

Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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IN THIS ISSUE

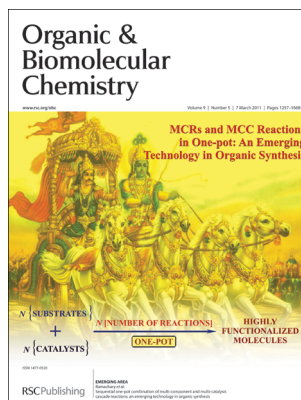
ISSN 1477-0520 CODEN OBCRAK 9(5) 1257–1668 (2011)



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

1277

Sequential one-pot combination of multi-component and multi-catalysis cascade reactions: an emerging technology in organic synthesis

Dhevalapally B. Ramachary* and Sangeeta Jain

Through the Emerging Area of one-pot sequential MCRs/MCC reactions, the chemical products (fine chemicals, agrochemicals and pharmaceuticals) that add value to our lives can be produced with less waste and greater economic benefits.



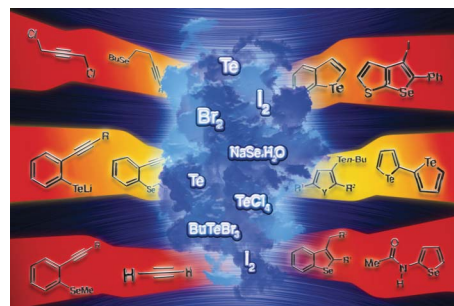
PERSPECTIVE

1301

New development of synthesis and reactivity of seleno- and tellurophenes

Cristiano R. B. Rhoden and Gilson Zeni*

Due to the many new and remarkable findings and applications published in recent years in seleno- and tellurophene chemistry, this review revisits different aspects of the chemistry, including synthesis, reactivity and applications in the field of heterocycles.



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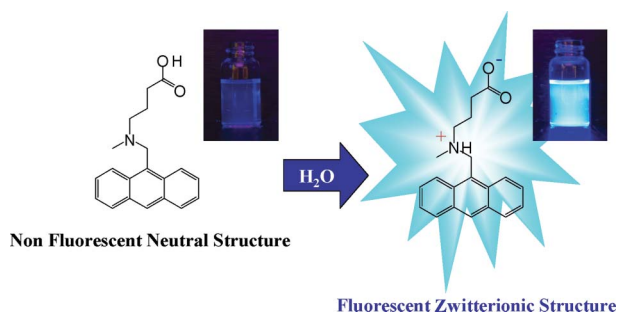
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1314

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.

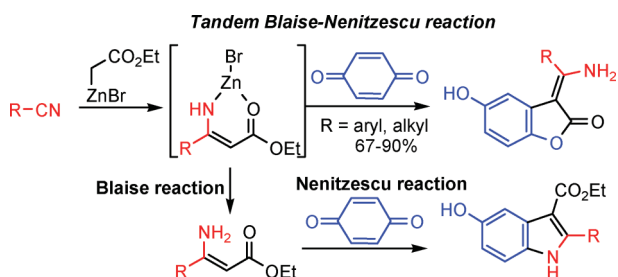


1317

Tandem Blaise–Nenitzescu reaction: one-pot synthesis of 5-hydroxy- α -(aminomethylene)benzofuran-2(3*H*)-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 -aminoesters, with benzoquinone affords 5-hydroxy- α -(aminomethylene)benzofuran-2(3*H*)-ones in good to excellent yields.

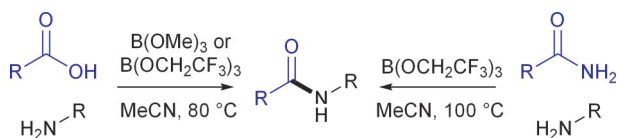


1320

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.

