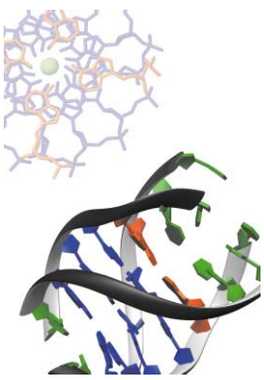
ISSN 1477–0520 OBCRAK(10) 1635–1826(2003)

Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



Cover
See Evripidis Gavathiotis and Mark S. Searle, page 1650.
NMR structure of the intermolecular DNA quadruplex formed from the human telomeric repeat.

contents

COMMUNICATIONS

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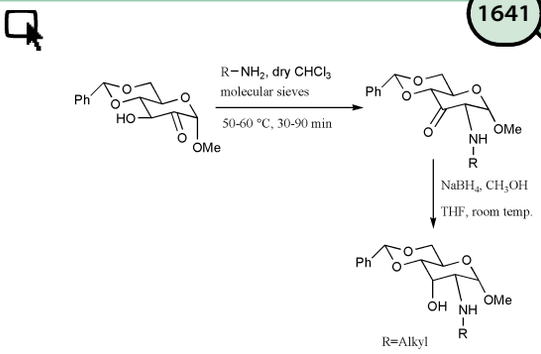
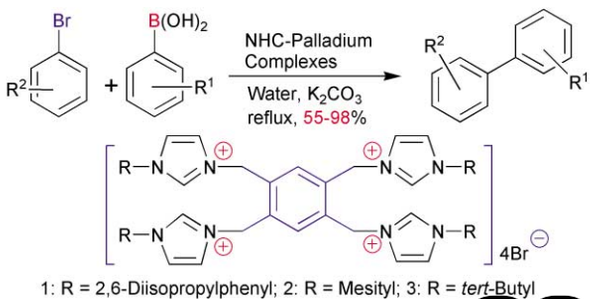


Stereoselective synthesis of 2-amino-2-deoxysugars: *N*-alkyl-D-allosamines

Hong-Min Liu, Fuyi Zhang and Shaomin Wang

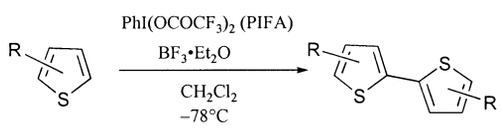
The first example of synthesis of *N*-alkyl-D-allosamines from a 2-oxo sugar.



Suzuki cross-coupling mediated by tetradentate *N*-heterocyclic carbene (NHC)–palladium complexes in an environmentally benign solvent

Yuanhong Zhao, Yongyun Zhou, Dandan Ma, Jingping Liu, Liang Li, Tony Y. Zhang and Hongbin Zhang

A highly effective, easy to handle and environmentally benign process for palladium mediated Suzuki cross-coupling was developed. By utilizing a solid support based NHC–palladium catalyst, cross couplings of aryl bromides with phenylboronic acid were achieved in neat water under air. A high ratio of substrate to catalyst was also realized.

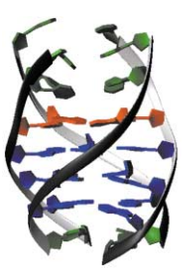


A novel and direct synthesis of alkylated 2,2′-bithiophene derivatives using a combination of hypervalent iodine(III) reagent and $BF_3{\cdot}Et_2O$

Hirofumi Tohma, Minako Iwata, Tomohiro Maegawa, Yorito Kiyono, Akinobu Maruyama and Yasuyuki Kita

A hypervalent iodine(III)-induced oxidative coupling of alkylthiophene derivatives gives the corresponding 2,2′-bithiophenes directly in the presence of $BF_3{\cdot}Et_2O$ without polymerization.

