Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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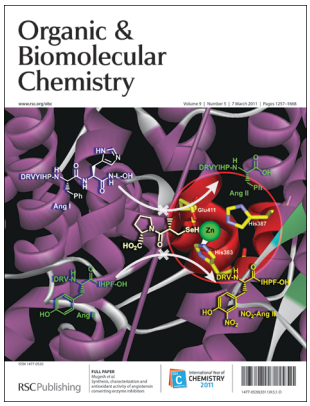
IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 9(5) 1257–1668 (2011)



Cover

See Mugesh *et al.*, pp. 1356–1365.

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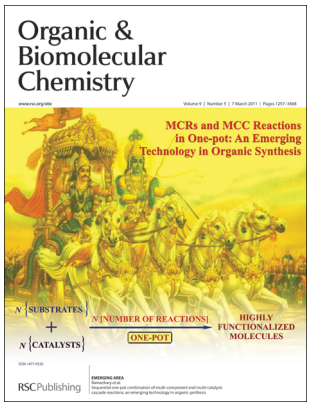

Inside cover

See Ramachary *et al.*, pp. 1277–1300. Warriors Arjuna and Srikrishna achieved many victories, protecting people from demons and keeping them in good spirits. Similarly, sequential one-pot combination of MCRs and MCC reactions will be victorious over many problems in synthetic organic chemistry.

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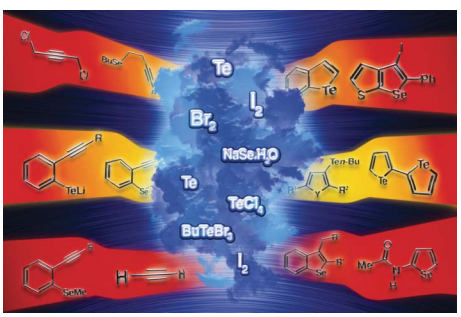
EMERGING AREA

PERSPECTIVE



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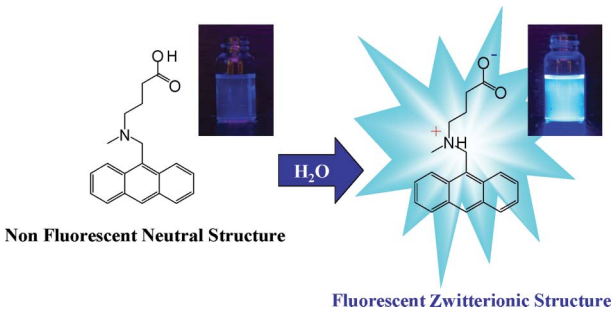
1314

Detection of water in organic solvents by photo-induced electron transfer method

Yousuke Ooyama, Minako Sumomogi, Tomoya Nagano, Kohei Kushimoto, Kenji Komaguchi, Ichiro Imae and Yutaka Harima*

A new class of fluorescence sensor for detection of water in organic solvents based on photo-induced electron transfer (PET) of a fluorophore skeleton coupled with an amino acid has been designed and developed.

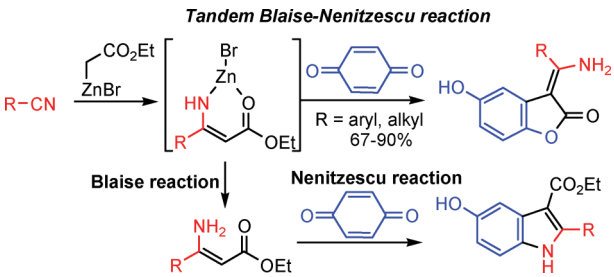


1317

Tandem Blaise–Nenitzescu reaction: one-pot synthesis of 5-hydroxy-α-(aminomethylene)benzofuran-2(*3H*)-ones from nitriles

Yu Sung Chun, Ka Yeon Ryu, Ju Hyun Kim, Hyunik Shin* and Sang-gi Lee*

The tandem one-pot reaction of the Blaise reaction intermediate, zinc bromide complex of β-enaminoesters, with benzoquinone affords 5-hydroxy-α-(aminomethylene)benzofuran-2(3*H*)-ones in good to excellent yields.