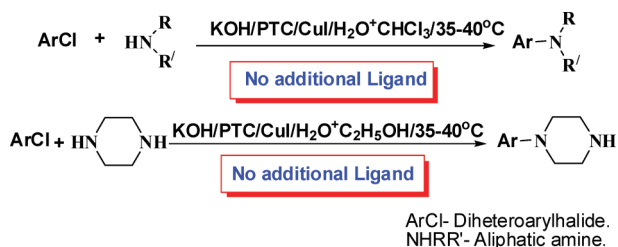


1324

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

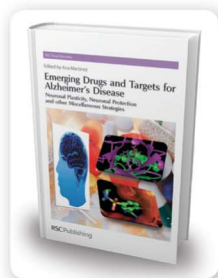
Sanjeev K. Verma, B. N. Acharya and M. P. Kaushik*

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.



ArCl- Diheteroarylhalide.
NHRR'- Aliphatic amine.

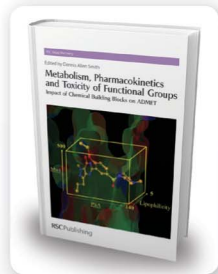
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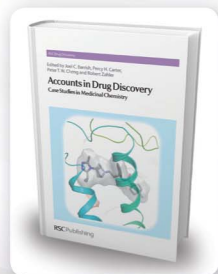
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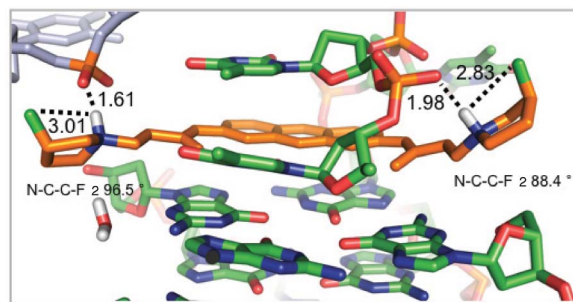
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1328

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

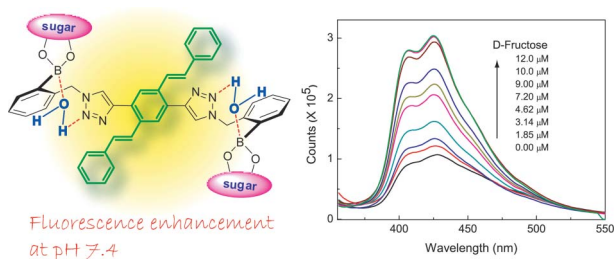


1332

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.

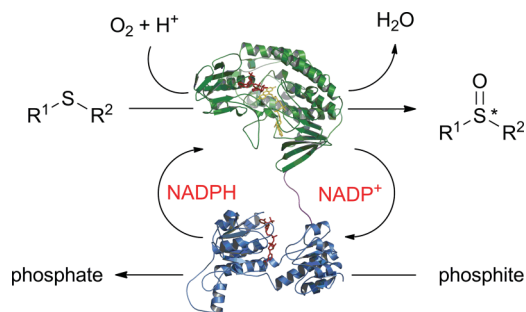


1337

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.

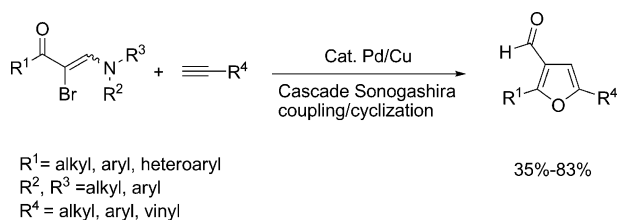


1342

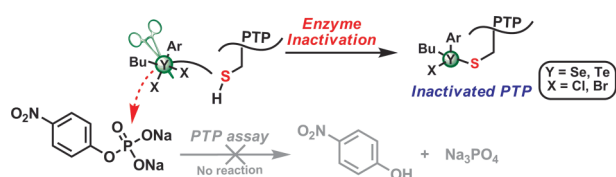
Pd/Cu-catalyzed cascade Sonogashira coupling/cyclization reactions to highly substituted 3-formyl furans

