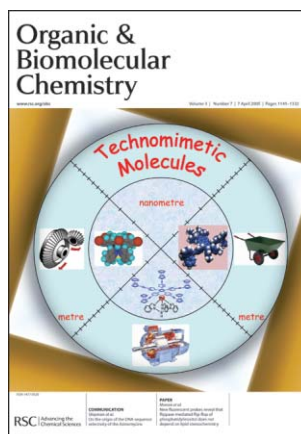
**Cover**

See K. Pagel, K. Seeger, B. Seiwert, A. Villa, A. E. Mark, S. Berger and B. Kokschi, pp. 1189–1194. Modelling structure of a *de novo* designed antiparallel α -helical coiled coil peptide.

Image reproduced by permission of Alessandra Villa and Kevin Pagel from *Org. Biomol. Chem.*, 2005, **3**, 1189.

**Inside Cover**

See G. Rapenne, pp. 1165–1169. Technomimetic molecules are molecules designed to imitate and transpose the motions of objects at the molecular level. On this cover are presented three macroscopic objects, a gear, a motor and a wheelbarrow with their molecular analogues in the centre of the viewfinder.

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CHEMICAL SCIENCE

C25

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Chemical Science

April 2005/Volume 2/Issue 4

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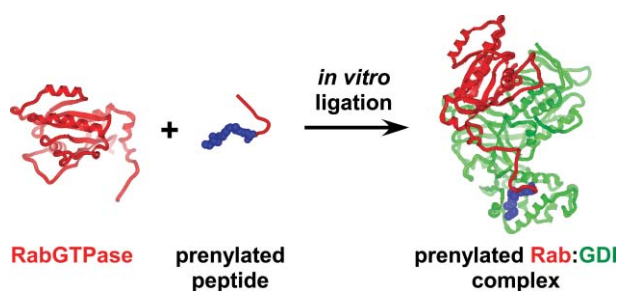
PERSPECTIVE

1157

Chemical biology of protein lipidation: semi-synthesis and structure elucidation of prenylated RabGTPases

Anja Watzke, Luc Brunsveld, Thomas Durek, Kirill Alexandrov, Alexey Rak, Roger S. Goody and Herbert Waldmann*

The semi-synthetic approach *via* Expressed Protein Ligation provides a powerful tool to get access to lipid-modified Rab proteins in amounts sufficient for structure elucidation.



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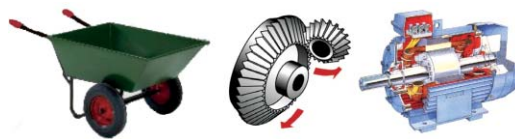
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1165

Synthesis of technomimetic molecules: towards rotation control in single-molecular machines and motors

Gwénaél Rapenne*

Following the bottom-up approach, the synthesis of technomimetic molecules grants access to the study of rotary motion at the molecular level.



COMMUNICATIONS

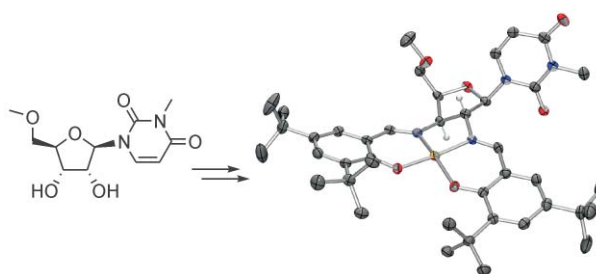
1170



Synthesis and crystal structure of a salen-type copper(II) complex derived from 3,5'-*O*-dimethyl-2',3'-dideoxy- β -D-xylo-uridine

Michael Gottschaldt,* Daniel Koth and Helmar Görls

Starting from uridine the first copper(II) complex of a xylo-2',3'-diamino substituted nucleoside was synthesised and structurally characterised.

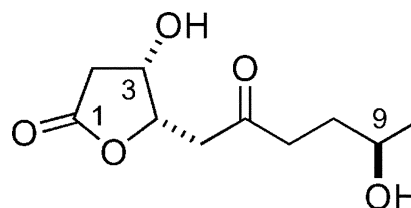


1172

Bassianolone: an antimicrobial precursor of cephalosporolides E and F from the entomoparasitic fungus *Beauveria bassiana*

Juan L. Oller-López, María Iranzo, Salvador Mormeneo, Eulalia Oliver, Juan M. Cuerva and J. Enrique Oltra*

The chemical structures of (+)-bassianolone and a furan derivative, from the fungus *Beauveria bassiana*, are presented.