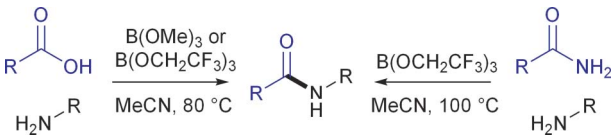


1320

Borate esters as convenient reagents for direct amidation of carboxylic acids and transamidation of primary amides

Pavel Starkov and Tom D. Sheppard*

Simple borate esters are effective reagents for the direct synthesis of secondary amides from either carboxylic acids or primary amides.

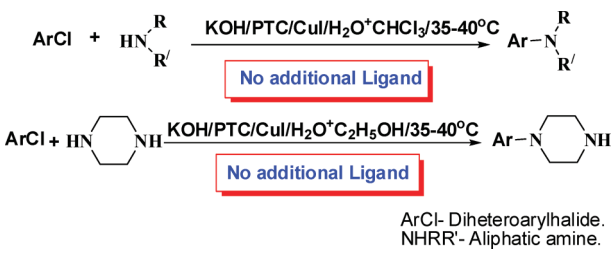


1324

Chemospecific and ligand free CuI catalysed heterogeneous N-arylation of amines with diheteroaryl halides at room temperature

Sanjeev K. Verma, B. N. Acharya and M. P. Kaushik*

A chemoselective/chemospecific, ligand free, copper-catalyzed N-arylation reaction of aliphatic amines with diheteroaryl halides in heterogeneous medium at room temperature has been developed. The protocol is very effective for low boiling amines and amines available in aqueous solution.



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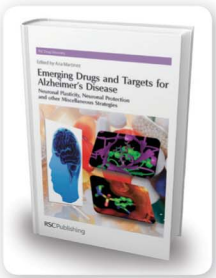

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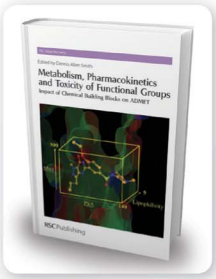

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Edited by Dennis A Smith | Pfizer Global R & D, UK
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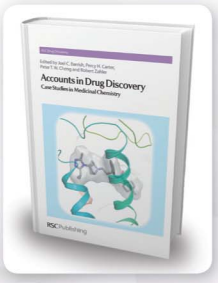

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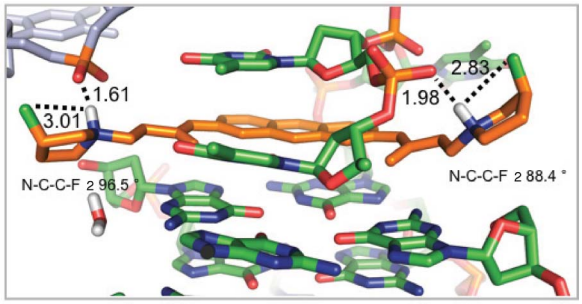
1328

Fluorine in medicinal chemistry: *β*-fluorination of peripheral pyrrolidines attached to acridine ligands affects their interactions with G-quadruplex DNA

Nancy H. Campbell, Daniel L. Smith, Anthony P. Reszka, Stephen Neidle* and David O'Hagan*

X-ray structure studies reveal that C–F bond incorporation into the peripheral pyrrolidine moieties of the G-quadruplex DNA binding ligand BSU6039 leads to a striking reversal of the pyrrolidinium ring N^+-H orientation

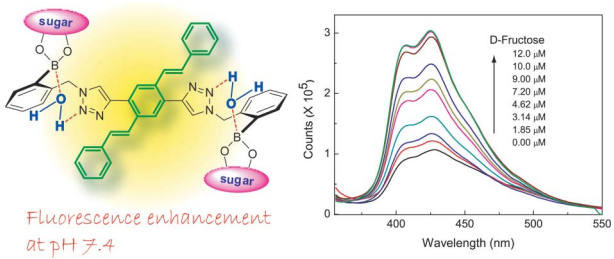


1332

Highly sensitive detection of saccharides under physiological conditions with click synthesized boronic acid-oligomer fluorophores

Karimulla Mulla, Prateek Dongare, Ningzhang Zhou, Guang Chen, David W. Thompson and Yuming Zhao*

A phenylboronic acid-attached cruciform oligomer acts as a highly sensitive fluorescence sensor for saccharides under physiological conditions.