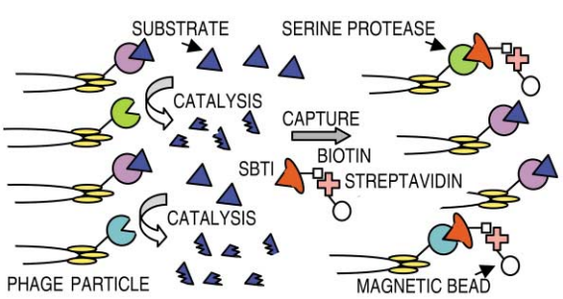
ARTICLES



Structure of the parallel-stranded DNA quadruplex $d(TTAGGGT)_4$ containing the human telomeric repeat: evidence for A-tetrad formation from NMR and molecular dynamics simulations

Evripidis Gavathiotis and Mark S. Searle

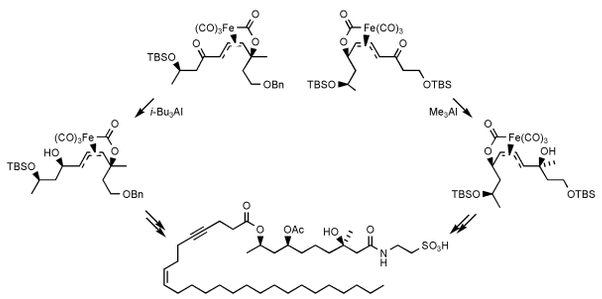
The structure of $d(TTAGGGT)_4$ provides a model system which can be exploited in the design of novel telomerase inhibitors that bind to and stabilise G-quadruplex structures.



Substrate turnover and inhibitor binding as selection parameters in directed evolution of blood coagulation factor X_a

Rikke H. Lorentsen, Charlotte H. Møller, Michael Etzerodt, Hans C. Thøgersen and Thor L. Holtet

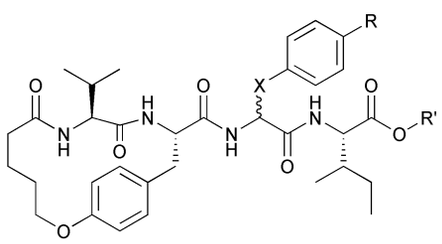
A robust selection strategy in directed evolution of enzymes, utilising substrate and inhibitors for selection of catalytically active clones.



Use of π-allyltricarbonyliron lactone complexes in the synthesis of taurospongin A: a potent inhibitor of DNA polymerase β and HIV reverse transcriptase

Christopher J. Hollowood, Shigeo Yamanoi and Steven V. Ley

Taurospongin A displays potent inhibitory action of DNA polymerase β and HIV reverse transcriptase. New syntheses of the two fatty acid components that are used to construct taurospongin A are demonstrated.

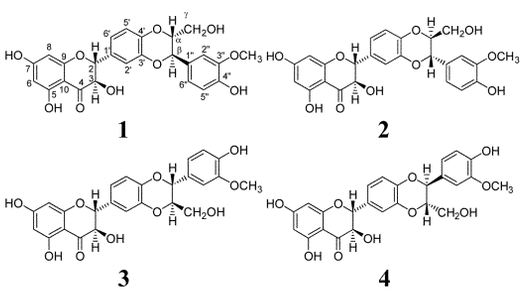


X = O, S, NH; R = H, alkoxy groups; R' = OH, ester group.

New β-strand macrocyclic peptidomimetic analogues containing α-(O-, S- or NH-)aryl substituted glycine residues: synthesis, chemical and enzymatic properties

Gilles Quéléver, Frédéric Bihel and Jean-Louis Kraus

Proteolytic enzymes are crucial for disease propagation and their selective inhibition appears to be a promising therapeutic route for the treatment of diseases as various as cancers, viral infections, such as HIV, or neurodegenerative disorders. Reported here is the synthesis of new β-strand macrocyclic peptidomimetic analogues which could affect HIV-1 protease.