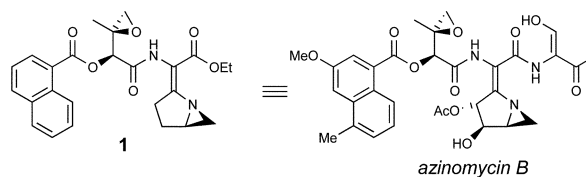


1174

On the origin of the DNA sequence selectivity of the azinomycins

Rachel C. LePla, Cyrille A. S. Landreau, Michael Shipman* and George D. D. Jones

Azinomycin analogue **1** preferentially induces DNA interstrand cross-links at the same sequence as azinomycin B indicating that noncovalent association between the drug and DNA duplex has little impact on sequence specificity.

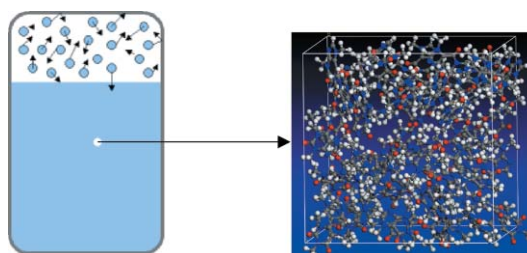


1176

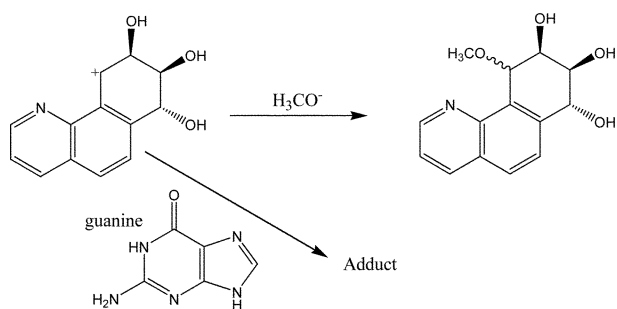
Prediction of vapour pressure using descriptors derived from molecular dynamics

Prem KC Paul

Vapour pressures of organic molecules can be predicted to a high degree of accuracy using solubility parameters derived from molecular dynamics simulations.



1180

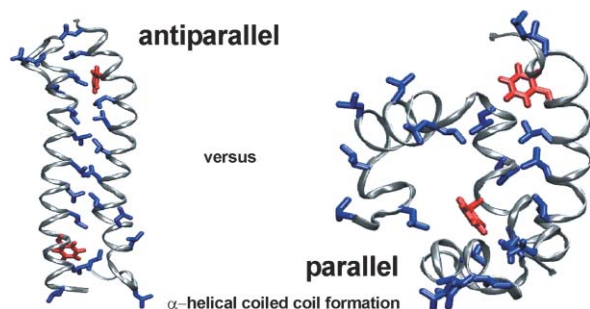


Theoretical study of aza-polycyclic aromatic hydrocarbons (aza-PAHs), modelling carbocations from oxidized metabolites and their covalent adducts with representative nucleophiles

Gabriela L. Borosky and Kenneth K. Laali*

A theoretical study modelling protonated aza-polycyclic aromatic hydrocarbons.

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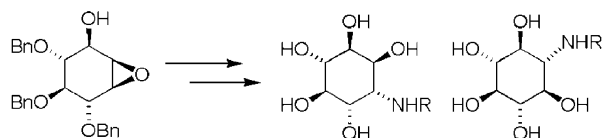


Advanced approaches for the characterization of a *de novo* designed antiparallel coiled coil peptide

Kevin Pagel, Karsten Seeger, Bettina Seiwert, Alessandra Villa, Alan E. Mark, Stefan Berger and Beate Kokschi*

Different analytical methods applied for the detailed characterization of a *de novo* designed antiparallel coiled coil peptide.

1195

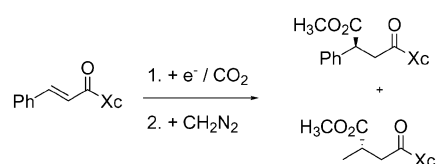


New aminocyclitols as modulators of glucosylceramide metabolism

Meritxell Egado-Gabás, Pedro Serrano, Josefina Casas, Amadeu Llebaria and Antonio Delgado*

The synthesis and biological study of new aminocyclitols as glucosylceramide hydrolase inhibitors is described.

