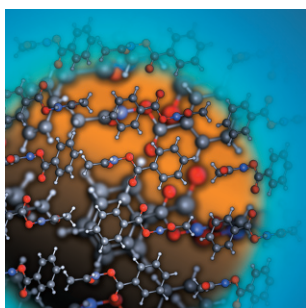


Organic & Biomolecular Chemistry

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Incorporating Acta Chemica Scandinavica

**Cover**

See Jan Schraml, Jan Sýkora, Pavel Fiedler, Jana Roithová, Jaromír Mindl, Vratislav Blechta, Ivana Čiřařová and Otto Exner, pp. 2311–2314.
Molecular packing of *N*-acetyl-*O*-benzoylhydroxylamine from the artist's perspective.

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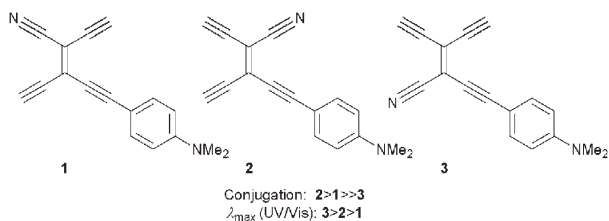
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contents

COMMUNICATIONS



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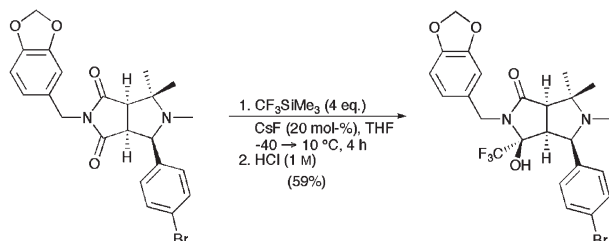
Limitations on the use of UV/Vis spectroscopy for the evaluation of conjugation effectiveness

Nicolle N. P. Moonen and François Diederich

A detailed study on *N,N*-dimethylanilino donor-substituted cyanoethynylethenes and tetraethynylethenes shows that there is no correlation between the effectiveness of the donor-acceptor conjugation pathway and the lowest-energy transition in the UV/Vis absorption spectrum.



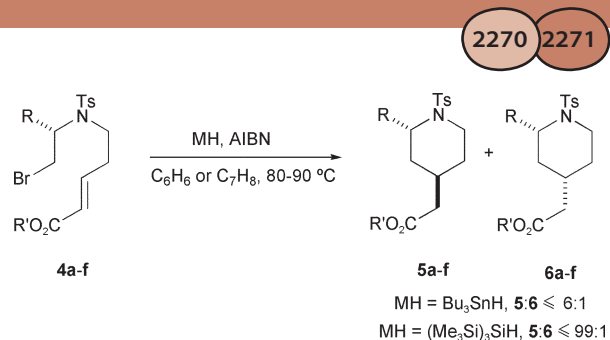
2267 2269



Nucleophilic trifluoromethylation of cyclic imides using (trifluoromethyl)trimethylsilane CF_3SiMe_3

Anja Hoffmann-Röder, Paul Seiler and François Diederich

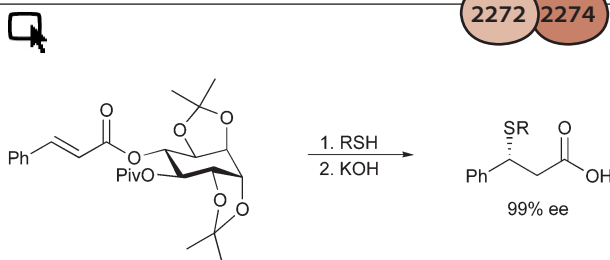
Various bi- and tricyclic imides can be efficiently trifluoromethylated in a regio- and diastereoselective manner using CF_3SiMe_3 under fluoride ion catalysis.



Tris(trimethylsilyl)silane: an unprecedented enhancement in the diastereoselectivity of radical cyclisations to give 2,4-disubstituted piperidines

Lucile A. Gandon, Alexander G. Russell and John S. Snaith

Cyclisation of bromides **4a–f** mediated by tributyltin hydride affords predominantly the *trans* piperidines **5a–f** with modest diastereomeric ratios, while cyclisation with tris(trimethylsilyl)silane affords the same products with diastereomeric ratios of up to 99:1.