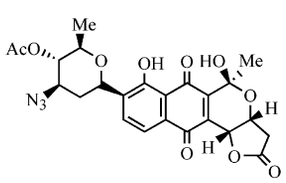


1 **2** **3** **4**

Complete isolation and characterization of silybins and isosilybins from milk thistle (*Silybum marianum*)

Nam-Cheol Kim, Tyler N. Graf, Charles M. Sparacino, Mansukh C. Wani and Monroe E. Wall

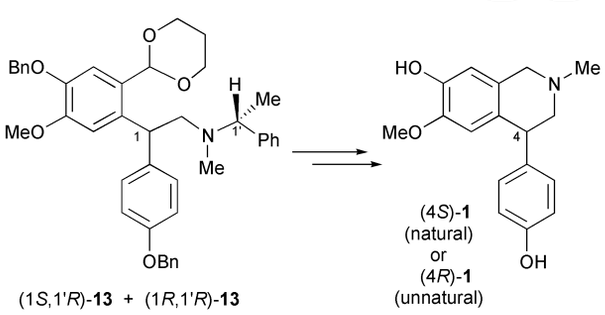
Complete isolation of hepatoprotective flavonolignans, silybins A (**1**) and B (**2**), and isosilybins A (**3**) and B (**4**), was achieved. Structures including absolute stereochemistries of isolates were characterized using NMR and CD methods.



Synthesis of 3-azido-2,3,6-trideoxy-β-D-*arabino*-hexopyranosyl pyranonaphthoquinone analogues of medermycin

Margaret A. Brimble, Roger M. Davey, Malcolm D. McLeod and Maureen Murphy

The synthesis of an isomeric mixture of azido analogues of the pyranonaphthoquinone antibiotic medermycin is reported *via* addition of 2-trimethylsilyloxyfuran to a *C*-azidoglycosyl-naphthoquinone followed by oxidative rearrangement of the resultant adducts.

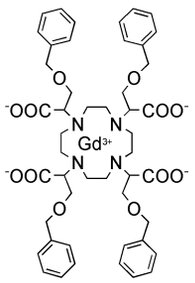


(1*S*,1'*R*)-**13** + (1*R*,1'*R*)-**13** → (4*S*)-**1** (natural) or (4*R*)-**1** (unnatural)

A new synthesis of (+)- and (−)-cherylline

Stéphane Lebrun, Axel Couture, Eric Deniau and Pierre Grandclaudon

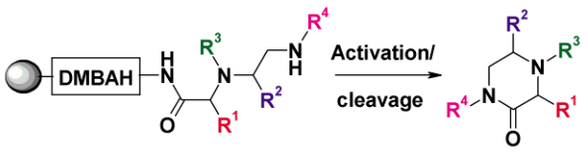
A new and concise synthesis of enantiopure antipodes of alkaloid cherylline has been devised. The synthetic strategy relies upon the separation of diastereopure diarylethylamines issued from asymmetric reduction of the corresponding enamines.



Preparation and *in vitro* evaluation of GdDOTA-(BOM)$_4$; a novel angiographic MRI contrast agent

Ragnar Hovland, Arne J. Aasen and Jo Klaveness

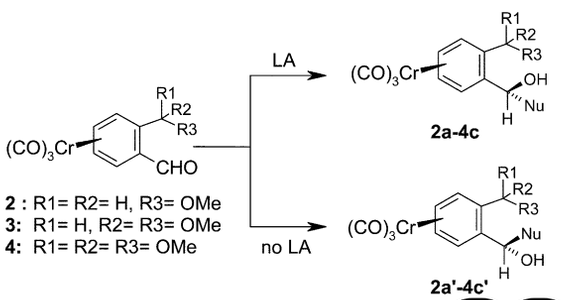
A novel Gd(III) complex, GdDOTA-(BOM)$_4$, has been prepared. The complex showed high T_1-relaxivity values in albumin solutions, blood and plasma.



The development and preparation of the 2,4-dimethoxybenzyl arylhydrazine (DMBAH) "latent" safety-catch linker: solid phase synthesis of ketopiperazines

Frédéric Berst, Andrew B. Holmes and Mark Ladlow

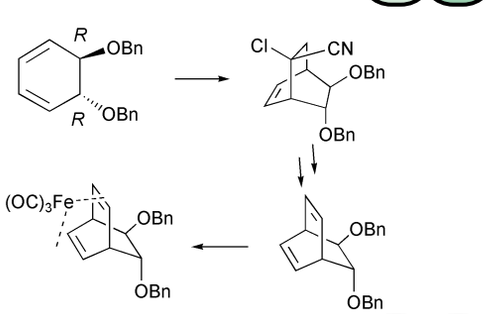
The preparation of a new "latent" safety-catch linker (DMBAH) and a study of cleavage conditions leading to mono-ketopiperazines is described.



