

Organic & Biomolecular Chemistry

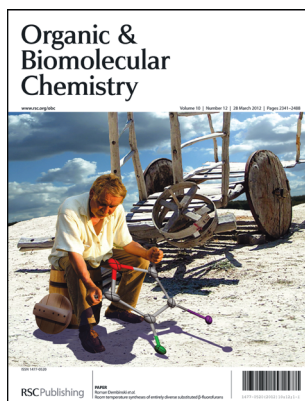
An international journal of synthetic, physical and biomolecular organic chemistry

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IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 10(12) 2341–2488 (2012)



Cover

See Roman Dembinski *et al.*, pp. 2395–2408.

The cover image is related to cycloisomerization and electrophilic cyclization reactions. The methodology allows the synthesis of diversely substituted β -fluorofurans, from propargyl ketones at room temperature. Cover art by Tomasz Sniady.

Image reproduced by permission of Roman Dembinski from *Org. Biomol. Chem.*, 2012, **10**, 2395.

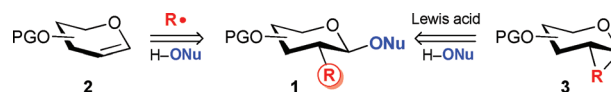
PERSPECTIVE

2351

Recent advances in the stereoselective synthesis of carbohydrate 2-C-analogs

Jian Yin and Torsten Linker*

A perspective summarizing recent syntheses of carbohydrate 2-C-analogs **1** by ring-opening of cyclopropanated sugars **3** and radical additions to glycols **2** is given.



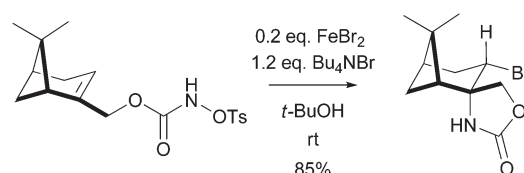
COMMUNICATIONS

2363

Intramolecular iron(II)-catalyzed aminobromination of allyl *N*-tosyloxycarbamates

Takuma Kamon, Daisuke Shigeoka, Tetsuaki Tanaka and Takehiko Yoshimitsu*

Allyl *N*-tosyloxycarbamates are found to be catalytically transformed into β -brominated oxazolidinones with FeBr_2 /*n*- Bu_4NBr in *t*-BuOH.



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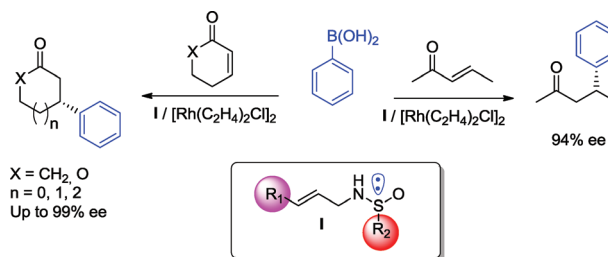
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COMMUNICATIONS

2366

“Sulfolefin”: Highly modular mixed S/Olefin ligands for enantioselective Rh-catalyzed 1,4-addition

Noureddine Khier,* Álvaro Salvador, Ahmed Chelouan, Ana Alcudia and Inmaculada Fernández*

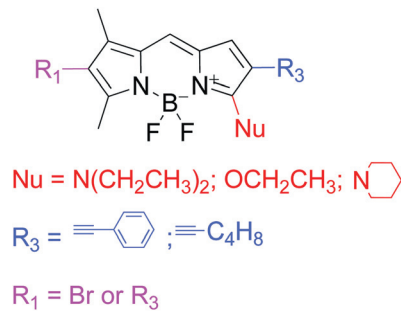
Sulfolefins **I** obtained in one step from DAG-sulfinate esters are excellent catalysts for the Rh-catalyzed 1,4-addition of boronic acids to cyclic and acyclic olefins.

2369

Diversity-oriented derivatization of BODIPY based on regioselective bromination

Xin Li, Shufang Huang and Yongzhou Hu*

Diversely substituted BODIPYs were achieved with a one-pot procedure.

