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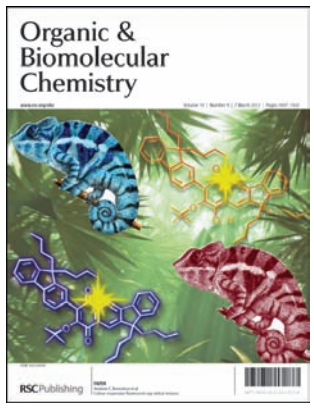
IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 10(9) 1697–1932 (2012)



Cover
See Andrew C. Benniston *et al.*, pp. 1775–1784.

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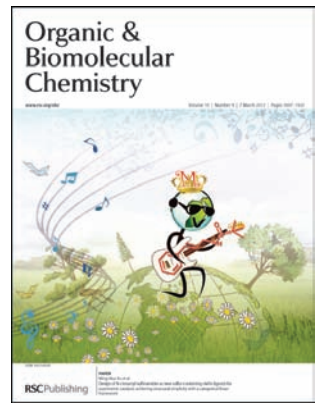

Inside cover
See Ming-Hua Xu *et al.*, pp. 1764–1768.

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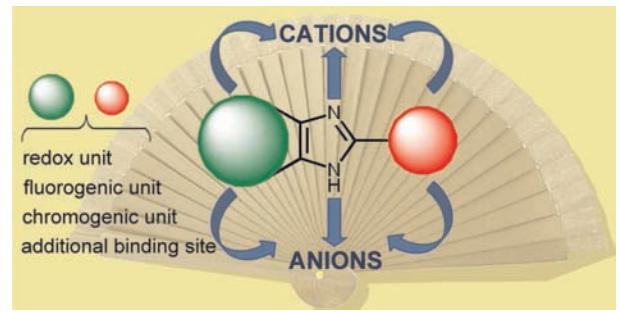
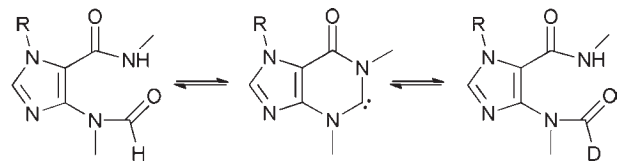
PERSPECTIVE



COMMUNICATIONS



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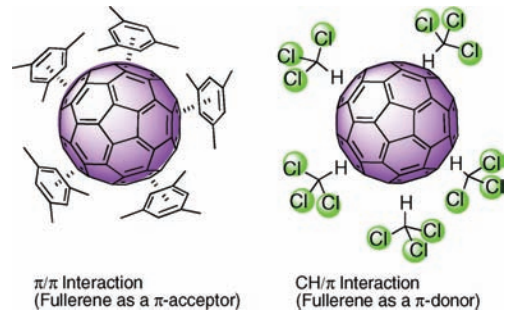
COMMUNICATIONS

1730

First kinetic evidence for the CH/π and π/π solute–solvent interaction of C_{60} in the Diels–Alder reaction with cyclohexadiene

Takumi Oshima,* Tsubasa Mikie, Naohiko Ikuma and Hajime Yakuma

The first CH/π solute–solvent interaction of C_{60} was evidenced by the kinetic solvent effects in the Diels–Alder reaction with 1,3-cyclohexadiene.

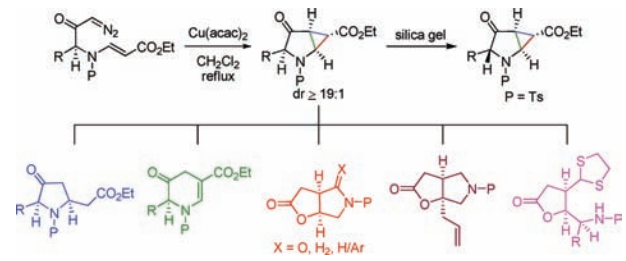


1735

Stereoselective synthesis and applications of nitrogen substituted donor–acceptor cyclopropanes (N-DACs) in the divergent synthesis of azacycles

Santosh J. Gharpure,* U. Vijayasree and S. Raja Bhushan Reddy

Stereoselective intramolecular cyclopropanation of vinylogous carbamates with carbenes using $Cu(acac)_2$ as the catalyst has been developed for the construction of N-DACs. Regioselective cleavage of each of the cyclopropane bonds of the N-DACs led to a diverse array of azacycles.