Chelation-control in nucleophilic addition to Cr(CO)$_3$-complexed aryl aldehydes

Suresh Kumar Tipparaju, Vedavati G. Puranik and Amitabha Sarkar

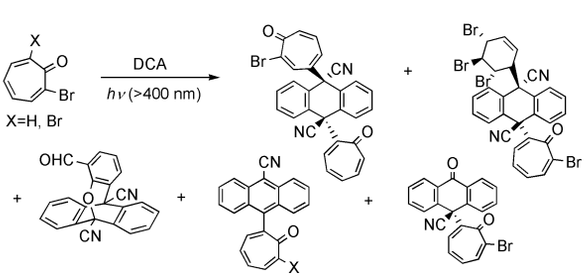
In the presence of Lewis acids, benzylic methoxy groups at the *ortho*-position facilitate chelation-controlled addition of nucleophiles to Cr(CO)$_3$-complexed aryl aldehydes.



Synthetic study of optically active and C_2-symmetric novel ligand, 7,8-bis(benzyloxy)bicyclo[2.2.2]octa-2,5-diene and a tricarbonyliron complex

Akiko Watanabe, Mariko Aso and Hiroshi Suemune

Novel diene compounds have been synthesised as potential chiral ligands for metal complexes.



Photochemical reactions of 2-bromotropone and 2,7-dibromotropone with 9,10-dicyanoanthracene

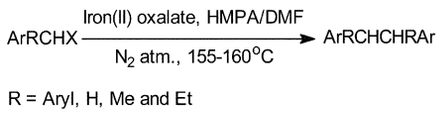
Akira Mori, Hiroko Kawakami, Nobuo Kato, Shu-Ping Wu and Hitoshi Takeshita

The reactions of halotropones with the excited state of 9,10-dicyanoanthracene give adducts derived from the [8+4]π intermediate with an oxabicyclo[3.2.2]nonane system.

Facile reductive coupling of benzylic halides with ferrous oxalate dihydrate

Jitender M. Khurana, Sushma Chauhan and Golak C. Maikap

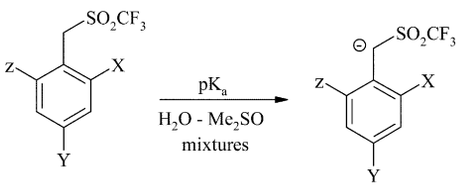
Reductive coupling of benzylic halides with ferrous oxalate dihydrate is reported at 155–160 °C in DMF or HMPA.



Super acidifiers: the origin of the exceptional electron transmission capability of the SO_2CF_3 group in carbanion stabilization

Régis Goumont, Elyane Kizilian, Erwin Buncel and François Terrier

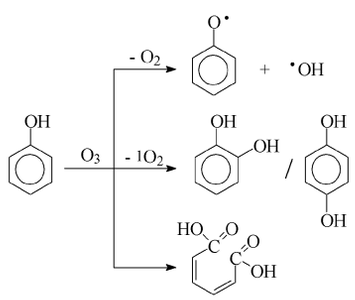
Because stabilization of negative charge by a SO_2CF_3 group is largely the result of polarizability effects, the relative acidity sequences of α-NO_2 and α-SO_2CF_3 activated carbon acids are strongly affected on transfer from H_2O to Me_2SO.



Ozonolysis of phenols in aqueous solution

Eino Mvula and Clemens von Sonntag

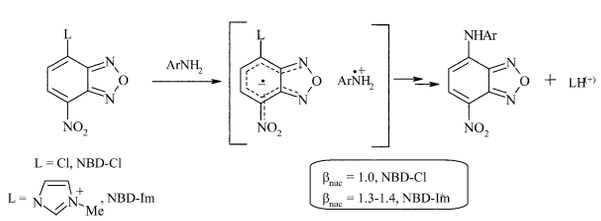
Ozonolysis of phenols in aqueous solution gives rise to large amounts of ˙OH and singlet dioxygen. The Criegee mechanism, typical for the ozonolysis of olefins, plays only a minor role.