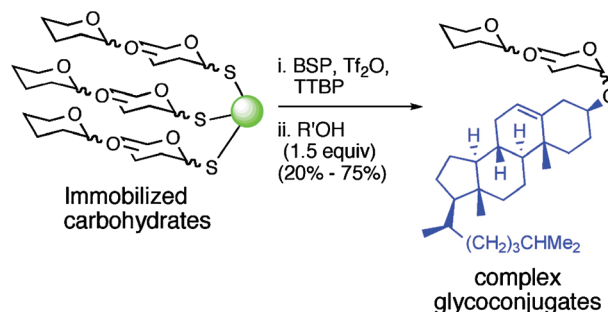


2373

Direct O-glycosidation of resin bound thioglycosides

Son Hong Nguyen, Adam H. Trotta, John Cao, Timothy J. Straub and Clay S. Bennett*

Glycoconjugate synthesis by the transfer of resin-immobilized carbohydrates to <2 equivalents of complex aglycones is described.

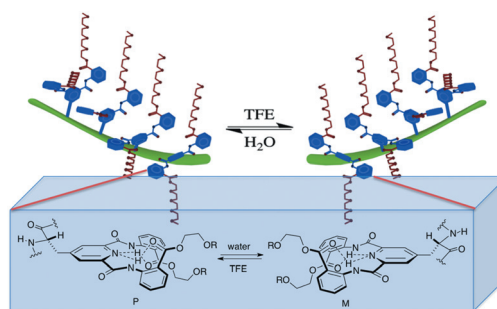


2377

Intramolecular chiral communication in peptide-dendron hybrids

Hui Shao, Nicholas A. Bewick and Jon R. Parquette*

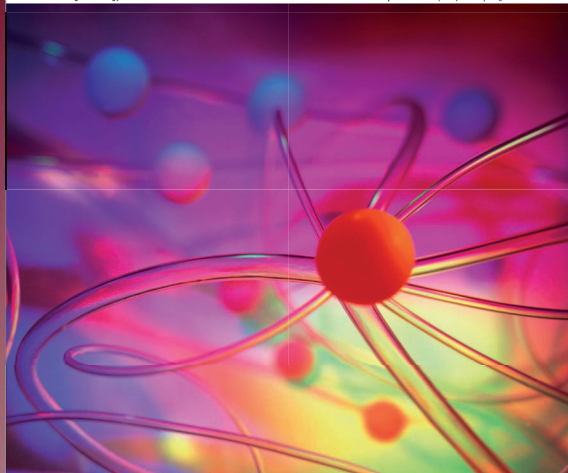
Intramolecular chirality transfer, amplification and solvent-mediated switching was observed in a series of random-coil peptide-dendron hybrids.



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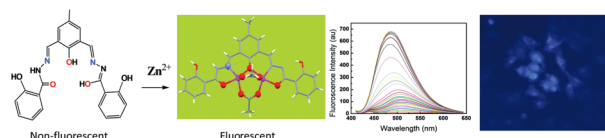
COMMUNICATIONS

2380

A highly selective and sensitive *in vivo* fluorosensor for zinc(II) without cytotoxicity

Tarun Mistri, Malay Dolai, Debrup Chakraborty, Anisur Rahman Khuda-Bukhsh, Kalyan Kumar Das and Mahammad Ali*

A highly selective and sensitive fluorescent Zn^{II}-sensor (**1**) features visible excitation and emission profiles with $K_d < 1 \text{ pM}^2$, LOD $< 1 \text{ ng L}^{-1}$ and 680 fold fluorescent enhancement along with intracellular Zn²⁺ sensing without noticeable cytotoxicity.

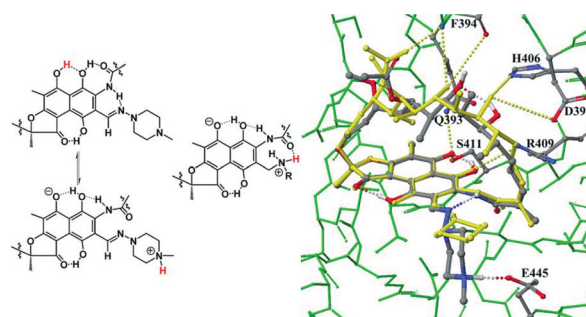


2385

Intramolecular proton transfer impact on antibacterial properties of ansamycin antibiotic rifampicin and its new amino analogues

Krystian Pyta, Piotr Przybylski,* Barbara Wicher, Maria Gdaniec and Joanna Stefańska

NMR and X-ray studies have provided evidence for the intramolecular proton transfer in rifampicin (**1**) and its amino analogues **2–9**. Biological tests of **1–9** in combination with the analysis of ligand–RNA polymerase interactions have revealed the relationship between the protonation site and extremely high antibacterial activity.

