Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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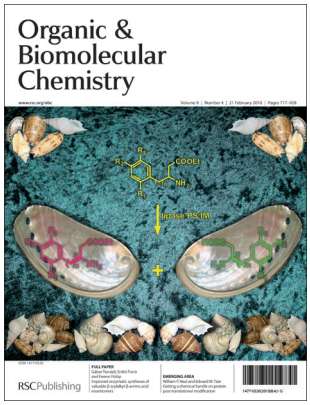
IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 8(4) 717–928 (2010)



Cover

See Ferenc Fülöp *et al.*, pp. 793–799.
The enantioselective *Burkholderia cepacia*-catalysed hydrolyses of biologically relevant β-arylalkyl-substituted β-amino esters were performed with high enantiomeric excesses and in good yields.

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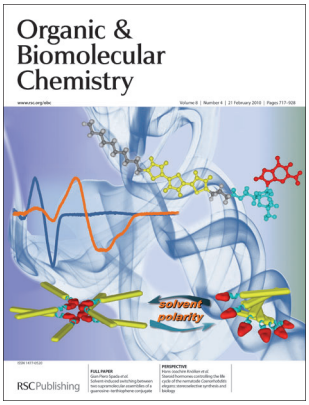

Inside cover

See Gian Piero Spada *et al.*, pp. 774–781.
Guanine or terthienyl: which one leads the self-assembly of the guanosine–terthiophene conjugate? Upon increasing solvent polarity, the supramolecular aggregate directed by guanine stacking is reversibly converted into a terthienyl stacked architecture.

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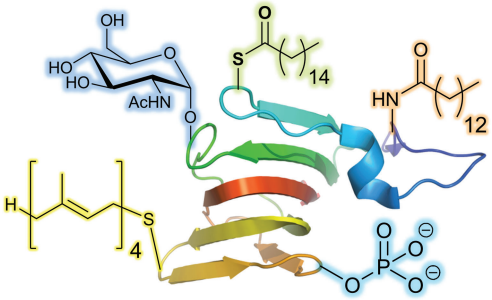
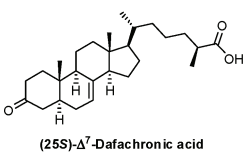
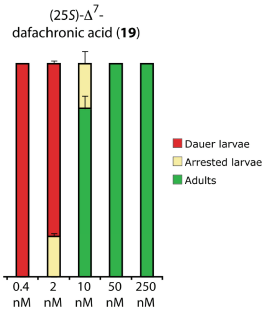
EMERGING AREA



PERSPECTIVE



(25*S*)-Δ^7-Dafachronic acid



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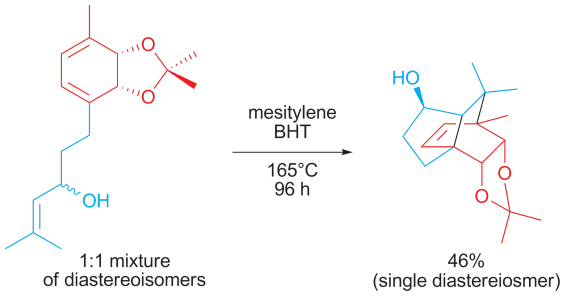
751

Chemoenzymatic and enantiodivergent routes to 1,2-ring-fused bicyclo[2.2.2]octane and related tricyclic frameworks

Kerrie A. B. Austin, Jon D. Elsworth, Martin G. Banwell* and Anthony C. Willis

The chemoenzymatically derived triene undergoes a facially-selective IMDA reaction to give an adduct incorporating the carbocyclic framework of the sesquiterpene (–)-khusiol.



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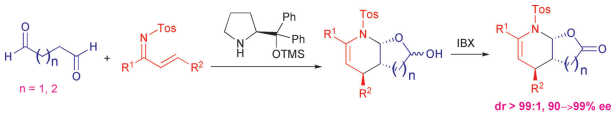
Enantioselective construction of lactone[2,3-*b*]piperidine skeletons *via* organocatalytic tandem reactions

Zhao-Quan He, Bo Han, Rui Li,* Li Wu and Ying-Chun Chen*

A highly enantioselective construction of δ- and γ-lactone[2,3-*b*]piperidine skeletons was accomplished by tandem aza-Diels–Alder reaction–hemiacetal formation–oxidation from *N*-Tos-1-aza-1,3-butadienes and aliphatic dialdehydes.