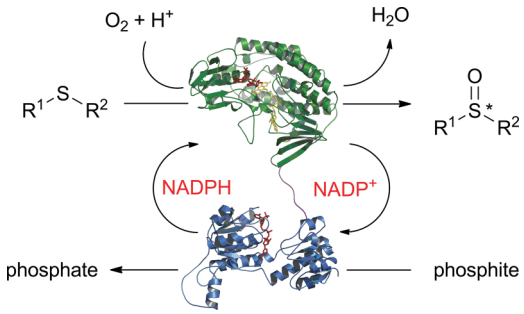


1337

Exploring the biocatalytic scope of a bacterial flavin-containing monooxygenase

Ana Rioz-Martínez, Malgorzata Kopacz, Gonzalo de Gonzalo,* Daniel E. Torres Pazmiño, Vicente Gotor and Marco W. Fraaije*

This study describes a biocatalytic exploration of a bacterial flavin-containing monooxygenase (FMO), fused to phosphite dehydrogenase. The FMO catalyzes enantioselective sulfoxidations and converts indole derivatives into the corresponding indigoid pigments.

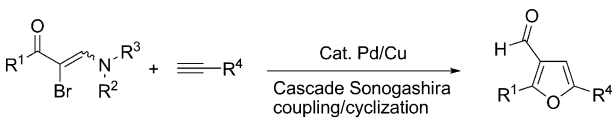


1342

Pd/Cu-catalyzed cascade Sonogashira coupling/cyclization reactions to highly substituted 3-formyl furans

Jingyu Yang, Chengyu Wang, Xin Xie, Hongfeng Li, Ende Li and Yanzhong Li*

Pd/Cu catalyzed cascade reactions of α-bromoenaminone with terminal alkyne to 3-formyl trisubstituted furans.

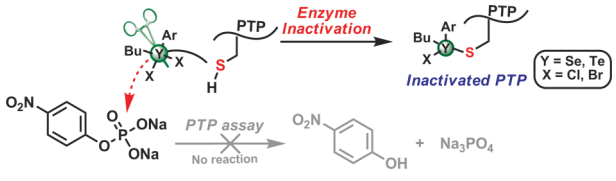


R^1= alkyl, aryl, heteroaryl
R^2, R^3 =alkyl, aryl
R^4 = alkyl, aryl, vinyl

35%-83%

COMMUNICATIONS

1347

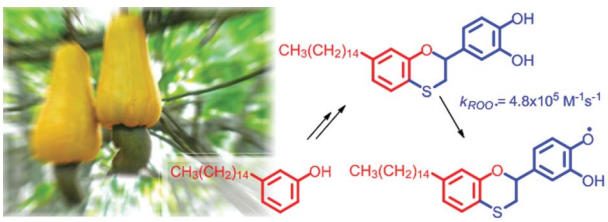


Hypervalent organochalcogenanes as inhibitors of protein tyrosine phosphatases

Leandro Piovan, Li Wu, Zhong-Yin Zhang* and Leandro H. Andrade*

Organochalcogenanes inactivate the PTPs in a time- and concentration-dependent fashion, most likely through covalent modification of the active site sulfur-moiety by the chalcogen atom.