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

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



1347

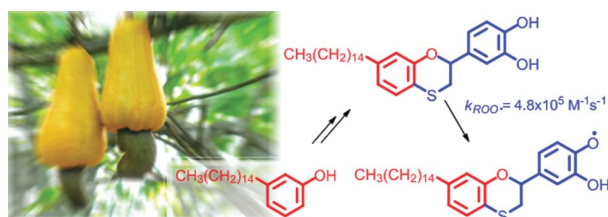


Hypervalent organochalcogenanes as inhibitors of protein tyrosine phosphatases

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



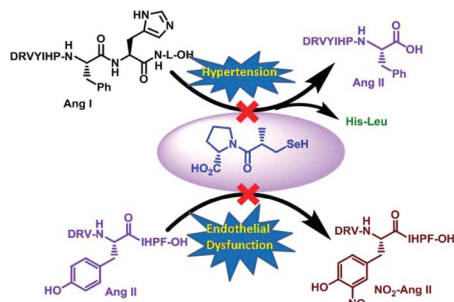
Amphiphilic antioxidants from “cashew nut shell liquid” (CNSL) waste

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

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

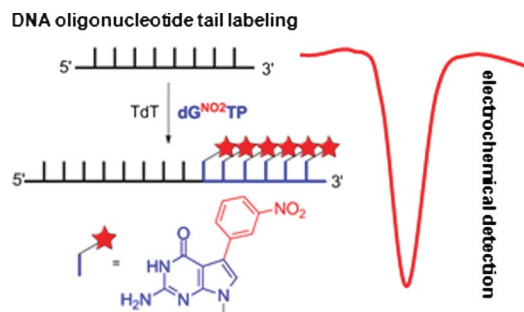


Synthesis, characterization and antioxidant activity of angiotensin converting enzyme inhibitors

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 transferase. 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*

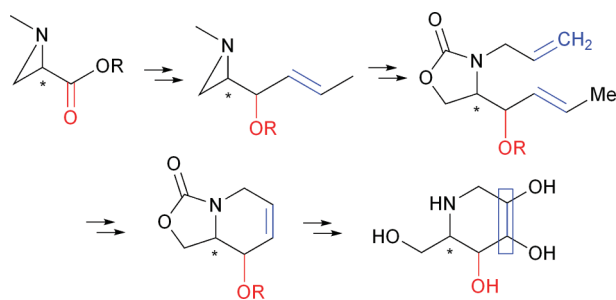
A simple approach to DNA labelling using terminal deoxynucleotidyl transferase and modified deoxynucleoside triphosphates.

1372

Asymmetric synthesis of 1-deoxyzasugars from chiral aziridines

Alok Singh, Bongchan Kim, Won Koo Lee* and Hyun-Joon Ha*

A general and facile synthesis of enantiopure 1-deoxyzasugars was achieved from stereoselective dihydroxylation of a common synthetic intermediate, piperidine ring fused oxazolidin-2-one, originating from a commercially available starting substrate, chiral aziridine-2-carboxylate, in high yields.

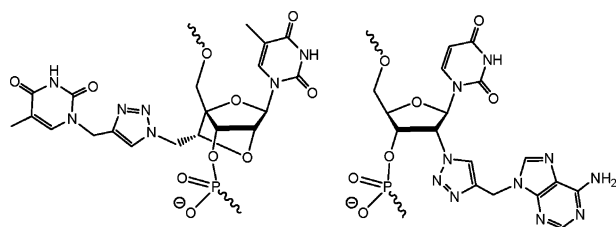


1381

The synthesis of double-headed nucleosides by the CuAAC reaction and their effect in secondary nucleic acid structures

Anna S. Jørgensen, Khalil I. Shaikh, Gerald Enderlin, Elise Ivarsen, Surender Kumar and Poul Nielsen*

Four double-headed nucleosides were synthesised by CuAAC reactions and investigated in secondary nucleic acid structures.