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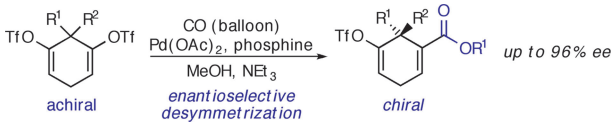
Enantioselective desymmetrizing palladium catalyzed carbonylation reactions: the catalytic asymmetric synthesis of quaternary carbon center containing 1,3-dienes

Simon J. Byrne, Anthony J. Fletcher, Paul Hebeisen and Michael C. Willis*

A desymmetrization protocol has been used to develop a palladium catalyzed enantioselective carbonylation process. Achiral cyclic bis-alkenyltriflates are converted to their corresponding monoester derivatives with selectivities of up to 96% ee.

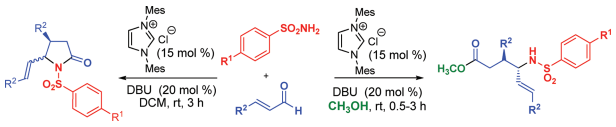


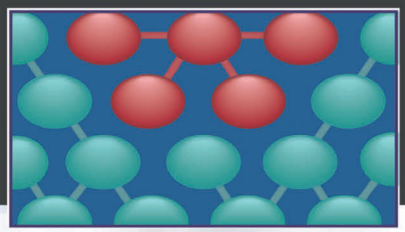
761

A novel pseudo four component reaction involving homoenolate for the synthesis of γ-aminobutyric acid (GABA) derivatives

Vijay Nair,* Vimal Varghese, Beneesh P. Babu, C. R. Sinu and Eringathodi Suresh

Homoenolate generated from α,β-unsaturated aldehydes by NHC catalysis underwent facile addition to conjugated sulfonimines and subsequent methanolysis to afford protected GABA derivatives stereoselectively and in high yields, thus constituting a novel pseudo four component reaction.





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Beining Chen, Senior Lecturer, Unviersity of Sheffield
Andreas Kuglstatter, Research Scientist, Hoffmann-La Roche
Gisber Schneider, Professor, Goethe Unviersity
Alexander Doemling, Associate Professor, Unviersity of Pittsburg
Rod Hubbard, Professor, York University
Asier Unciti-Broceta, Senior Research Fellow, University of Edinburgh
Edgar Jacoby, Group Leader, Novartis
György Keseru, Head of Discovery Chemistry, Gedeon Richter
Chiara Ghiron, Head of Department, Siena Biotech
Bernd Wendt, Senior Scientist, Elara Pharmaceuticals
Peter Oledzki, Application Scientist, BioSolveIT
Mark Bagley, Reader, Cardiff University

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Agenda Topics to include:

- Compound Management
- Chemogenomics
- Fragment Based Lead Detection
- Formulation

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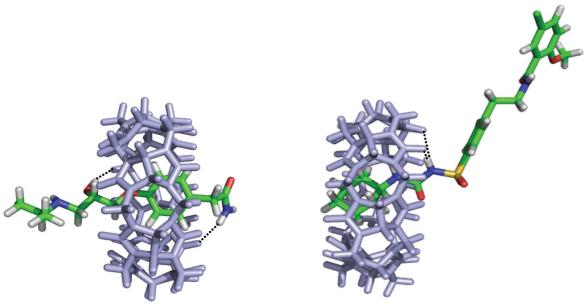