1352



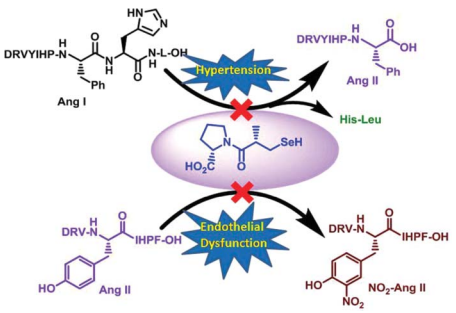
Amphiphilic antioxidants from "cashew nut shell liquid" (CNSL) waste

Riccardo Amorati,* Orazio A. Attanasi, Gianfranco Favi, Stefano Menichetti,* Gian Franco Pedulli and Caterina Viglianisi

Cardanol and cardols from cashew-nut oil are easily transformed into 4-thiaflavane antioxidants bearing a long alkyl chain and a catechol group.

PAPERS

1356

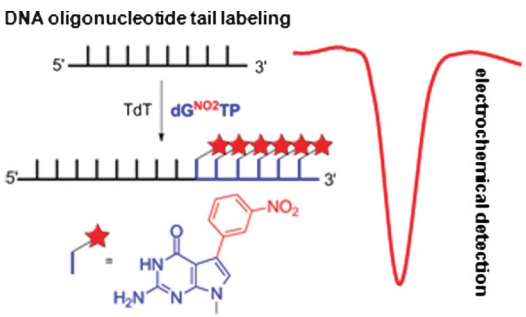


Synthesis, characterization and antioxidant activity of angiotensin converting enzyme inhibitors

Bhaskar J. Bhuyan and Govindasamy Mugesh*

It is shown for the first time that the selenium analogues of captopril not only inhibit angiotensin converting enzyme but also protect against peroxynitrite-mediated nitration of peptides and proteins. Synthesis of Sec-Pro and Cys-Pro dipeptides and their ACE inhibition and PN-scavenging activities are discussed. This study reveals that the ACE inhibitors with significant antioxidant activity may be beneficial in the treatment of hypertension.

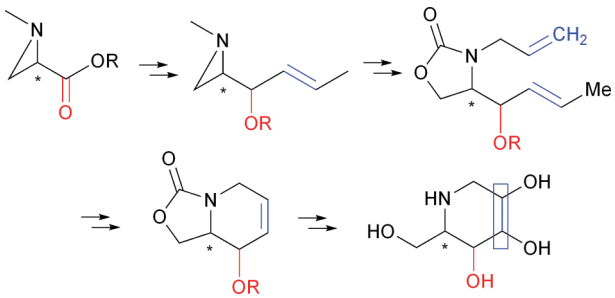
1366

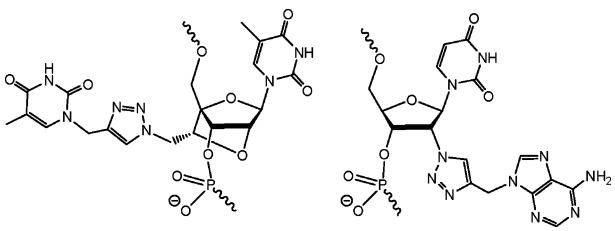


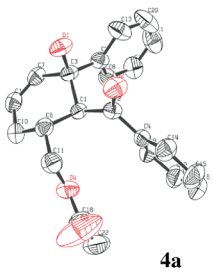
Tail-labelling of DNA probes using modified deoxynucleotide triphosphates and terminal deoxynucleotidyl tranferase. Application in electrochemical DNA hybridization and protein-DNA binding assays

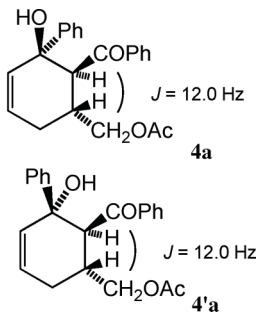
Petra Horáková, Hana Macíčková-Cahová, Hana Pivoňková, Jan Špaček, Luděk Havran, Michal Hocek* and Miroslav Fojta*

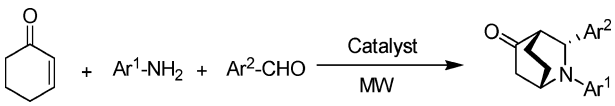
A simple approach to DNA labelling using terminal deoxynucleotidyl transferase and modified deoxynucleoside triphosphates.