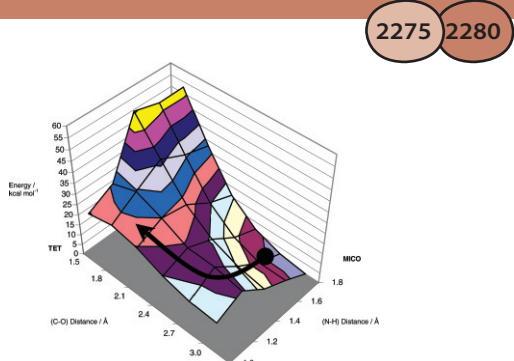


Inositols as chiral templates: 1,4-conjugate addition to tethered cinnamic esters

Ghislaine Cousins, Andrew Falshaw and John O. Hoberg

With inositols as chiral templates, excellent ee's and yields are obtained in conjugate addition reactions.

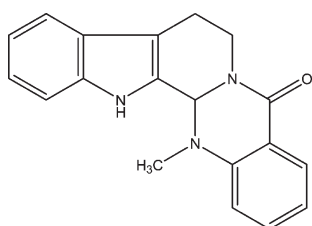
ARTICLES



Theoretical analysis of peptidyl α -ketoheterocyclic inhibitors of human neutrophil elastase: Insight into the mechanism of inhibition and the application of QM/MM calculations in structure-based drug design

M. Paul Gleeson, Ian H. Hillier and Neil A. Burton

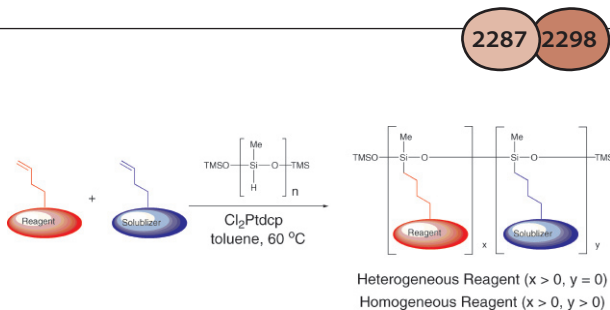
We use QM/MM methods to investigate the mechanism of inhibition of elastase by peptidyl α -ketoheterocyclic inhibitors.



Evodiamine functions as an agonist for the vanilloid receptor TRPV1

Larry V. Pearce, Pavel A. Petukhov, Tamas Szabo, Noemi Kedei, Fero Bizik, Alan P. Kozikowski and Peter M. Blumberg

Evodiamine functions as a novel full agonist, like capsaicin, for the heterologously expressed rat TRPV1.



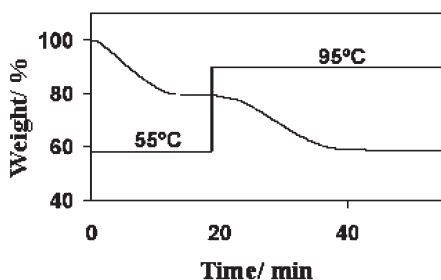
Polysiloxane-bound ligand accelerated catalysis: a modular approach to heterogeneous and homogeneous macromolecular asymmetric dihydroxylation ligands

Michael S. DeClue and Jay S. Siegel

The modular scaffold polysiloxane allows high catalyst loadings providing exceptionally reactive heterogeneous and homogeneous macromolecular reagents.



2299 2304

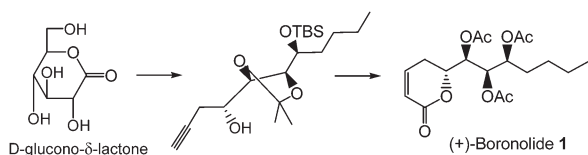


Inclusion by a fluorenyl host with volatile guests: structures, thermal stability and kinetics

Mino R. Caira, Tanya le Roex, Luigi R. Nassimbeni, John A. Ripmeester and Edwin Weber

The kinetics of desorption of several host–guest compounds are correlated to their structures.