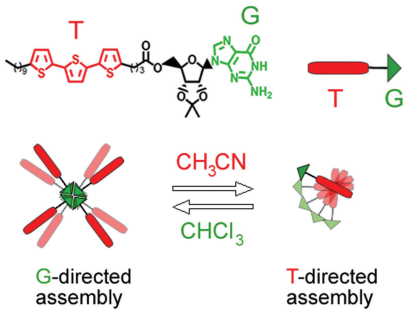

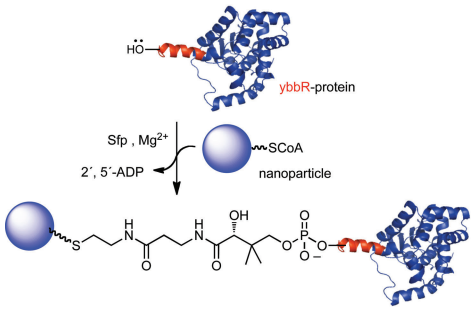

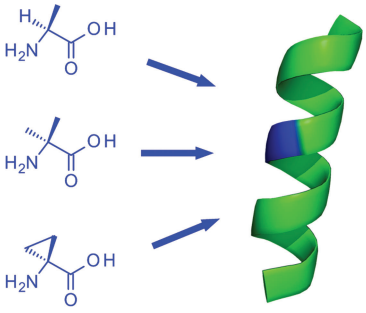

2010 Meetings (in chronological order)

NF-κB in Inflammation & Disease
Advances in Biopharmaceuticals
Structural Biology
Structural Genomics: Expanding the Horizons of Structural Biology
Triglycerides & Triglyceride-Rich Particles in Health & Disease (new!)
Alzheimer's Disease Beyond Aβ
Molecular Basis for Biological Membrane Organization & Dynamics
HIV Biology & Pathogenesis
RNA Silencing: Mechanism, Biology & Application
Molecular Basis for Chromatin Structure & Regulation
Hypoxia: Molecular Mechanisms of Oxygen Sensing & Response Pathways
Adipose Tissue Biology
Neuronal Control of Appetite, Metabolism & Weight*
New Insights into Healthspan & Diseases of Aging
Role of Inflammation in Oncogenesis
Molecular and Cellular Biology of Immune Escape in Cancer
Advances in Molecular Mechanisms of Atherosclerosis
The Macrophage: Intersection of Pathogenic & Protective Inflammation
Antibiotics & Resistance: Challenges & Solutions (new!)
Stem Cell Differentiation & Dedifferentiation
Cell Biology of Virus Entry, Replication & Pathogenesis
RNA Silencing Mechanisms in Plants (new!)
Tolerance & Autoimmunity
Cilia, Signaling & Human Disease
Lymphocyte Activation & Gene Expression
Angiogenesis in Health & Disease
Cardiovascular Development & Repair
Biomolecular Interaction Networks: Function & Disease (new!)
Cell Death Pathways: Apoptosis, Autophagy & Necrosis
Metabolism & Cancer Progression (new!)
Receptors and Signaling in Plant Development & Biotic Interactions
HIV Vaccines
Viral Immunity
Nuclear Receptors: Signaling, Gene Regulation & Cancer
Nuclear Receptors: Development, Physiology & Disease
New Paradigms in Cancer Therapeutics
Integration of Developmental Signaling Pathways
G Protein-Coupled Receptors
Dynamics of Eukaryotic Transcription During Development
Synapses: Formation, Function & Misfunction
Towards Defining the Pathophysiology of Autistic Behavior
Malaria: New Approaches to Understanding Host-Parasite Interactions
Molecular Targets for Control of Vector-Borne Diseases: Bridging Lab & Field Research*
Islet Biology
Diabetes
Computer-Aided Drug Design
New Directions in Small Molecule Drug Discovery (new!)
Developmental Origins & Epigenesis in Human Health and Disease (new!)
Bioactive Lipids: Biochemistry & Diseases
Innate Immunity: Mechanisms Linking with Adaptive Immunity

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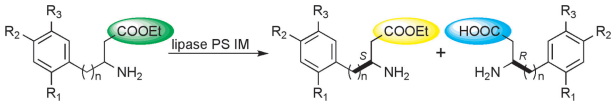
Improved enzymatic syntheses of valuable β-arylalkyl-β-amino acid enantiomers

Gábor Tasnádi, Enikő Forró and Ferenc Fülöp*

The enantioselective ($E \sim 200$) *Burkholderia cepacia*-catalysed hydrolyses of β-amino esters with H_2O (0.5 equiv.) in *t*-BuOMe or in *i*-Pr_2O at 45 °C are described. The enantiomers were prepared with high enantiomeric excesses (*ee* >96%) and in good yields (>42%).