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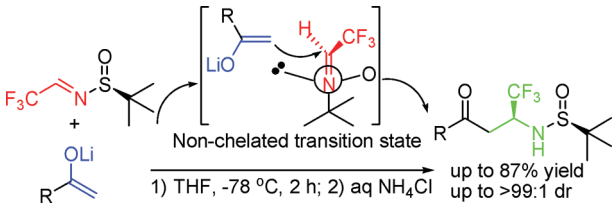
1402

A facile process for the asymmetric synthesis of β-trifluoromethylated β-amino ketones *via* addition of ketone enolates to sulfinylimine

Haibo Mei, Yiwen Xiong, Jianlin Han* and Yi Pan*

A facile method was developed for asymmetric synthesis of β-trifluoromethylated β-amino ketones with good yields and excellent diastereoselectivities, even on the large scale preparation.

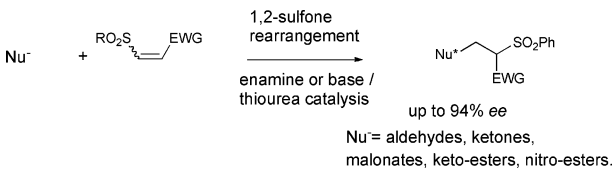


1407

1,2-Sulfone rearrangement in organocatalytic reactions

Adrien Quintard and Alexandre Alexakis*

1,2-Sulfone rearrangement resulting from nucleophilic addition to bis activated vinyl-sulfones has been extensively studied. Different nucleophiles activated by different types of catalysts (enamine, Brönsted base, thiourea) are able to promote such rearrangement in excellent yields and moderate to excellent enantioselectivities (up to 94% *ee*). Mechanistic studies have led to a better understanding of the mechanism and allowed its application to other electrophiles such as vinyl-sulfone acrylates.

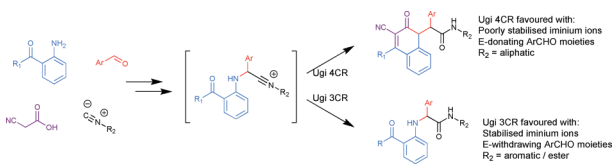


1419

Investigation of the one-pot synthesis of quinolin-2-(1*H*)-ones and the discovery of a variation of the three-component Ugi reaction

Christopher P. Gordon, Kelly A. Young, Lacey Hizartzidis, Fiona M. Deane and Adam McCluskey*

Cyanoacetic acid diverts the sequential Ugi–Knoevenagel, 4 component reaction to quinolin-2-(1*H*)-ones to an Ugi 3 component reaction and the synthesis of alpha-amino amides.

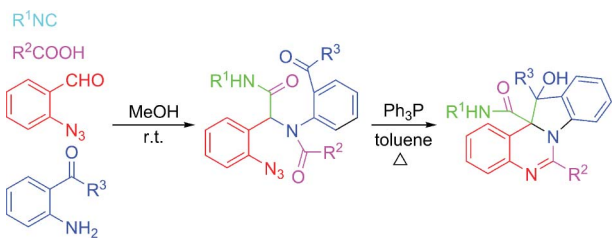


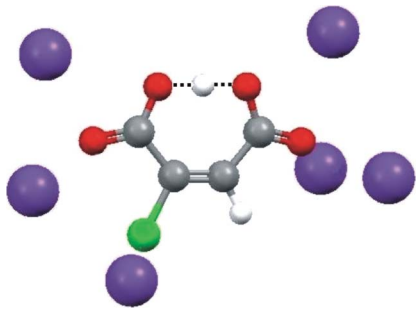
1429

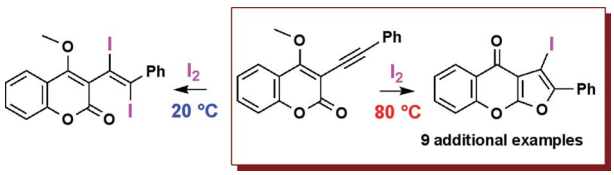
Unexpected synthesis of indolo[1,2-*c*]quinazolines by a sequential Ugi 4CC–Staudinger–aza-Wittig–nucleophilic addition reaction