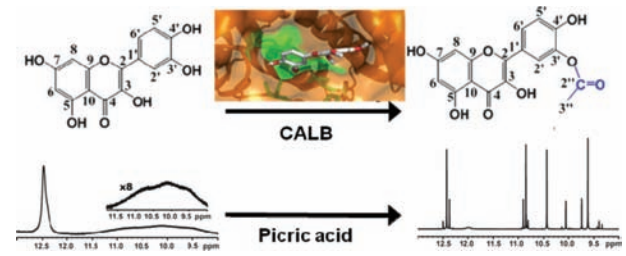


1739

Unexpected enzyme-catalyzed regioselective acylation of flavonoid aglycones and rapid product screening

Eleni Kyriakou, Alexandra Primikyri, Pantelis Charisiadis, Maria Katsoura, Ioannis P. Gerothanassis, Haralambos Stamatis and Andreas G. Tzakos*

CALB-mediated regioselective polyphenol aglycon transformations are reported and rapid product formation screening is achieved through an internal sensor.

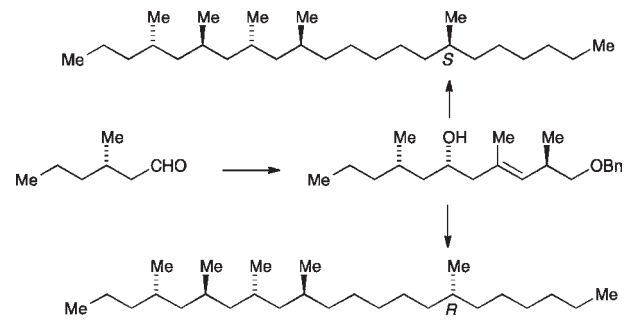


1743

Total synthesis of a cuticular hydrocarbon from the cane beetle *Antitrogus parvulus*: confirmation of the relative stereochemistry

Norazah B. Basar, Hao Liu, Devendra Negi, Hasnah M. Sirat, Gareth A. Morris and Eric J. Thomas*

Synthesis and comparison of (4*S*,6*R*,8*R*,10*S*,16*S*)- and (4*S*,6*R*,8*R*,10*S*,16*R*)-4,6,8,10,16-pentamethyldocosanes confirmed that the (16*S*)-epimer was the hydrocarbon isolated from *Antitrogus parvulus*.



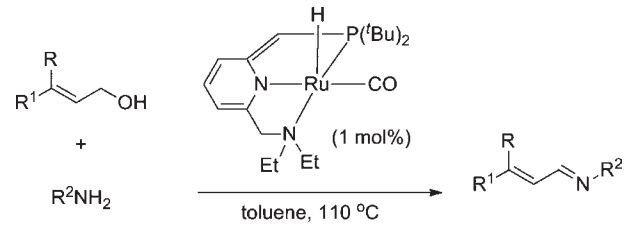
COMMUNICATIONS

1746

α,β-Unsaturated imines *via* Ru-catalyzed coupling of allylic alcohols and amines

Jared W. Rigoli, Sara A. Moyer, Simon D. Pearce and Jennifer M. Schomaker*

The conversion of allylic alcohols and amines to α,β-unsaturated imines is reported using 1 mol% of a Ru-pincer complex.

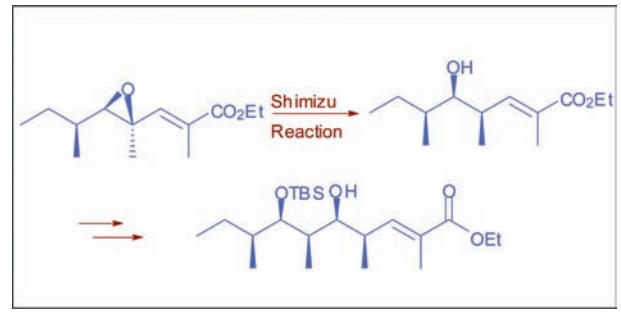


1750

An iterative Shimizu non-aldol approach for the stereoselective synthesis of C13-C22 fragment of callystatin A

Sandip A. Pujari and Krishna P. Kaliappan*

A stereoselective synthesis of C13-C22 fragment of callystatin A by using an iterative Shimizu non-aldol approach is reported.