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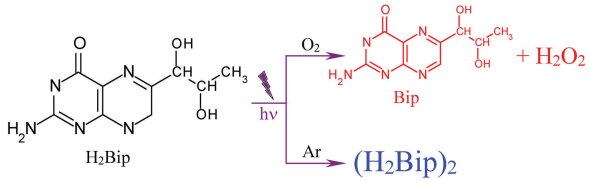
Photochemistry of dihydrobiopterin in aqueous solution

Mariana Vignoni, Franco M. Cabrerizo, Carolina Lorente, Catherine Claparols, Esther Oliveros* and Andrés H. Thomas*

Photooxidation of pterins takes place *in vivo* under pathological conditions. We have investigated the photochemistry of dihydrobiopterin and discuss the mechanisms involved.

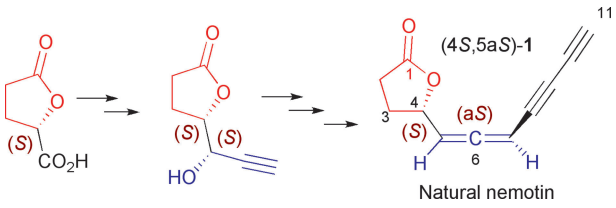


811

The enantioselective total synthesis of nemotin

Ya-Jun Jian and Yikang Wu*

The gross structure of nemotin was established in the 1950s, but the stereochemistry remains unknown to date. Now, with the aid of an enantioselective synthesis, the (4*S*,5a*S*) configuration among the four possible alternatives is shown to represent the natural product.

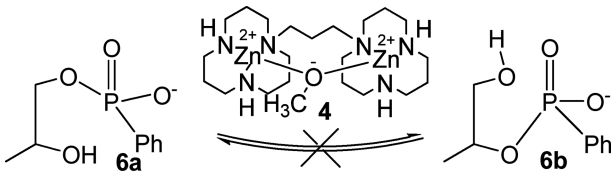


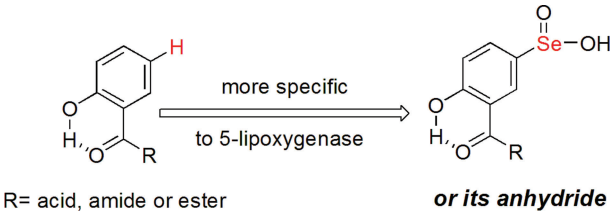
822

On the question of stepwise *vs.* concerted cleavage of RNA models promoted by a synthetic dinuclear Zn(II) complex in methanol: implementation of a noncleavable phosphonate probe

David R. Edwards, Wing-Yin Tsang, Alexei A. Neverov and R. Stan Brown*

$Zn(II)_2$ complex (**4**) does not promote the interconversion of isomeric phosphonates (**6a**, **6b**), the only products of the reaction being 1,2-propanediol and *O*-methyl phenylphosphonate.

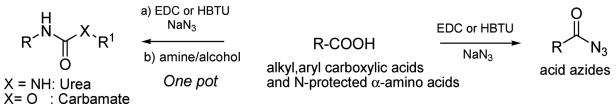




5-Selenization of salicylic acid derivatives yielded isoform-specific 5-lipoxygenase inhibitors

Sun-Chol Yu, Hartmut Kuhn,* Constantin-Gabriel Daniliuc, Igor Ivanov, Peter G. Jones and Wolf-Walther du Mont*

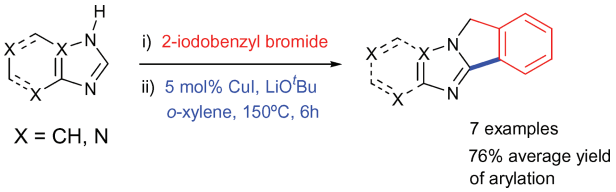
5-Seleninic acids or anhydrides of salicylic acid amides or esters are promising inhibitors more selective to recombinant human 5-lipoxygenase than to rabbit reticulocyte 12/15-lipoxygenase.



