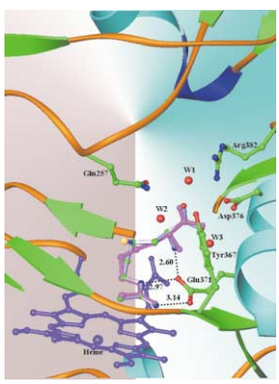
ISSN 1477–0520 OBCRAK(20) 3471–3624(2003)

Indexed in Medline from issue 1

Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

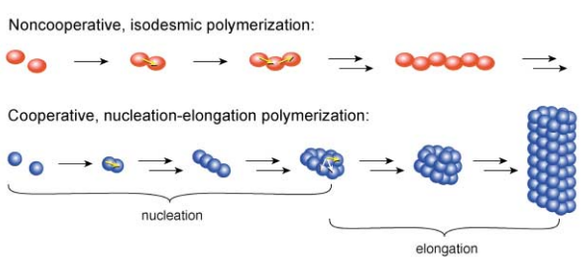
Incorporating Acta Chemica Scandinavica



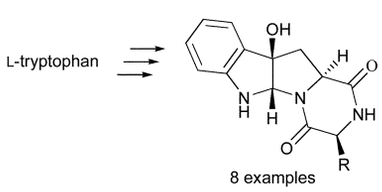
Cover
See E. Ann Hallinan, Steven W. Kramer, Stephen C. Houdek, William M. Moore, Gina M. Jerome, Dale P. Spangler, Anna M. Stevens, Huey S. Shieh, Pamela T. Manning and Barnett S. Pitzele, page 3527.
The cover illustrates a ribbon presentation of the arginine binding pocket of the oxygenase domain (residues 66-498) of mouse iNOS complexed with compound **12** (white and grey). L-NIL (magenta) is docked into the pocket for comparison.

contents

PERSPECTIVE



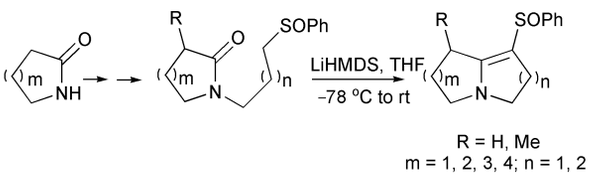
COMMUNICATIONS



COMMUNICATIONS

A general synthetic route to 1-azabicyclo[*m.n.*0]alkenes *via* cyclisation based on α-sulfinyl carbanions

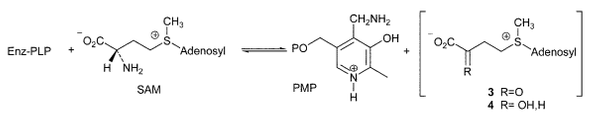
Manat Pohmakotr, Pornthep Numechai, Saisuree Prateeptongkum, Patoomratana Tuchinda and Vichai Reutrakul



The intramolecular nucleophilic addition of α-sulfinyl carbanions derived from the corresponding sulfinyl lactams afforded 1-azabicyclo[*m.n.*0]alkenes in good yields.

The mechanism of 7,8-diaminopelargonate synthase; the role of *S*-adenosylmethionine as the amino donor

Rachel S. Breen, Dominic J. Campopiano, Scott Webster, Mhairi Brunton, Rory Watt and Robert L. Baxter

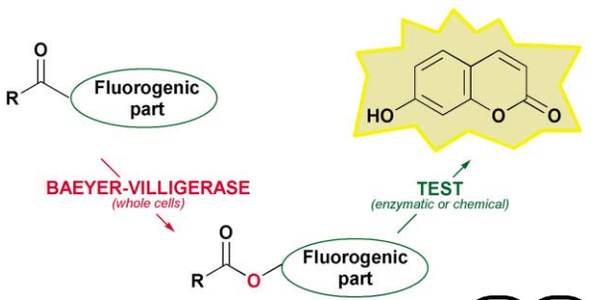


The product of the first transamination step in the reaction catalysed by diaminopelargonate (DAPA) synthase has been shown to be 4-(*S*-adenosyl)-2-oxobutanoate, which has been trapped as the corresponding alcohol.