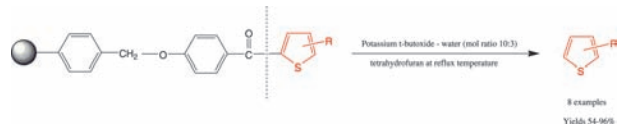
PAPERS

1754

Polymer-supported syntheses of thiophene-containing compounds using a new type of traceless linker

Abderrazak Ben-Haida and Philip Hodge*

A traceless linker that is based on the Haller–Bauer cleavage of polymer-supported aryl 2-thienyl ketones is described.

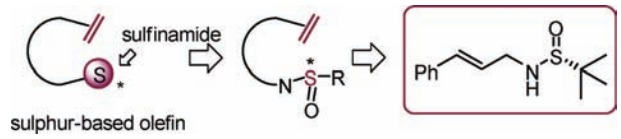


1764

Design of *N*-cinnamyl sulfinamides as new sulfur-containing olefin ligands for asymmetric catalysis: achieving structural simplicity with a categorical linear framework

Shen-Shuang Jin, Hui Wang, Ting-Shun Zhu and Ming-Hua Xu*

The design and development of an extraordinarily simple new class of chiral sulfur–olefin hybrid ligands with remarkable structural simplicity were described. These unique sulfinamide–olefin ligands have been proved to be highly effective ligands in Rh-catalyzed asymmetric 1,4-additions.



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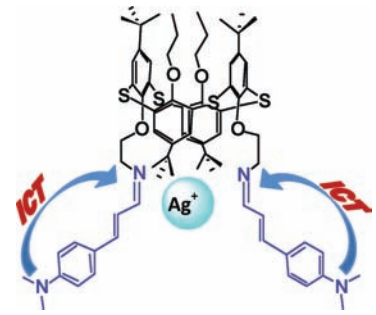
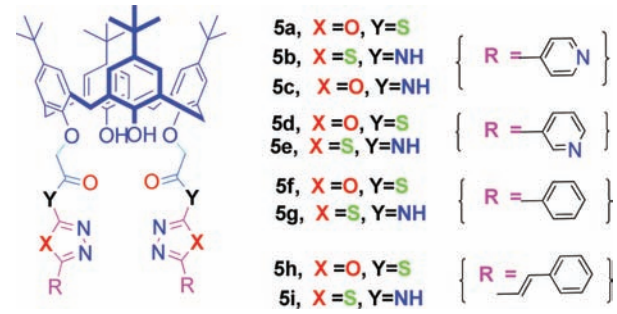
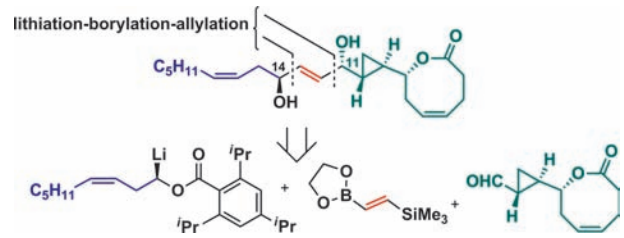




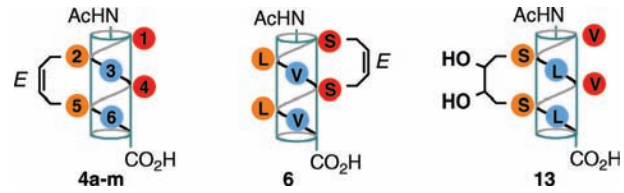


1802

Conformational stability studies of a stapled hexa-β^3-peptide library

Romila D. Gopalan, Mark P. Del Borgo, Ylva E. Bergman, Sharon Unabia, Roger J. Mulder, Matthew C. J. Wilce, Jacqueline A. Wilce, Marie-Isabel Aguilar* and Patrick Perlmutter*

An extensive library of new, 14-helical, hexa β^3-peptides demonstrates that appropriately stapled hexa-β^3-peptides can allow for a number of variations, including staple size, location and functionalization, without significant perturbation of the 14-helix.