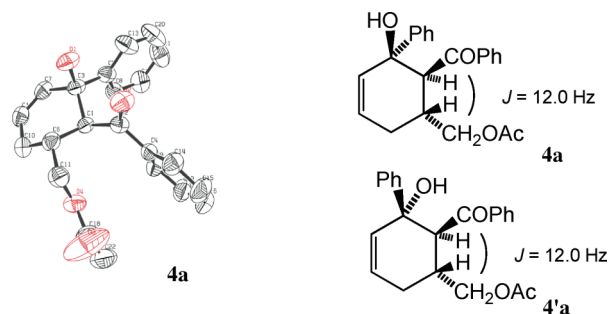


1389

A tandem reaction of organozinc reagent prepared from palladium-catalyzed umpolung method: diastereoselective formation of cyclohexene derivatives bearing three adjacent stereocenters

Mutsumi Sada, Kenichi Nomura and Seiji Matsubara*

In the presence of a palladium catalyst, treatment of γ -acyloxy- α,β -unsaturated ketone with bis(iodozinc)methane caused umpolung of π -allylpalladium to give a zinc dienolate.

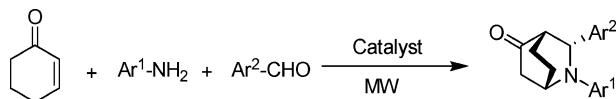


1394

Heteropoly acid-catalyzed microwave-assisted three-component aza-Diels–Alder cyclizations: diastereoselective synthesis of potential drug candidates for Alzheimer's disease

Dmitry Borkin, Elena Morzhina, Silpi Datta, Aleksandra Rudnitskaya, Abha Sood, Marianna Török and Béla Török*

A highly diastereoselective microwave-assisted three component synthesis of azabicyclo[2.2.2]octan-5-ones by a silicotungstic acid-catalyzed aza-Diels–Alder cyclization is described.



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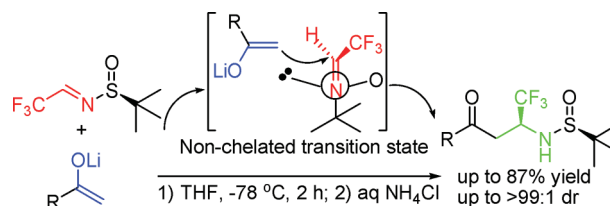
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1402

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.

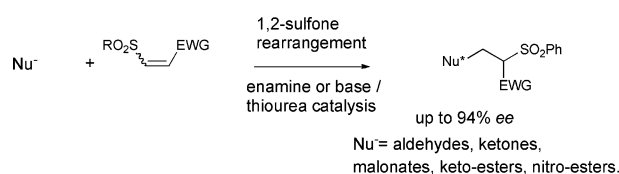


1407

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, Brønsted 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.

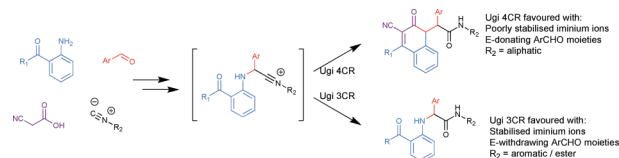


1419

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.