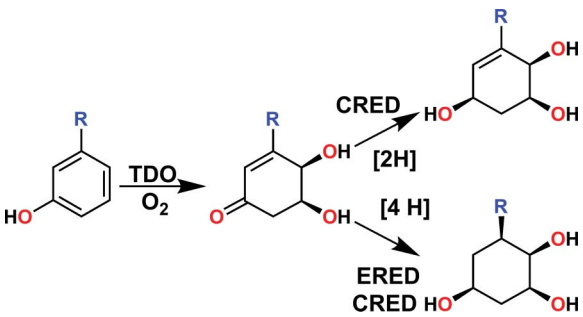
Ping He, Yi-Bo Nie, Jing Wu and Ming-Wu Ding*

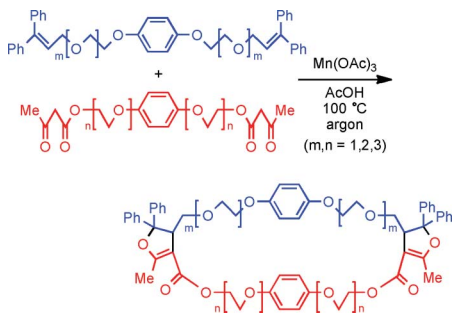
A new sequential Ugi–Staudinger–aza-Wittig–nucleophilic addition reaction was developed to construct indolo[1,2-*c*]quinazoline derivatives.