ARTICLES

The first fluorogenic assay for detecting a Baeyer–Villigerase activity in microbial cells

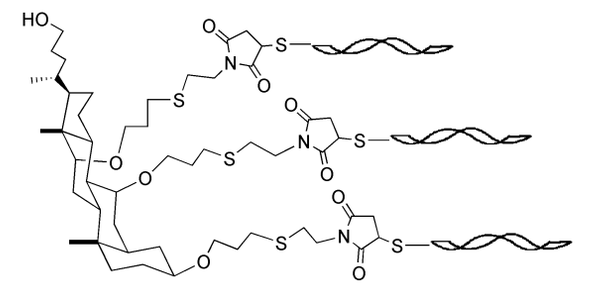
María C. Gutiérrez, Arthur Sleegers, Helen D. Simpson, Véronique Alphand and Roland Furstoss



A fluorimetric assay for detection of Baeyer–Villigerase activities, with potential applicability in high throughput screening (HTS) strategies, is described. A fluorescent signal is produced by liberation of umbelliferone upon oxidation of the test ketone.

Cholic acid as template for multivalent peptide assembly

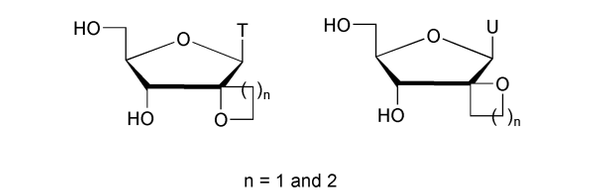
Hengguang Li and Lai-Xi Wang



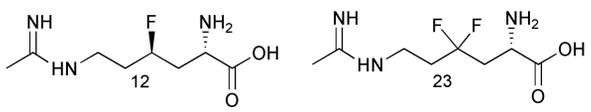
HIV-1 gp41 peptides assembled on the cholic acid template form α-helix bundles that may mimic conformational epitopes.

2′-Spiro ribo- and arabinonucleosides: synthesis, molecular modelling and incorporation into oligodeoxynucleotides

B. Ravindra Babu, Lise Keinicke, Michael Petersen, Claus Nielsen and Jesper Wengel



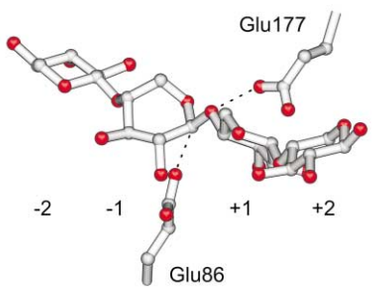
Four conformationally restricted bicyclic 2′-spiro nucleosides were synthesized *via* 2′-*C*-allyl nucleosides as key intermediates.



4-Fluorinated L-lysine analogs as selective i-NOS inhibitors: methodology for introducing fluorine into the lysine side chain

E. Ann Hallinan, Steven W. Kramer, Stephen C. Houdek, William M. Moore, Gina M. Jerome, Dale P. Spangler, Anna M. Stevens, Huey S. Shieh, Pamela T. Manning and Barnett S. Pitzele

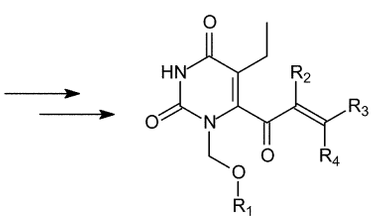
The synthesis of iNOS inhibitors, 4-fluoro-L-NIL and 4,4-difluoro-L-NIL are described.



MM-PBSA free energy analysis of *endo*-1,4-xylanase II (XynII)–substrate complexes: binding of the reactive sugar in a skew boat and chair conformation

Tuomo Laitinen, Juha Rouvinen and Mikael Peräkylä

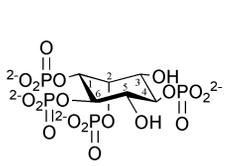
In the skew boat conformation the glycosidic linkage is in the *pseudo*-axial orientation ready for facile bond cleavage.



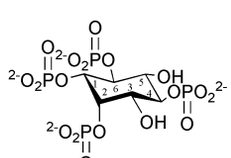
Synthesis and evaluation of new potential HIV-1 non-nucleoside reverse transcriptase inhibitors. New analogues of MKC-442 containing Michael acceptors in the C-6 position

Lene Petersen, Carsten H. Jessen, Erik B. Pedersen and Claus Nielsen

Analogues of MKC-442 capable of undergoing Michael addition reactions were synthesised in order to investigate the activity against the HIV-1 mutant (Y181C).