High Brønsted β_{nuc} values in S_NAr displacement. An indicator of the SET pathway?

François Terrier, Malika Mokhtari, Régis Goumont, Jean-Claude Hallé and Erwin Buncel

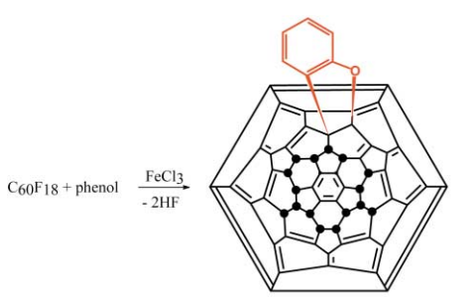
Nucleophilic substitutions of substituted anilines with 4-chloro-7-nitrobenzofurazan and 3-methyl-1-(4-nitrobenzofurazanyl)-imidazolium ions highlight the possible role of the Brønsted β_{nuc} parameter as an indication of a single electron transfer process.



Electrophilic substitution of $C_{60}F_{18}$ into phenols: HF elimination between OH and a 1,3-shifted fluorine giving benzofurano[2′,3′:10,26]hexadecafluoro[60]fullerene and derivatives

Adam D. Darwish, Anthony G. Avent, Joan M. Street and Roger Taylor

Substitution of phenols into $C_{60}F_{18}$ followed by further HF elimination leads to formation of benzofurano[60]fullerene derivatives.



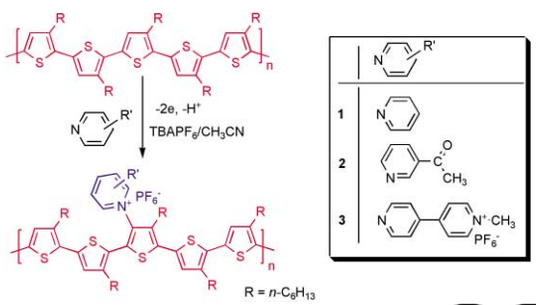
Generation of neutrals from ionic precursors in the gas phase. The rearrangement of CCCCCHO to HCCCCCO

Mark Fitzgerald, John H. Bowie and Suresh Dua

HCCCCCO and CCCCCHO are made by neutralisation of precursor ions. Energised CCCCCHO rearranges as follows: CCCCCHO to CCCCHCO to CCCHCCO to HCCCCCO.

Efficient anodic pyridination of poly(3-hexylthiophene) toward post-functionalization of conjugated polymers

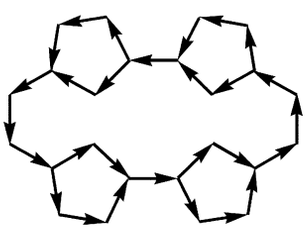
Yi Li, Kaori Kamata, Sadayuki Asaoka, Takamichi Yamagishi and Tomokazu Iyoda



Pyridinium-modified poly(3-hexylthiophene)s were obtained by anodic pyridination reactions, which were characterized by FT-IR, cyclic voltammetry, and spectroelectrochemical methods.

The four-electron diamagnetic ring current of porphycene

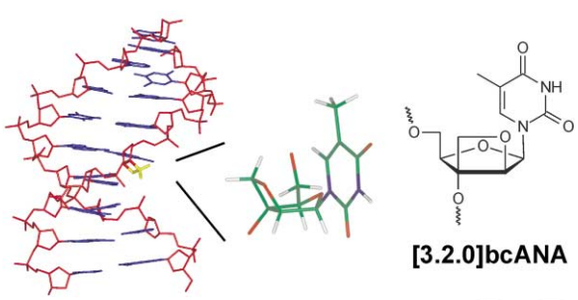
Erich Steiner and Patrick W. Fowler



Porphycene is shown to be a close model of porphin in that it possesses a macrocyclic ring current related to its frontier-orbital electronic structure.