2305 2310



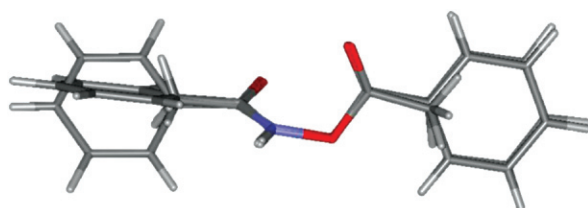
Stereoselective synthesis of (+)-boronolide and its 8-epimer

Shou-Gang Hu, Tai-Shan Hu and Yu-Lin Wu

The δ -butenolactone segment of **1** can be prepared *via* propargylation and three of the four chiral centers can be taken from D-glucono- δ -lactone directly.



2311 2314



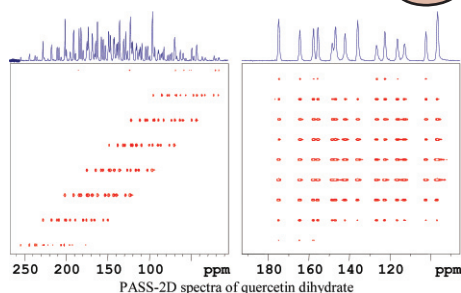
N,O-diacylhydroxylamines—structures in crystals and solutions

Jan Schraml, Jan Sýkora, Pavel Fiedler, Jana Roithová, Jaromír Mindl, Vratislav Blechta, Ivana Císařová and Otto Exner

N,O-Diacylhydroxylamines (RCOHNOCOR', R, R' = Me, Ph) have NH tautomer structure both in the solid state and in DMSO solutions.



2315 2322



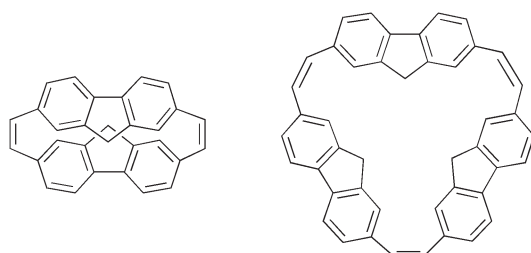
Solid state NMR studies and density functional theory (DFT) calculations of conformers of quercetin

Sebastian Olejniczak and Marek J. Potrzebowski

A comparative analysis of two crystallographic modifications of quercetin is presented; the existence of dihydrated and unhydrated forms of quercetin in the solid state is confirmed by several experimental techniques.



2323 2326

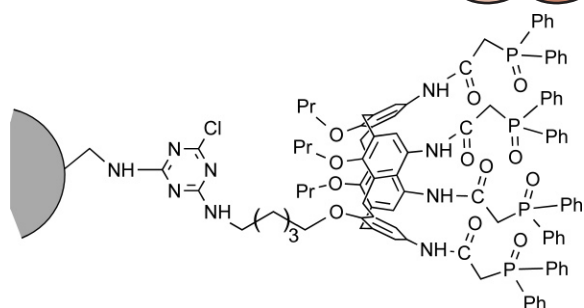


[2.2](2,7)-Fluorenophanediene, [2.2.2](2,7)-fluorenophanetriene, and their fluorenyl ions

Kouzou Matsumoto, Hiroaki Minami, Takeshi Kawase and Masaji Oda

The McMurry coupling of 2,7-diformylfluorene affords a dimer, *anti*-[2.2](2,7)-fluorenophanediene, and a trimer, [2.2.2](2,7)-fluorenophanetriene, as cyclic oligomers.