D-Ins(1,2,5,4,6)P_4
IC_{50} = 3.8 μM for Ins(1,4,5)P_3 5-phosphatase

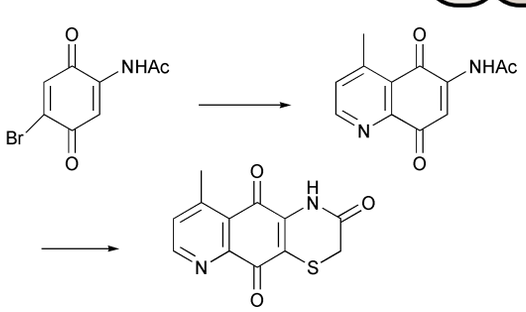


L-Ins(1,2,4,6)P_4
IC_{50} = 14 μM for Ins(1,4,5)P_3 5-phosphatase

Synthesis of D- and L-*myo*-inositol 1,2,4,6-tetrakisphosphate, regioisomers of *myo*-inositol 1,3,4,5 tetrakisphosphate: activity against Ins(1,4,5)P_3 binding proteins

Stephen J. Mills, Katrien Backers, Christophe Erneux and Barry V. L. Potter

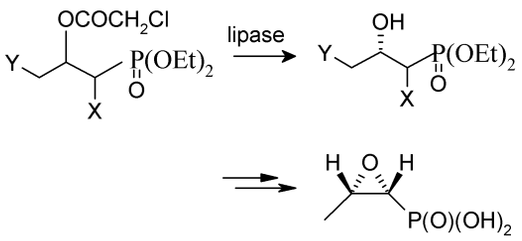
Synthesis of the enantiomers of inositol polyphosphate Ins(1,2,4,6)P_4 is described; Both D- and L- isomers are Ins(1,4,5)P_3 5-phosphatase inhibitors, but not of Ins(1,4,5)P_3 3-kinase.



Synthesis of 9-methyl-1*H*-[1,4]thiazino[3,2-*g*]quinoline-2,5,10(3*H*)-trione, the B,C,D ring core of the shermilamine alkaloids

Norman O. Townsend and Yvette A. Jackson

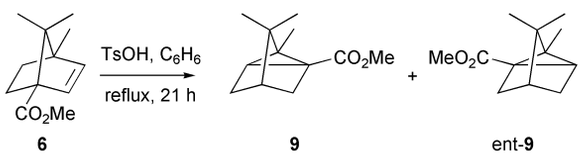
The B,C,D ring core of the shermilamine alkaloids has been prepared in 4 steps and 18% overall yield from *N*-(4-bromo-2,5-dimethoxyphenyl)acetamide.



Enzymatic synthesis of phosphocarnitine, phosphogabob and fosfomycin

Ke Wang, Yonghui Zhang and Chengye Yuan

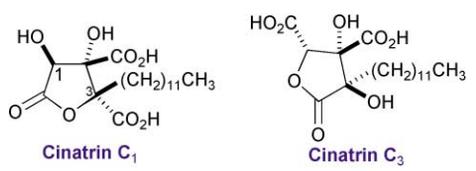
Lipase catalyzed alcoholysis was reported as an efficient methodology for the preparation of optically pure phosphocarnitine, phosphogabob and fosfomycin.



A tricycloheptane product in cationic rearrangements

John E. Davies, Ian Fleming and Jonathan M. Goodman

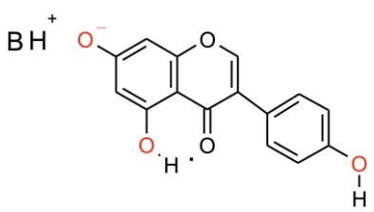
The ester **6** rearranged cleanly to the racemic ester **9**, in spite of the latter having three contiguous quaternary centres.



Enantiospecific synthesis of the phospholipase A_2 inhibitors (−)-cinatrin C_1 and (+)-cinatrin C_3

Anthony N. Cuzzupe, Romina Di Florio, Jonathan M. White and Mark A. Rizzacasa

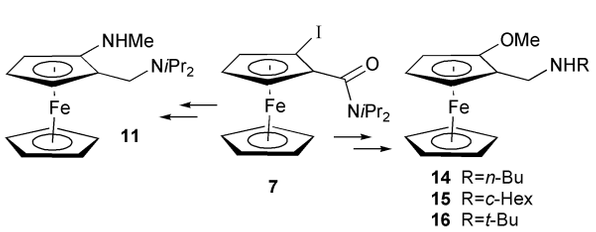
The enantiospecific synthesis of (−)-cinatrin C_1 (**3**) and (+)-cinatrin C_3 (**5**) from a common precursor is described which utilises an Ireland–Claisen rearrangement as a key step.