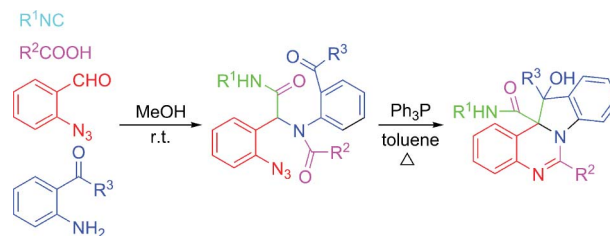


1429

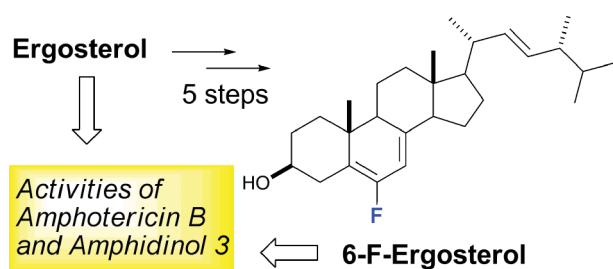
Unexpected synthesis of indolo[1,2-*c*]quinazolines by a sequential Ugi 4CC–Staudinger–aza-Wittig–nucleophilic addition reaction

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.



1437



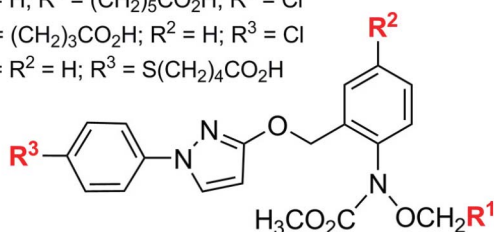
Synthesis of 6-F-ergosterol and its influence on membrane-permeabilization of amphotericin B and amphidinol 3

Yusuke Kasai, Nobuaki Matsumori,* Hiroyuki Ueno, Kenichi Nonomura, Shinya Yano, Murata Michio* and Tohru Oishi

6-F-Ergosterol was synthesized from ergosterol in 5 steps, and its activity of promoting pore formation of amphotericin B and amphidinol 3 was examined.

1443

PY: $R^1 = R^2 = H; R^3 = Cl$
PYa6: $R^1 = H; R^2 = (CH_2)_5CO_2H; R^3 = Cl$
PYo5: $R^1 = (CH_2)_3CO_2H; R^2 = H; R^3 = Cl$
PYs5: $R^1 = R^2 = H; R^3 = S(CH_2)_4CO_2H$

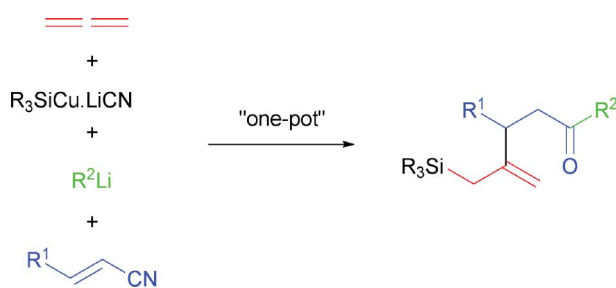


Synthesis of site-heterologous haptens for high-affinity anti-pyralostrobin antibody generation

Josep V. Mercader, Consuelo Agulló, Antonio Abad-Somovilla* and Antonio Abad-Fuentes*

Site-heterology of pyraclostrobin bioconjugates has been investigated using synthetic derivatives (haptens) with equivalent spacer arms that introduce minimal electronic modifications

1454

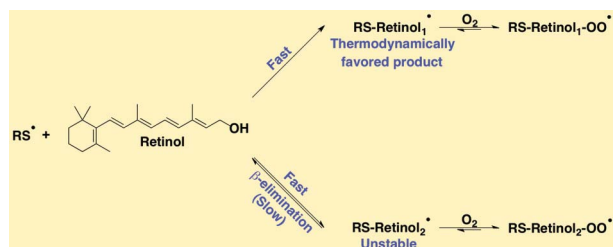


One-pot multicoupling reaction of silylcopper reagents, organolithium compounds and α,β -unsaturated nitriles

Francisco J. Pulido,* Asunción Barbero* and Yolanda Blanco

A new multicomponent reaction is described in which the assembly of four components is allowed in a simple and efficient protocol.