1202

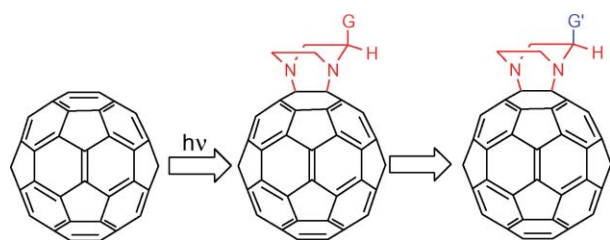


Stereoselective electrochemical carboxylation: 2-phenylsuccinates from chiral cinnamic acid derivatives

Monica Orsini, Marta Feroci,* Giovanni Sotgiu and Achille Inesi*

The diastereoselective electrochemical carboxylation of chiral cinnamic acid derivatives has been achieved to yield dimethyl phenylsuccinate in pure enantiomeric form.

1209



Piperazine additions to C₆₀—a facile approach to fullerene substitution

Craig P. Butts* and Mikael D. S. Jazdyk

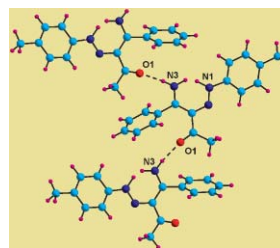
A range of fullerene monoadducts can be generated *via* the photochemical reaction of C₆₀ with piperazine derivatives and subsequent transformations.

1217

Solution and solid state structure and tautomerism of azo coupled enaminone derivatives of benzoylacetone

Petr Šimůnek,* Valerio Bertolasi, Markéta Pešková,
Vladimír Macháček and Antonín Lyčka

Tautomeric equilibrium of azo coupled enaminone derivatives of benzoylacetone was studied both in solution and in the solid state by means of NMR and X-ray diffraction.

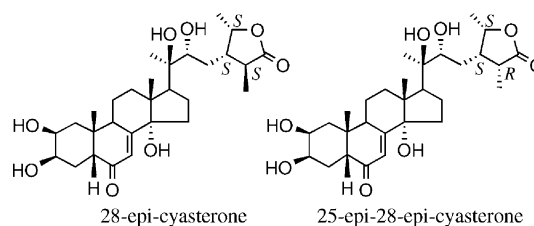


1227

Structure elucidation of cyasterone stereoisomers isolated from *Cyathula officinalis*

Keiko Okuzumi, Noriyuki Hara, Hidehiro Uekusa and
Yoshinori Fujimoto*

Structures of two phytoecdysteroids, isolated from *Cyathula officinalis*, were determined to be 28-epi- and 25-epi-28-epi-cyasterones.

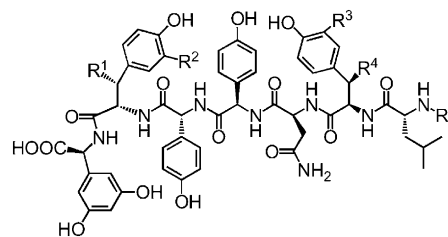


1233

An improved solid-phase methodology for the synthesis of putative hexa- and heptapeptide intermediates in vancomycin biosynthesis

Dong Bo Li and John A. Robinson*

Peptide intermediates in vancomycin biosynthesis have been synthesized by methods that largely avoid the use of side chain protecting groups.

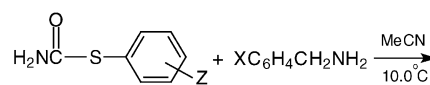


1240

Kinetics and mechanism of the aminolysis of aryl thiocarbamates: effects of the non-leaving group

Hyuck Keun Oh, Young Cheul Jin, Dae Dong Sung and
Ikchoon Lee*

Polar (σ^*) and steric (E_s) effects of the non-leaving group (NH_2) are insignificant, consistent with a concerted mechanism ($\rho_{XZ} = -0.38$).

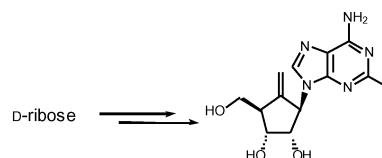


1245

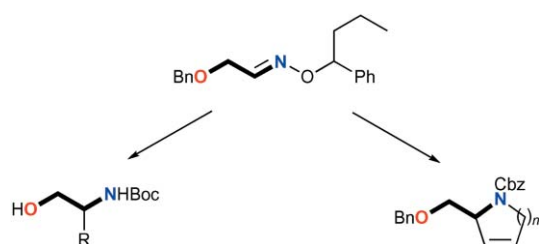
Synthesis of 5'-methylenearisteromycin and its 2-fluoro derivative with potent antimalarial activity due to inhibition of the parasite *S*-adenosylhomocysteine hydrolase¹

Chieko Takagi, Makoto Sukeda, Hye-Sook Kim, Yusuke
Wataya, Saori Yabe, Yukio Kitade, Akira Matsuda and
Satoshi Shuto*

2-Fluoro-5'-methylenearisteromycin (**5**) was synthesized and identified as a potent antimalarial agent due to its inhibitory effect on the malarial parasite AdoHcy hydrolase.