New and simple synthesis of acid azides, ureas and carbamates from carboxylic acids: application of peptide coupling agents EDC and HBTU

Vommina V. Sureshbabu,* H. S. Lalithamba, N. Narendra and H. P. Hemantha

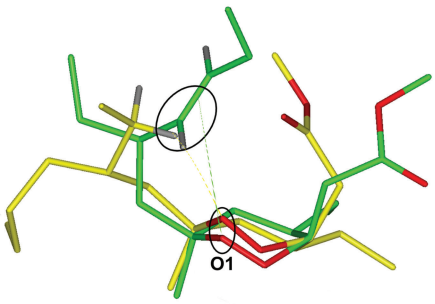
Acid azides have been efficiently prepared from carboxylic acids using peptide coupling agents EDC or HBTU; and the reaction has been extended to the one pot synthesis of ureas and carbamates from carboxylic acids



Ligand-free copper(I)-catalysed intramolecular direct C–H functionalization of azoles

Nekane Barbero, Raul SanMartin* and Esther Domínguez*

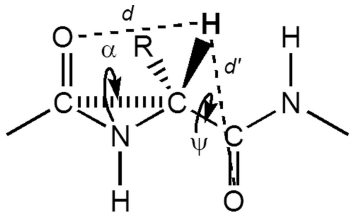
The first examples of copper-catalysed intramolecular direct C-arylation of azaheterocycles for the synthesis of complex heterofused compounds is presented, featuring an unprecedented arylation *via* C–H activation of 9*H*-purine and 4-azabenzimidazole.



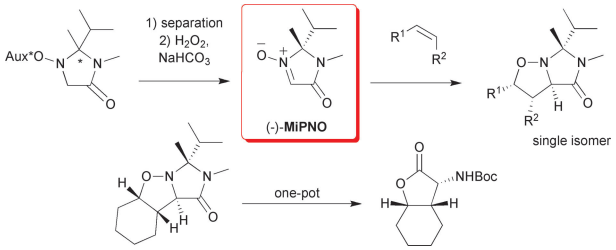
Insight into the mechanism of action of plakortins, simple 1,2-dioxane antimalarials

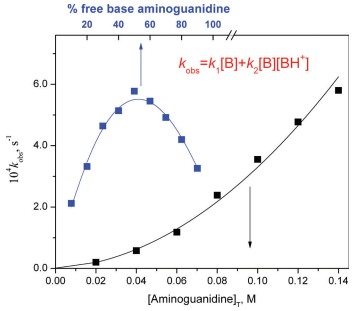
Orazio Taglialatela-Scafati, Ernesto Fattorusso, Adriana Romano, Fernando Scala, Vincenzo Barone, Paola Cimino, Emiliano Stendardo, Bruno Catalanotti, Marco Persico and Caterina Fattorusso*

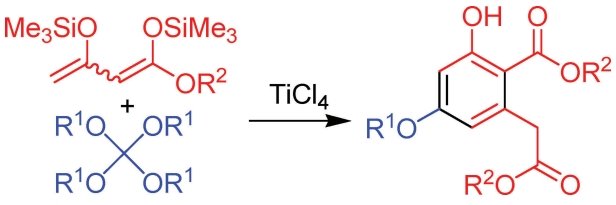
Computational calculations and chemical reactions give insight into the mechanism of the antimalarial action of plakortin and dihydroplakortin, simple 1,2-dioxanes isolated from a marine sponge.



$$\delta = 2.87 + \sigma_R + 1.32\cos^2\frac{(\alpha - 25)}{d} + 0.75\cos^2\frac{(\psi - 10)/2}{d'}$$







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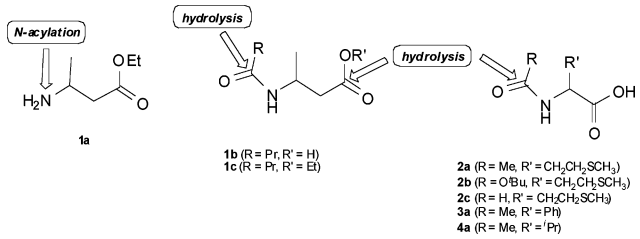
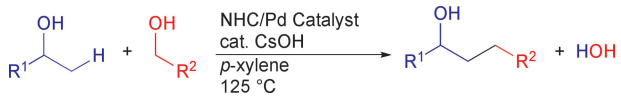