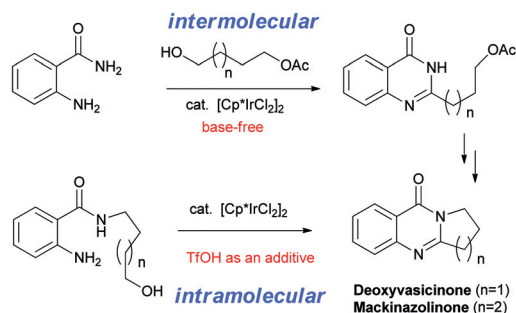


2389

Efficient syntheses of 2,3-disubstituted natural quinazolinones *via* iridium catalysis

Jie Fang and Jianguang Zhou*

Syntheses of natural quinazolinones *via* Ir-catalysis were described, in which both intermolecular and intramolecular reactions were successfully employed.

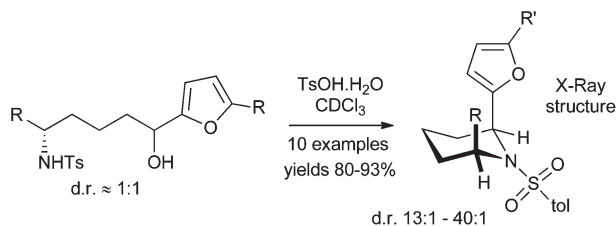


2392

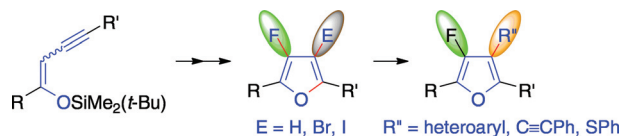
Furanyl cyclic amines: a diastereoselective synthesis of 2,6-*syn*-disubstituted piperidines under thermodynamic control

Matthew O'Brien,* Andrew Leach, Roly J. Armstrong, Keting Chong and Ross Sheridan

A highly diastereoselective synthesis of 2,6-disubstituted piperidines utilises an electron rich furan group to facilitate acid catalysed epimerisation.



2395

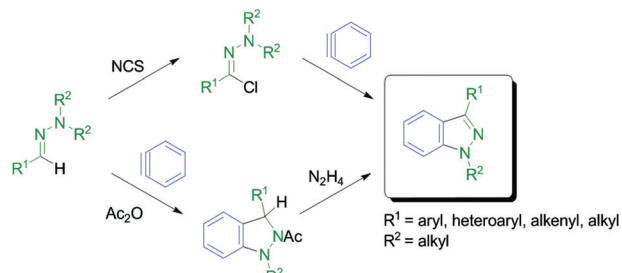


Room temperature syntheses of entirely diverse substituted β -fluorofurans

Yan Li, Craig A. Wheeler and Roman Dembinski*

Synthetic methods for the preparation of 3-fluorofurans, 3-bromo-4-fluorofurans, and 3-fluoro-4-iodofurans are elaborated.

2409

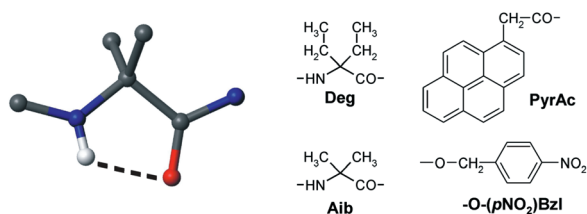


One-pot synthesis of 1-alkyl-1H-indazoles from 1,1-dialkylhydrazones *via* aryne annulation

Nataliya A. Markina, Anton V. Dubrovskiy and Richard C. Larock

The reaction of readily accessible 1,1-dialkylhydrazones with commercially available *o*-(trimethylsilyl)aryl triflates provides a direct one-step route to pharmaceutically important 1-alkylindazoles.