1252

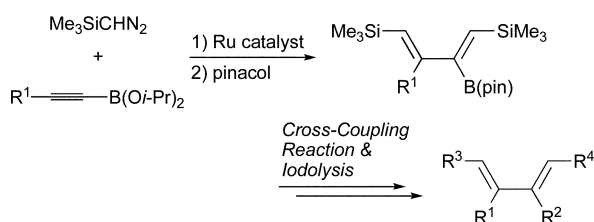


Chiral oxime ethers in asymmetric synthesis. *O*-(1-Phenylbutyl)-benzyloxyacetaldoxime, a versatile reagent for the asymmetric synthesis of protected 1,2-aminoalcohols, α -amino acid derivatives, and 2-hydroxymethyl nitrogen heterocycles including iminosugars

Tracey S. Cooper, Alexander S. Larigo, Pierre Laurent, Christopher J. Moody* and Andrew K. Takle

O-(1-Phenylbutyl)benzyloxyacetaldoxime is a versatile reagent for the asymmetric synthesis of protected 1,2-aminoalcohols, α -amino acid derivatives, and 2-hydroxymethyl nitrogen heterocycles including iminosugars.

1263

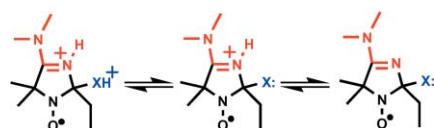


Synthesis of multisubstituted 1,3-butadienes using the ruthenium-catalysed double addition of trimethylsilyldiazomethane to alkynylboronates

Ryotaro Morita, Eiji Shirakawa,* Teruhisa Tsuchimoto and Yusuke Kawakami

Double addition of trimethylsilyldiazomethane to C \equiv C bonds was applied to alkynylboronates. The boryl and silyl groups of the products could be converted to organic groups to give multisubstituted 1,3-butadienes.

1269

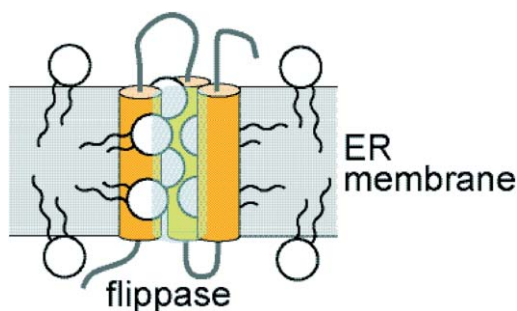


Nitroxides with two pK values—useful spin probes for pH monitoring within a broad range

Igor A. Kirilyuk,* Andrey A. Bobko, Valery V. Khrantsov and Igor A. Grigor'ev

4-Dialkylamino-2,5-dihydroimidazole nitroxides modified at the 2 position of the imidazole ring were prepared. The EPR spectra of the nitroxides undergo changes in the nitrogen hyperfine coupling constant over a broad pH-range.

1275

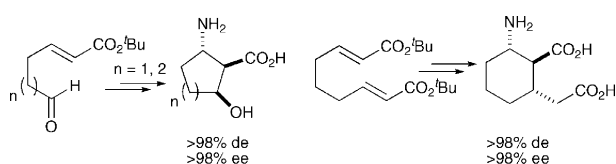


New fluorescent probes reveal that flippase-mediated flip-flop of phosphatidylinositol across the endoplasmic reticulum membrane does *not* depend on the stereochemistry of the lipid

Ram A. Vishwakarma,* Stefanie Vehring, Anuradha Mehta, Archana Sinha, Thomas Pomorski, Andreas Herrmann and Anant K. Menon*

Fluorescence-labeled forms of all four diastereoisomers of phosphatidylinositol have been synthesized and their flippase catalyzed transport across biological membranes evaluated.