Formation and hydrolysis of amide bonds by lipase A from *Candida antarctica*; exceptional features

Arto Liljeblad,* Pauli Kallio, Marita Vainio, Jarmo Niemi and Liisa T. Kanerva

Exceptional lipase: the ability of lipase A from *Candida antarctica* (CAL-A) to form and hydrolyze amide bonds was studied with **1a–c**, **2a–c**, **3a** and **4a**. The possible role of enzyme contaminants in the reactions was studied by fractionation and sequence-based identification of the commercial CAL-A preparation Cat#ICR-112 (Codexis).

896



Cross-coupling reaction of alcohols for carbon–carbon bond formation using pincer-type NHC/palladium catalysts

Osamu Kose and Susumu Saito*

A cross-coupling reaction of different alcohols was achieved using a pincer-type NHC/PdBr complex as the catalyst precursor, and the reaction, under either Ar or H_2 gas, displayed a broad substrate scope with respect to both primary and secondary alcohol components, with high product alcohol selectivity.

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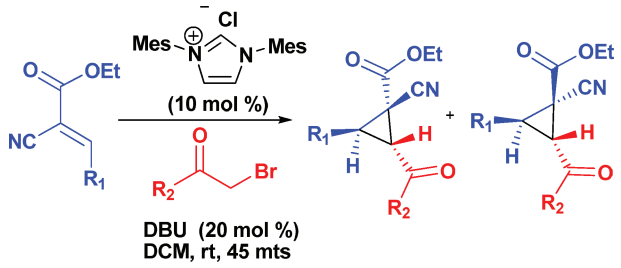

Nucleophilic heterocyclic carbene as a novel catalyst for cyclopropanation of cyano acrylates

Anabha E. Raveendran, Rony Rajan Paul, Eringathodi Suresh and Vijay Nair*

Nucleophilic heterocyclic carbenes (NHCs) have been used or the first time as catalysts in the cyclopropanation of ethyl cyanocinnamates with phenacyl bromide by Michael-initiated ring-closure (MIRC).

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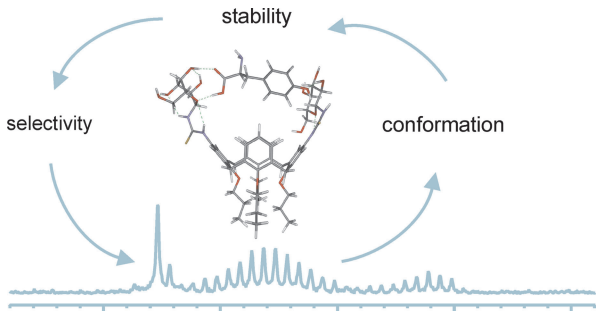
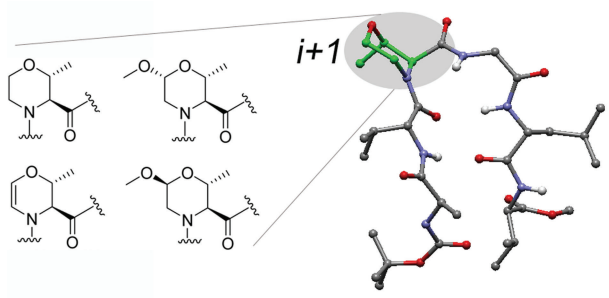


Glucosylthioureidocalix[4]arenes: Synthesis, conformations and gas phase recognition of amino acids

Mika Torvinen, Raisa Neitola, Francesco Sansone, Laura Baldini, Rocco Ungaro, Alessandro Casnati,* Pirjo Vainiotalo* and Elina Kalenius*

Conformational properties of glucosylcalixarenes and their selective complexation with amino acids have been clarified in solution and gas-phase.



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Electronic supplementary information (ESI) is available *via* the online article (see http://www.rsc.org/esi for general information about ESI).

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