2413

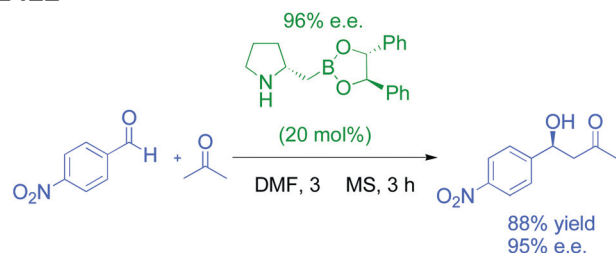


Novel peptide foldameric motifs: a step forward in our understanding of the fully-extended conformation/ 3_{10} -helix coexistence

Fernando Formaggio,* Marco Crisma, Gema Ballano, Cristina Peggion, Mariano Venanzi and Claudio Toniolo*

Fluorescent PyrAc-(Deg)_n-O-(*p*NO₂)Bzl peptides exist as mixtures of fully-extended (right) and 3_{10} -helical conformers, the latter typical of (Aib)_n oligomers.

2422



Mechanism and optimisation of the homoboroproline bifunctional catalytic asymmetric aldol reaction: Lewis acid tuning through *in situ* esterification

Irene Georgiou and Andrew Whiting*

The novel enamine-Lewis acid based chiral catalyst homoboroproline undergoes *in situ* esterification of the boronic acid to provide a highly effective asymmetric aldol catalyst.

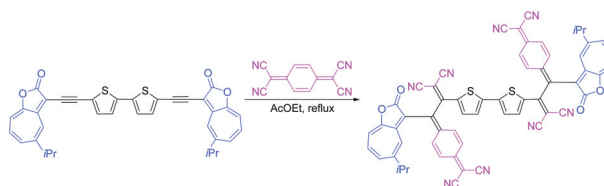
PAPERS

2431

Synthesis of donor–acceptor chromophores by the [2 + 2] cycloaddition of arylethynyl-2*H*-cyclohepta[*b*]furan-2-ones with 7,7,8,8-tetracyanoquinodimethane

Taku Shoji,* Junya Higashi, Shunji Ito, Tetsuo Okujima, Masafumi Yasunami and Noboru Morita

A series of 2*H*-cyclohepta[*b*]furan-2-one-substituted dicyanoquinodimethanes (DCNQs) were synthesized by the formal [2 + 2] cycloaddition–cycloreversion sequence of the corresponding acetylene derivatives with TCNQ.

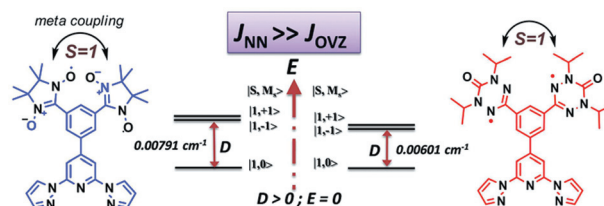


2439

Syntheses, optical and intramolecular magnetic properties of mono- and di-radicals based on nitronyl-nitroxide and oxoverdazyl groups appended to 2,6-bispyrazolylpyridine cores

Pramiti Hui, Khaja Md. Arif and Rajadurai Chandrasekar*

This paper presents the synthesis of a series of nitronyl-nitroxide (NN), oxoverdazyl (OVZ) based mono-, and bi-radicals attached to 4-phenyl-2,6-bispyrazolylpyridine coupling units, their optical, and electron spin resonance (ESR) spectroscopy studies.

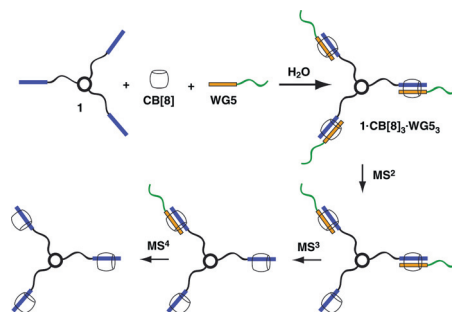


2447

Probing the stability of multicomponent self-assembled architectures based on cucurbit[8]uril in the gas phase

Monika Cziferszky, Frank Biedermann, Markus Kalberer and Oren A. Scherman*

An investigation of supramolecular stoichiometrically-controlled assemblies with CB[8] in water and their gas phase stabilities as measured by HCD fragmentation.