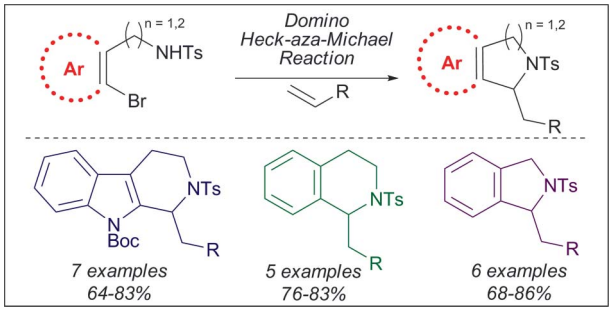


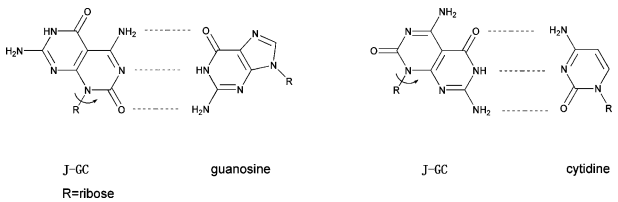


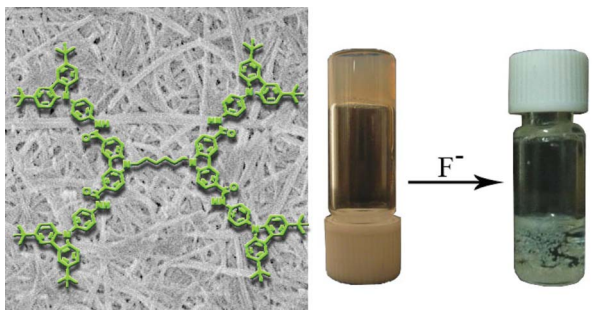


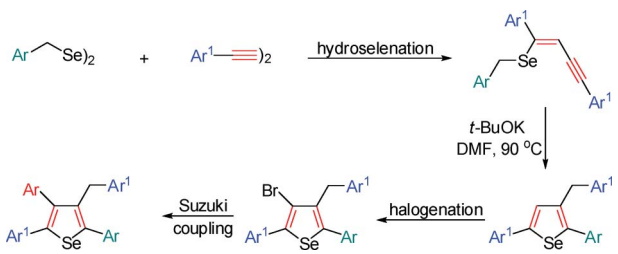










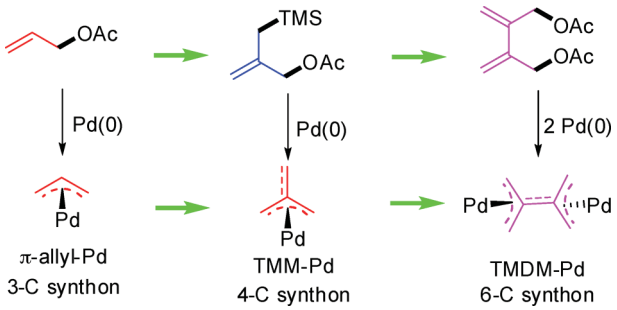


1572

New strategy to construct fused/bridged/spiro carbocyclic scaffolds based on the design of novel 6-C synthon precursor

Jia Liu, Xi Wang, Chang-Liang Sun, Bi-Jie Li, Zhang-Jie shi and Min Wang*

In this article we designed a new strategy to build fused/spiro/bridged carbocyclic systems with a novel 6-C synthon from readily available diallyl diacetates through the sequential Pd-catalyzed double allyl alkylation and Diels Alder annulation. Further exploration on the application of this strategy can construct useful complex scaffolds.

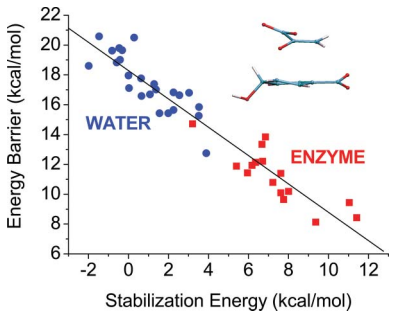


1578

Analysis of chorismate mutase catalysis by QM/MM modelling of enzyme-catalysed and uncatalysed reactions

Frederik Claeyssens, Kara E. Ranaghan, Narin Lawan, Stephen J. Macrae, Frederick R. Manby, Jeremy N. Harvey and Adrian J. Mulholland*

Comparison of multiple enzymic and solution pathways shows that transition state stabilization is important for catalysis in chorismate mutase.

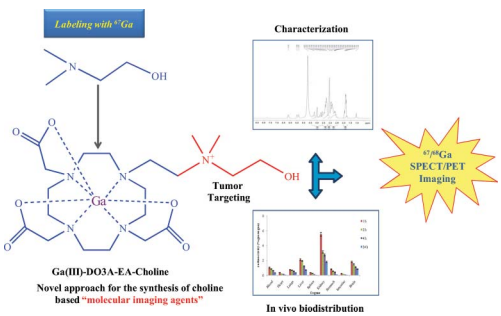


1591

Design, synthesis and biological evaluation of choline based SPECT imaging agent: Ga(III)-DO3A-EA-Choline

Jasleen K. Uppal, Puja P. Hazari, Raunak, Krishna Chuttani, Michele Allard, Narender K. Kaushik and Anil K. Mishra*

An expedient strategy for the synthesis of choline functionalized macrocyclic chelating agent (DO3A-EA-Choline) and its radiocomplexation with ^{67}Ga has been reported. The compound is a promising candidate for oncologic imaging and SPECT/PET applications.

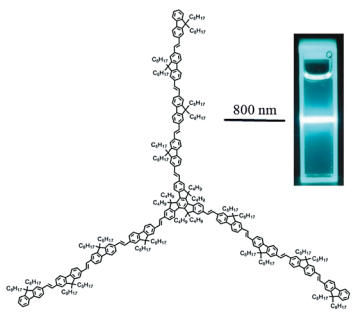


1600

Synthesis of star-shaped monodisperse oligo(9,9-di-n-octylfluorene-2,7-vinylene)s functionalized truxenes with two-photon absorption properties

Huipeng Zhou, Xin Zhao, Tianhao Huang, Ran Lu,* Hanzhuang Zhang, Xiaohui Qi, Pengchong Xue, Xingliang Liu and Xiaofei Zhang

New star-shaped oligo(9,9-di-n-octylfluorene-2,7-vinylene)s functionalized truxenes without strong donor and acceptor units yield high TPA cross sections.



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