2327 2334

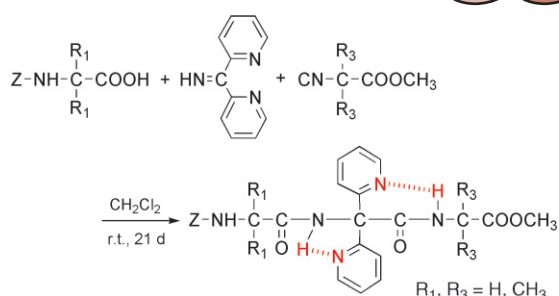


Separation of lanthanides and actinides using magnetic silica particles bearing covalently attached tetra-CMPO-calix[4]arenes

Volker Böhmer, Jean-François Dozol, Cordula Grüttner, Karine Liger, Susan E. Matthews, Sandra Rudershausen, Mohamed Saadioui and Pingshan Wang

Magnetic silica particles coated with covalently linked calix[4]arene derivatives were used to remove Eu(III) and Am(III) from aqueous nitric acid.

2335 2339

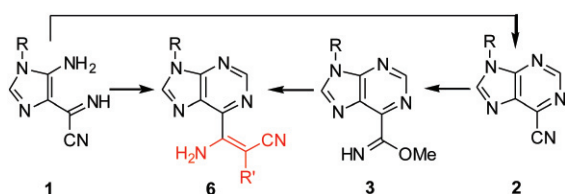


A novel intramolecular hydrogen bonding between a side-chain pyridine ring and an amide hydrogen of the peptide backbone in tripeptides containing the new amino acid, α,α -di(2-pyridyl)glycine

Takashi Yamada, Tomoyuki Ichino, Masayuki Hanyu, Daisuke Ninomiya, Ryoji Yanagihara, Toshifumi Miyazawa and Takashi Murashima

Tripeptides containing the new amino acid, α,α -di(2-pyridyl)glycine (2Dpy), synthesized by the modified Ugi reaction adopt a unique conformation.

2340 2345

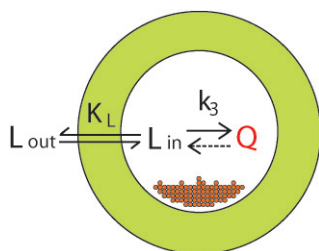


Synthesis of novel 6-enaminopurines

M. Alice Carvalho, Magdi E. A. Zaki, Yolanda Álvares, M. Fernanda Proença and Brian L. Booth

6-Enaminopurines **6** were prepared in excellent yield either from imidazole **1** or from purine **3** in a mild one-step reaction.

2346 2351

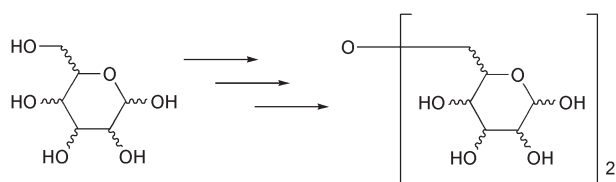


New insights into iron release from ferritin: direct observation of the neurotoxin 6-hydroxydopamine entering ferritin and reaching redox equilibrium with the iron core

Guy N. L. Jameson, Reginald F. Jameson and Wolfgang Linert

The ability of 6-hydroxydopamine to enter ferritin and reduce the iron is examined in detail.

2352 2358

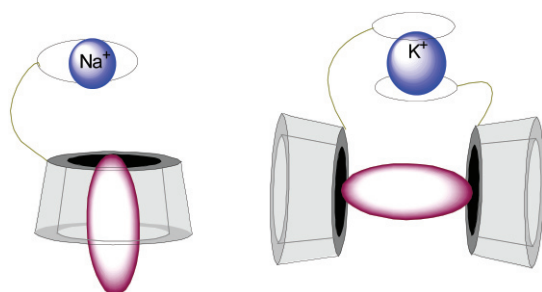


Synthesis of 6,6'-ether linked disaccharides from D-allose, D-galactose, D-glucose and D-mannose; evidence on the structure of coyolosa

Alan H. Haines

NMR spectroscopic data on 6,6'-linked ethers of hexopyranoses indicate the hypoglycemic compound coyolosa does not possess this type of structure.

