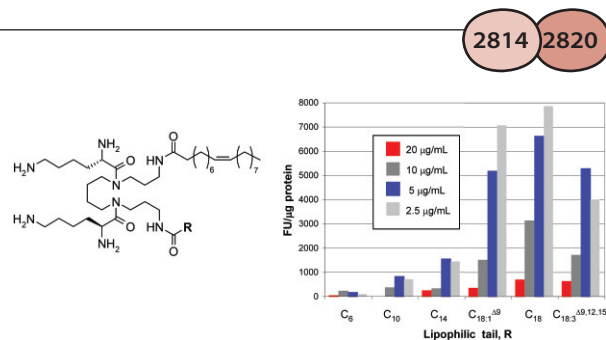
Insertion of an amino group in position 7 of the flavylium cation opens a new reaction channel that allows us to define an unidirectional pH driven reaction cycle.



Thiazolidin-4-one formation. Mechanistic and synthetic aspects of the reaction of imines and mercaptoacetic acid under microwave and conventional heating

Adele Bolognese, Gaetano Correale, Michele Manfra, Antonio Lavecchia, Ettore Novellino and Vincenzo Barone

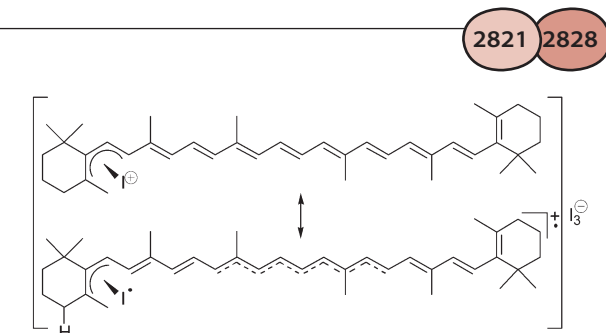
Two mechanisms for the title reaction are hypothesized on the basis of solvent effect and of the transient species detected by ¹H-NMR and predicted by DFT calculations.



Effect of chain length on transfection properties of spermine-based gemini surfactants

Mariano Castro, Derek Griffiths, Alpesh Patel, Nicola Patrick, Chris Kitson and Mark Ladlow

The preparation of a series of both symmetrical and unsymmetrical gemini surfactants is reported and their efficacies as non-viral vectors mediating gene transfection are contrasted and used to derive associated structure–activity relationships.

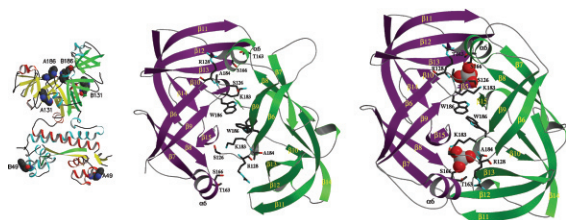


On the structure of carotenoid iodine complexes

Bjart Frode Lutnaes, Jostein Krane and Synnøve Liaaen-Jensen

The reaction between β,β -carotene and iodine has been reinvestigated. Spectroscopic and chemical data are compatible with a π -complex with cationic/radical cationic properties.

2829 2837

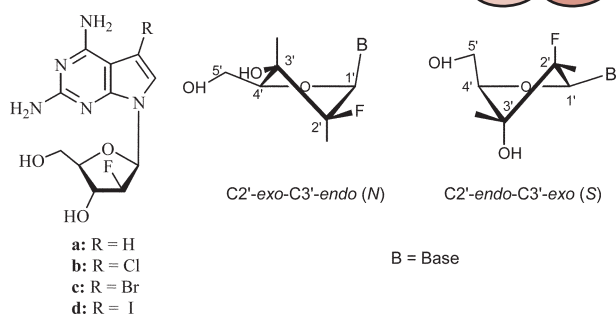


Sensing of remote oxyanion binding at the DNA binding domain of the molybdate-dependent transcriptional regulator, ModE

David H. Boxer, Han Zhang, David G. Gourley, William N. Hunter, Sharon M. Kelly and Nicholas C. Price

Linkage between the DNA-binding and molybdate-binding sites (some 55 Å apart) has been shown.

2838 2846

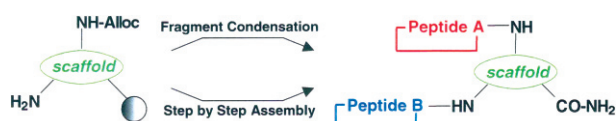


Halogenated 7-deazapurine nucleosides: stereoselective synthesis and conformation of 2'-deoxy-2'-fluoro-beta-D-arabinonucleosides

Xiaohua Peng and Frank Seela

Stereoselective synthesis of **a–d**, and the influence of halogen substituents on the sugar conformation and nucleobase properties.