Solution and solid state ^{13}C NMR and X-ray studies of genistein complexes with amines. Potential biological function of the C-7, C-5, and C-4′-OH groups

Lech Kozerski, Bogdan Kamieński, Robert Kawęcki, Zofia Urbanczyk-Lipkowska, Wojciech Bocian, Elżbieta Bednarek, Jerzy Sitkowski, Katarzyna Zakrzewska, Kim T. Nielsen and Poul Erik Hansen

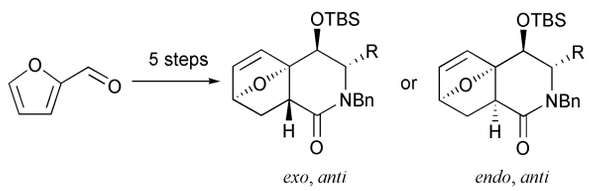
Three hydroxyl groups of the title compound display different donor–acceptor properties as potential HB partners in interactions with biomolecules.



Synthesis of planar chiral ferrocenyl 1,3-diamines and 1,3-amino ethers

James C. Anderson, Alexander J. Blake and Jennifer C. Arnall-Culliford

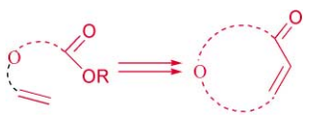
A novel series of planar chiral ferrocenyl 1,3-diamine and 1,3-amino ether ligands have been efficiently synthesised from (*pR*)-*N*,*N*-diisopropyl-2-iodoferrocenecarboxamide.



Stereochemistry of intramolecular Diels–Alder furan (IMDAF) reactions of furyl-substituted chiral ethanolamides

Reynier A. Tromp, Johannes Brussee and Arne van der Gen

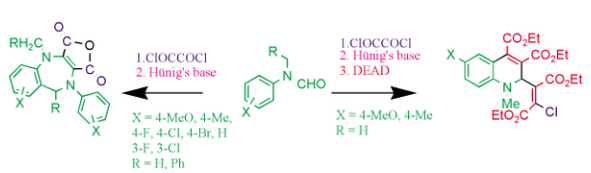
A description of the stereoselective outcome of the intramolecular Diels–Alder furan (IMDAF) reaction of substituted (2*S*,3*S*)-ethanolamides, which were synthesised from a furyl substituted cyanohydrin.



Construction of medium-ring oxacycloalkenones. Extension towards benzo-fused cyclic ethers

Frédéric Lecornué and Jean Ollivier

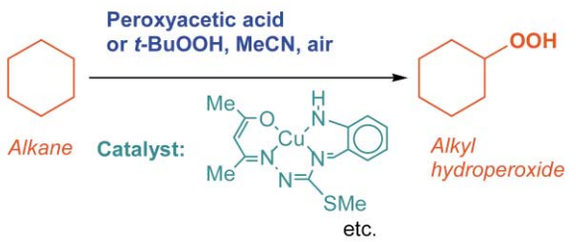
A rapid route to medium-sized cyclic ether skeletons as well as benzo-fused ones is achieved by Kulinkovich cyclopropanation and Saegusa oxidation.



The surprising nucleophilic addition of aminochlorocarbenes to diethyl acetylenedicarboxylate and to oxalyl chloride: quinolines and benzo[1,4]diazepines from *N*-alkylformanilides and oxalyl chloride in the presence of Hünig's base

Ying Cheng, Hua Yang and Otto Meth-Cohn

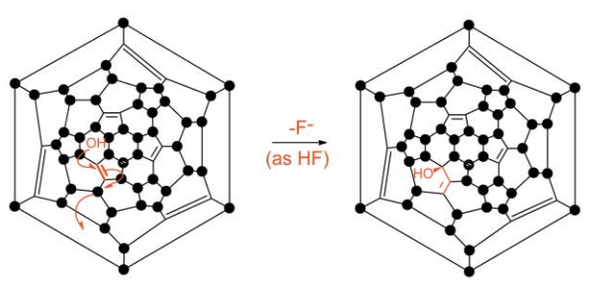
4-Methyl- and 4-methoxyphenylaminochlorocarbene reacted with diethyl acetylenedicarboxylate to give 1 : 2 quinoline adducts, while all arylaminochlorocarbenes examined yielded benzodiazepine derivatives from the 1 : 1 interaction of the carbene with oxalyl chloride under the same reaction conditions.



Alkane hydroperoxidation with peroxides catalysed by copper complexes

Georgiy B. Shul'pin, Julieta Gradinaru and Yuriy N. Kozlov

Various copper(I) and copper(II) derivatives catalyse very efficient oxidation of saturated hydrocarbons with peroxyacetic acid or *tert*-butyl hydroperoxide in acetonitrile solution at 60 °C.



Evidence for the S_N2' mechanism in hydrolysis of $C_{60}F_{48}$: origin of the stability of trannulenes

Brian W. Clare, David L. Kepert and Roger Taylor

Facile S_N2' hydrolysis of fluorofullerenes requires the presence of a specific motif, consequently only twelve fluorines are readily lost from $C_{60}F_{48}$.

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