2359 2364

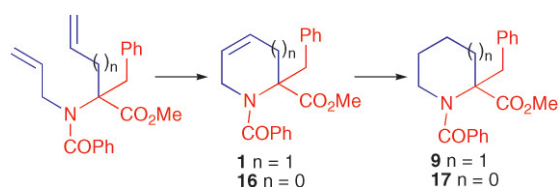


Cooperative self-assembly and molecular binding behavior of cyclodextrin–crown ether conjugates mediated by alkali metal ions

Yu Liu, Zhong-Yu Duan, Yong Chen, Jian-Rong Han and Lv Cui

K⁺-mediated self-assembly of cyclodextrin–crown ether conjugates possessing a dimeric structure results in enhanced recognition abilities towards guest molecules.

2365 2370

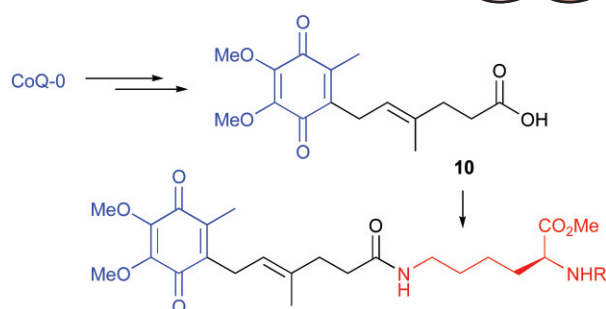


Synthesis and solid state conformation of phenylalanine mimetics constrained in a proline-like conformation

James Gardiner and Andrew D. Abell

Five- and six-membered cyclic phenylalanine mimics (**1**, **9**, **16**, and **17**) constrained in a proline-like conformation have been synthesised and the solid state structures of **1**, **9** and **16** have been determined by X-ray crystallography.

2371 2375

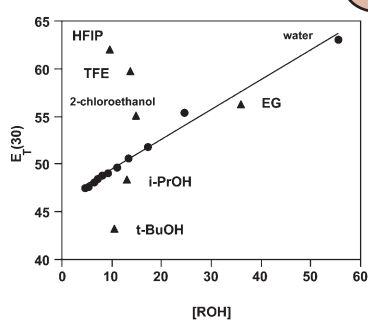


The preparation of side chain functionalized analogues of coenzyme Q for protein conjugation studies

Alison M. Daines and Andrew D. Abell

Two analogues of CoQ (**10** and **13**) have been prepared and **10** conjugated with the side chain of *N*-Ac-L-Lys-OMe and *N*-Ac-Gly-L-Lys-OMe as a first step to raising a monoclonal antibody against CoQ.

2376 2380

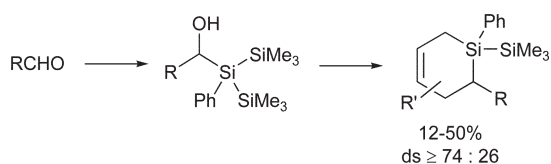


Role of hydroxyl concentrations in solvatochromic measures of solvent polarity of alcohols and alcohol–water mixtures—evidence that preferential solvation effects may be overestimated

T. William Bentley and In Sun Koo

The correlation shown for a series of primary alcohols is extended to aqueous mixtures by summing alcohol and water concentrations.

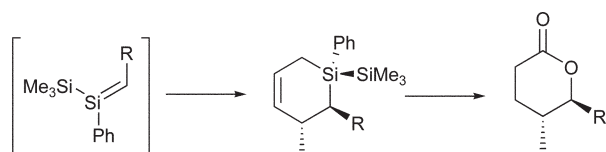
2381 2392



Silenes as novel synthetic reagents: identification of a practical method for silene generation and trapping

Malcolm B. Berry, Russell J. Griffiths, Mahesh J. Sanganee, Patrick G. Steel and Daniel K. Whelligan

The presence of a sub-stoichiometric amount of soluble lithium salts (LiBr) is crucial for the generation of highly reactive transient silenes through the silyl modified Peterson olefination.



Stereochemistry of the reaction of Si-phenyl silenes with butadienes: elaboration of the silacycloadducts to provide a novel route to substituted lactones

Mahesh J. Sanganee, Patrick G. Steel and Daniel K. Whelligan

Silenes, generated through a modified Peterson reaction, combine with alkyl butadienes to afford silacycles with good chemo- and stereoselectivity. These provide access to diols and lactone *via* a phenyl triggered Fleming–Tamao oxidation.

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