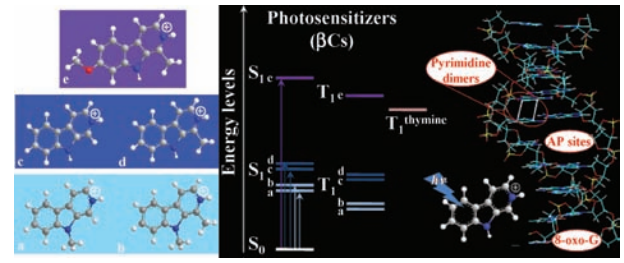


1807

Photosensitization of DNA by β-carbolines: Kinetic analysis and photoproduct characterization

M. Micaela Gonzalez, Mariana Vignoni, Magali Pellon-Maison, Matias A. Ales-Gandolfo, Maria R. Gonzalez-Baro, Rosa Erra-Balsells, Bernd Epe* and Franco M. Cabrerizo*

The type and extent of DNA modifications photosensitized by β-carboline alkaloids strongly depend on both the pH and the chemical structure of the photosensitizer.

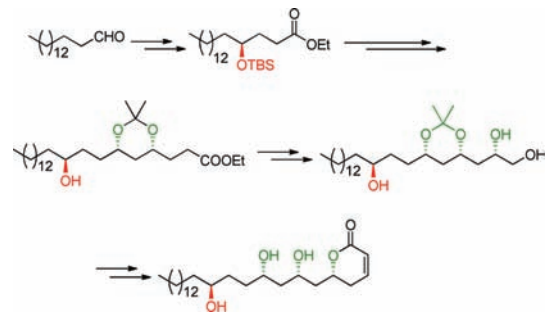


1820

Organocatalytic stereoselective synthesis of passifloricin A

Pradeep Kumar,* Menaka Pandey, Priti Gupta and Dilip D. Dhavale

An efficient enantioselective synthesis of passifloricin A has been achieved in high diastereomeric excess by a combination of iterative proline-catalyzed sequential α-aminoxylation, Horner–Wadsworth–Emmons olefination and ring-closing metathesis.

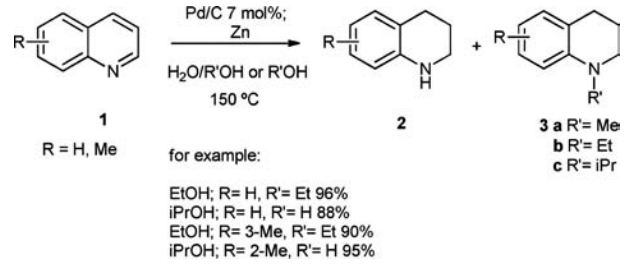


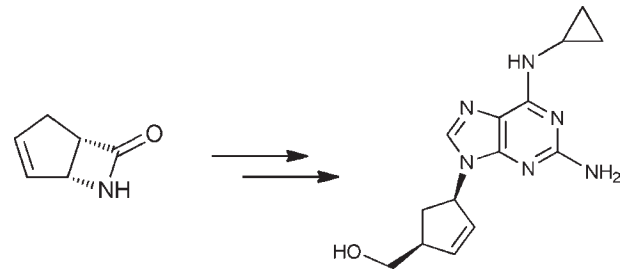
1826

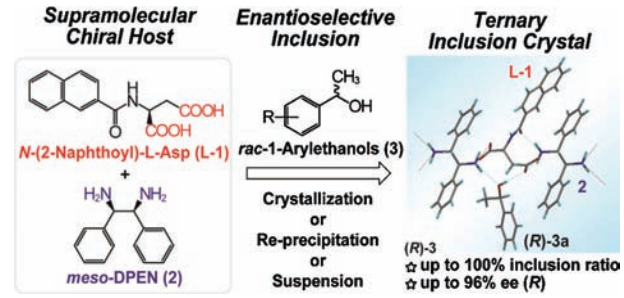
An efficient one pot transfer hydrogenation and N-alkylation of quinolines with alcohols mediated by Pd/C/Zn