2847 2851

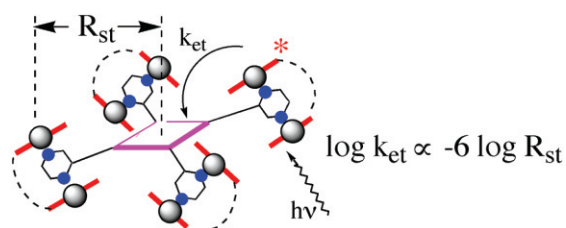


Loops on loops: generation of complex scaffolded peptides presenting multiple cyclic fragments

Raimo Franke, Christian Doll, Victor Wray and Jutta Eichler

Scaffolded peptides presenting two different cyclic peptide fragments through a cyclic peptidomimetic scaffold in a site-selective fashion, were generated by stepwise solid phase synthesis, as well as fragment condensation.

2852 2860

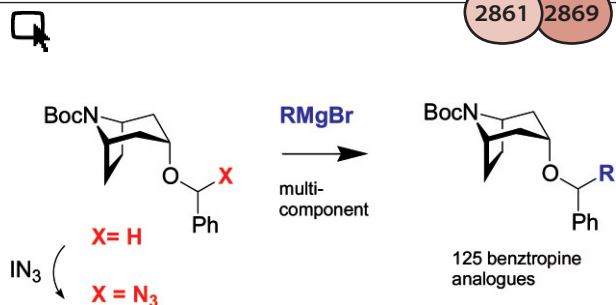


Nonameric porphyrin assemblies – formation and intra-assembly energy transfer reactions

Ken Sasaki, Kenji Sugou, Koji Miyamoto, Jyun-ichi Hirai, Shigetaka Tsubouchi, Hiroshi Miyasaka, Akira Itaya and Yasuhisa Kuroda

The series of nonameric porphyrin assemblies show an effective antenna effect and successive energy transfer to the central free base porphyrin.

2861 2869

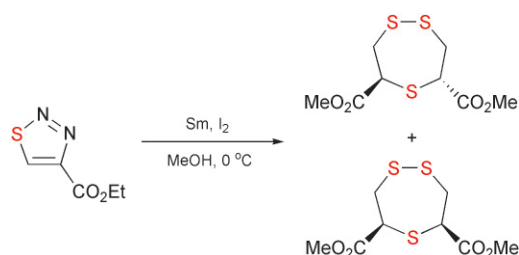


Combinatorial synthesis of benzotropine libraries and their evaluation as monoamine transporter inhibitors

Hanne Pedersen, Steffen Sinning, Anne Bülow, Ove Wiborg, Lise Falborg and Mikael Bols

Radical azidation and substitution of azide with multicomponent Grignard reagents are the key features of a new combinatorial synthesis method.

2870 2873

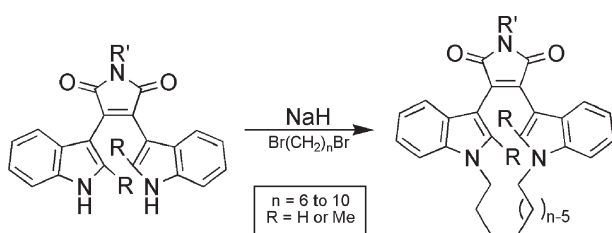


Attempted reduction of 1,2,3-thiadiazole-4-carboxylates with samarium/iodine in methanol. Unexpected ring enlargement to 1,2,5-trithiepan-4,6-dicarboxylates

Kazuhiro Miyawaki, Hitomi Suzuki and Hiromichi Morikawa

Attempted reduction of ethyl 1,2,3-thiadiazole-4-carboxylate with samarium and iodine in methanol led to a *cis/trans*-isomeric mixture of dimethyl 1,2,5-trithiepan-4,6-dicarboxylates.

2874 2883



Evaluation of alternative approaches for the synthesis of macrocyclic bisindolylmaleimides

Stephen Bartlett and Adam Nelson

Alternative approaches for the synthesis of macrocyclic bisindolylmaleimides, a class of potent and selective protein kinase inhibitors, are described.

2884

Stephen Hermitage, Judith A. K. Howard, David Jay, Robin G. Pritchard, Michael R. Probert and Andrew Whiting

Mechanistic studies on the formal aza-Diels–Alder reactions of *N*-aryl imines: evidence for the non-concertedness under Lewis-acid-catalysed conditions

Toshifumi Takeuchi, Satoshi Ugata, Shuichi Masuda, Jun Matsui and Masayoshi Takase

Atrazine transformation using synthetic enzymes prepared by molecular imprinting