NMR solution structure of dsDNA containing a bicyclic D-*arabino*-configured nucleotide fixed in an O4′-*endo* sugar conformation

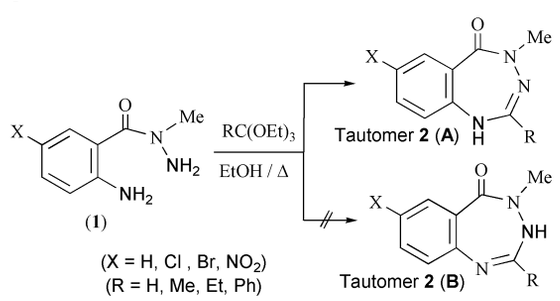
Henning V. Tømmerholt, Nanna K. Christensen, Poul Nielsen, Jesper Wengel, Paul C. Stein, Jens Peter Jacobsen and Michael Petersen



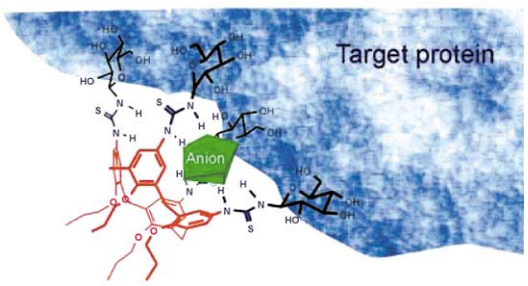
The structure reveals that the [3.2.0]bcANA nucleotide adopts an O4′-*endo* sugar pucker and that it causes only minute disruption of the B-form framework of the dsDNA duplex.

Investigations on the structure of 4-methyldihydro-1,3,4-benzotriazepin-5-ones. Tautomer reassignment

Jalal A. Zahra, Mustafa M. El-Abadelah, Musa Z. Nazer, Kais A. K. Ebraheem and Roland Boese



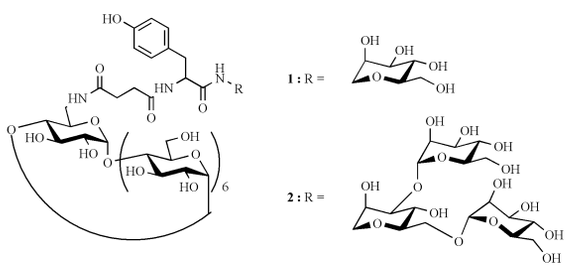
Dihydro-1,3,4-benzotriazepin-5-ones exist in the 1,4- (and not 3,4-) dihydro tautomeric forms as evidenced from X-ray and computational data.



Thiourea-linked upper rim calix[4]arene neoglycoconjugates: synthesis, conformations and binding properties

Francesco Sansone, Elisa Chierici, Alessandro Casnati and Rocco Ungaro

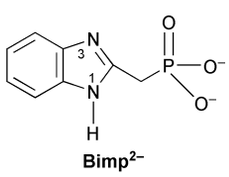
Calix[4]arene based glycoconjugates which bind anions and specifically interact with lectins are described.



Synthesis and characterization of mannosyl mimetic derivatives based on a β-cyclodextrin core

Duplex Yockot, Vincent Moreau, Gilles Demailly and Florence Djedaïni-Pilard

Novel glycosylated β-cyclodextrins **1** and **2** were prepared as potential inhibitors of HIV-1 envelope glycoprotein gp120/ macrophage interactions.



Synthesis and acid–base properties of (1*H*-benzimidazol-2-yl-methyl)phosphonate ($Bimp^{2-}$). Evidence for intramolecular hydrogen-bond formation in aqueous solution between (N-1)H and the phosphonate group

María José Sánchez-Moreno, Raquel B. Gómez-Coca, Alfonso Fernández-Botello, Justyn Ochocki, Andrzej Kotynski, Rolf Griesser and Helmut Sigel

The intramolecular hydrogen bond between the (N-1/N-3)H site and the phosphonate group of $Bimp^{2-}$ reaches a formation degree of 98%!

CONFERENCE DIARY

xi

Dates, venues and contact details of forthcoming events.

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