1284



Cyclic β -amino acid derivatives: synthesis *via* lithium amide promoted tandem asymmetric conjugate addition–cyclisation reactions

Stephen G. Davies,* David Díez, Sara H. Dominguez, Narciso M. Garrido, Dennis Kruchinin, Paul D. Price and Andrew D. Smith

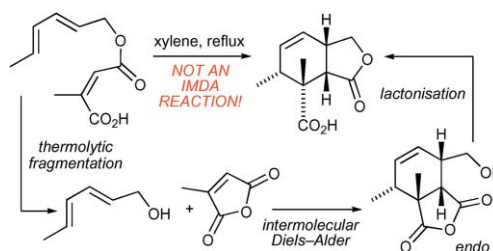
Tandem double conjugate addition and conjugate addition–aldol reactions initiated by a homochiral lithium amide proceed with high stereoselectivity, giving a range of functionalised cyclic β -amino esters in high de and ee after deprotection.

1302

On the Diels–Alder reactions of pentadienyl maleates and citraconates

Tory N. Cayzer, Michael J. Lilly, Rachel M. Williamson, Michael N. Paddon-Row* and Michael S. Sherburn*

The anomalous *endo*-selectivities of intramolecular Diels–Alder (IMDA) reactions of sorbyl half esters of maleic and citraconic acids are explained.

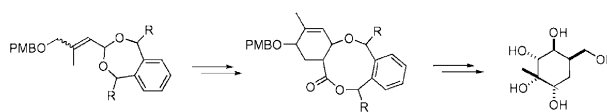


1308

Ring fission of chiral cyclic acetals plus intramolecular [4 + 2] cycloaddition: a sequential access to medium-size lactones. Application to the synthesis of carbasugars

Loïc Lemiègre, Richard L. Stevens, Jean-Claude Combret and Jacques Maddaluno*

A base-induced conjugate elimination transforms starting dioxepanes into the corresponding trienes which undergo intramolecular cyclisation under high pressure.

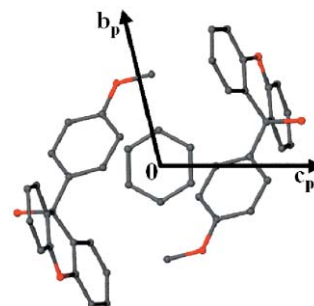


1319

Xanthenol clathrates: structure, thermal stability, guest exchange and kinetics of desolvation

Ayesha Jacobs,* Luigi R. Nassimbeni, Hong Su and Benjamin Taljaard

The xanthenol host, 9-(4-methoxyphenyl)-9*H*-xanthen-9-ol, displays similar structures with a variety of aromatic guests.

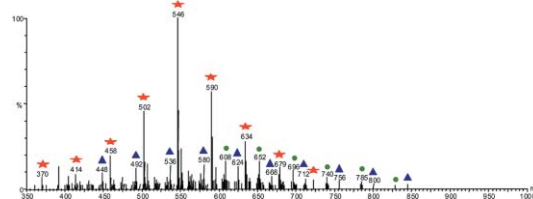


1323

Complete ozonolysis of alkyl substituted ethenes at $-60\text{ }^{\circ}\text{C}$: distributions of ozonide and oligomeric products

Matthew Barton, John R. Ebdon,* Andrew B. Foster and Steve Rimmer*

The ozonolysis of 3-methylpent-2-ene and *trans*-hex-2-ene yields predominantly cyclic ozonate oligomers containing both carbonyl oxide and aldehyde units. Small amounts of open chain oligomers are also identified.



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[3+3] Cycloadditions and related strategies in alkaloid natural product synthesis

Joseph P. A. Harrity and Olivier Provoost (DOI: 10.1039/b502349c)

Ethyl (benzothiazol-2-ylsulfonyl)acetate: a new reagent for the stereoselective synthesis of α,β -unsaturated esters from aldehydes

Paul R. Blakemore, Danny K. H. Ho and W. Mieke Nap (DOI: 10.1039/b500713e)

A chiral molecular recognition approach to the formation of optically active quaternary centres in aza-Henry reactions

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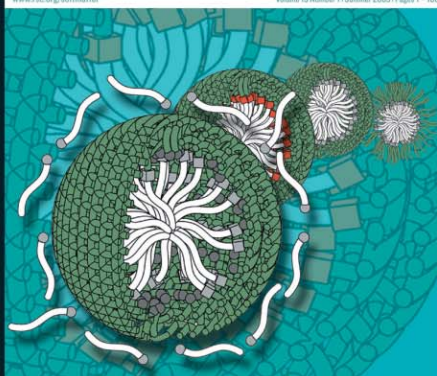
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