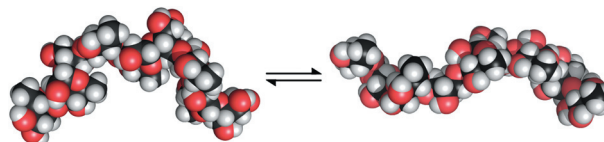


2453

Studies on the conformational flexibility of α -L-rhamnose-containing oligosaccharides using ^{13}C -site-specific labeling, NMR spectroscopy and molecular simulations: implications for the three-dimensional structure of bacterial rhamnan polysaccharides

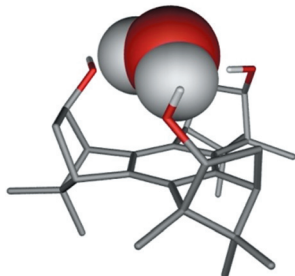
K. Hanna M. Jonsson, Elin Säwén and Göran Widmalm*

Conformational preferences and dynamics of constituent disaccharides are possible to translate to a description of polysaccharide three-dimensional structure.



2464

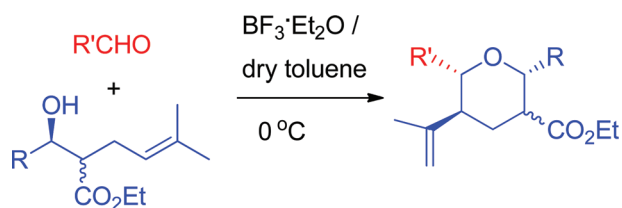
Make one's mouth water

**(+)-*syn*-Benzotriborneol an enantiopure C₃-symmetric receptor for water**

Fabrizio Fabris,* Ottorino De Lucchi, Ilaria Nardini, Marco Crisma, Andrea Mazzanti, Sax A. Mason, Marie-Hélène Lemée-Cailleau, Francesca A. Scaramuzzo and Cristiano Zonta*

The enantiopure C₃-symmetric triol forms stable complexes with water. This is due to the ability of the host to form three hydrogen bonds with water, to act simultaneously as a hydrogen-bond acceptor and donor, and to a geometrical match between the pair.

2470



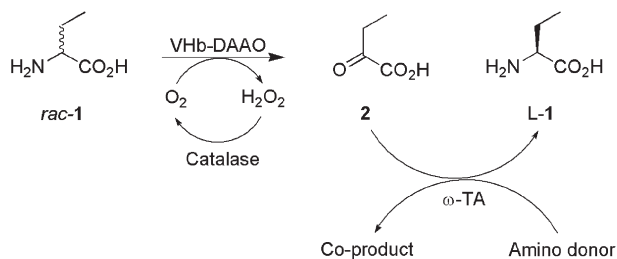
Where R = Me, Et, Ph; R' = alkyl, aryl 55-92%

Synthesis of 2,3,5,6-tetrasubstituted tetrahydropyrans via (3,5)-oxonium-ene reaction

Pipas Saha, Anup Bhunia and Anil K. Saikia*

2,3,5,6-Tetrasubstituted tetrahydropyrans can be efficiently synthesized from the reaction of aldehydes and ethyl 2-(1-hydroxyalkyl/hydroxy(phenyl)methyl)-5-methylhex-4-enoate via (3,5)-oxonium-ene reaction in good yields under mild conditions.

2482

**Deracemization of unnatural amino acid: homoalanine using D-amino acid oxidase and ω-transaminase**

Young-Man Seo, Sam Mathew, Han-Seop Bea, Yong-Ho Khang, Sang-Hyeup Lee, Byung-Gee Kim and Hyungdon Yun*

A deracemization method was developed to generate optically pure L-homoalanine from racemic homoalanine using D-amino acid oxidase and ω-transaminase.