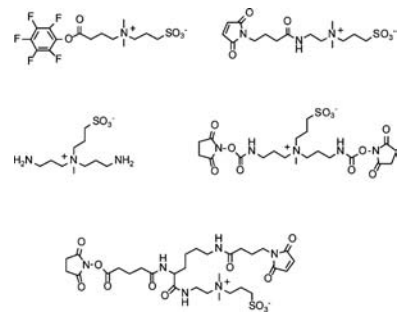
Belén Abarca,* Rosa Adam and Rafael Ballesteros*

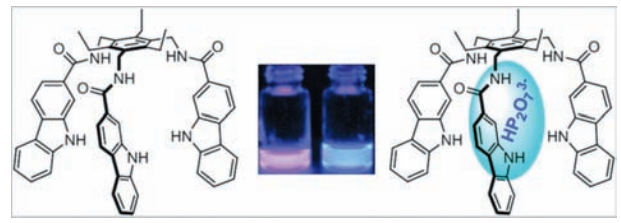
1,2,3,4-Tetrahydroquinolines and N-alkylated tetrahydroquinolines from quinolines have been obtained with excellent yields in one step.





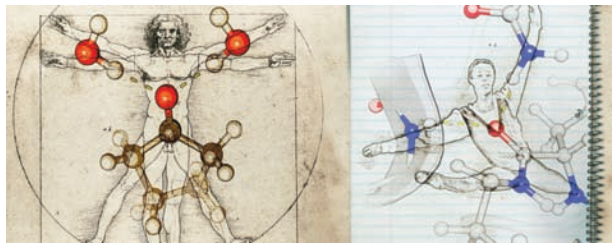






PAPERS

1905

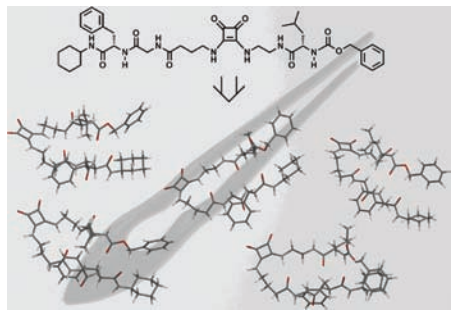


Hydrogen-bond stabilization in oxyanion holes: *grand jeté* to three dimensions

Luis Simón* and Jonathan M. Goodman*

Molecular dynamics and ONIOM calculations reaffirm the conclusion from crystallographic studies that oxyanion holes are not usually stabilized by planar arrangements of H-bonds, but by 3D arrangements. This sub-optimal transition state stabilization leads to better overall catalysis.

1914

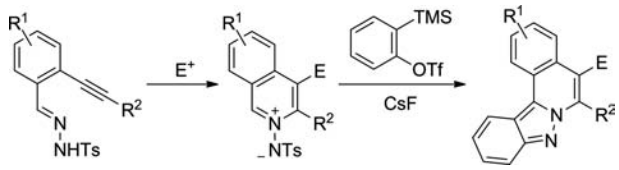


Synthesis and conformational studies of peptido-squaramide foldable modules: a new class of turn-mimetic compounds

Luis Martínez, Angel Sampedro, Elena Sanna, Antoni Costa* and Carmen Rotger*

The combination of a disecondary squaramide with 4-aminobutyric acid affords a new turn module that can be functionalized with dipeptide chains to induce the formation of a hairpin-like structure.

1922



Aryne [3 + 2] cycloaddition with *N*-sulfonylpyridinium imides and *in situ* generated *N*-sulfonylisoquinolinium imides: a potential route to pyrido[1,2-*b*]indazoles and indazolo[3,2-*a*]isoquinolines

Jingjing Zhao, Pan Li, Chunrui Wu,* Hongli Chen, Wenying Ai, Renhong Sun, Hailong Ren, Richard C. Larock and Feng Shi*

N-Tosylpyridinium imides and *in situ* generated *N*-tosylisoquinolinium imides react with arynes in a [3 + 2] cycloaddition fashion and readily afford pyrido[1,2-*b*]indazoles and indazolo[3,2-*a*]-isoquinolines after elimination of a sulfinate anion.