1459



Kinetic studies of retinol addition radicals

Ali El-Agamey,* Shunichi Fukuzumi,* K. Razi Naqvi and David J. McGarvey

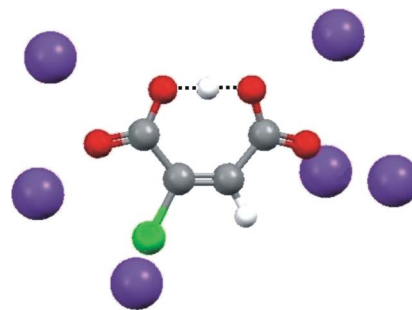
The dynamics of β -elimination for retinol thiyl addition radicals and their reactions with oxygen were examined for the first time.

1466

The influence of potassium cation on a strong OHO hydrogen bond

Irena Majerz*

The strong OHO hydrogen bond can be modified by the potassium cation.

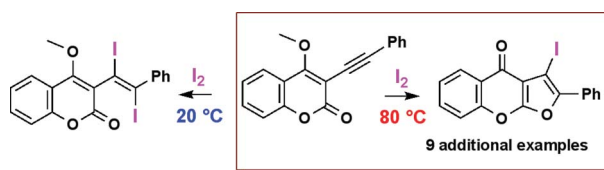


1474

Iodocyclization versus diiodination in the reaction of 3-alkynyl-4-methoxycoumarins with iodine: Synthesis of 3-iodofuro[2,3-*b*]chromones

Guillaume Raffa, Sébastien Belot, Geneviève Balme and Nuno Monteiro*

The reaction of 3-alkynyl-4-methoxycoumarins with molecular iodine in hot 1,2-dichloroethane offers a practical, high-yielding access to 3-iodofurochromones, whereas diiodoethenylcoumarins are predominantly produced at room temperature.

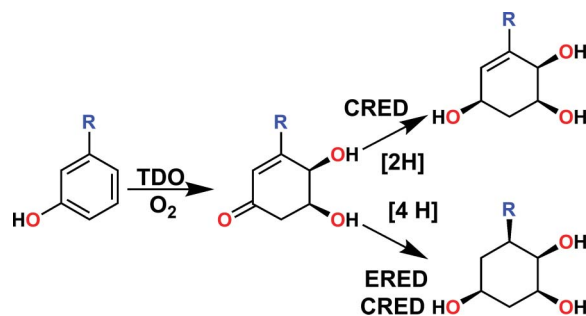


1479

Dioxygenase-catalysed *cis*-dihydroxylation of *meta*-substituted phenols to yield cyclohexenone *cis*-diol and derived enantiopure *cis*-triol metabolites

Derek R. Boyd,* Narain D. Sharma, Paul J. Stevenson, Marine Blain, Colin McRoberts, John T. G. Hamilton, José M. Argudo, Harpinder Mundi, Leonid A. Kulakov and Christopher C. R. Allen

Dioxygenase-catalysed dihydroxylation of phenols in bacterial cells yielded cyclohexenone *cis*-diols as primary metabolites with some of the corresponding cyclohexene *cis*-triols and cyclohexane *cis*-triols as secondary metabolites

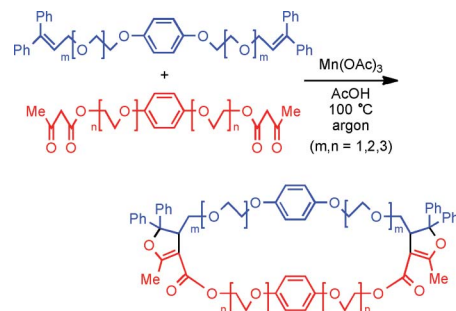


1491

One-pot synthesis of cyclophane-type macrocycles using manganese(III)-mediated oxidative radical cyclization

Yosuke Ito, Yuichi Tomiyasu, Takahiro Kawanabe, Keisuke Uemura, Yuu Ushimizu and Hiroshi Nishino*

A convenient synthesis of interesting cyclophanes from 21 to 56 members was achieved using the Mn(III)-mediated oxidative radical cyclization.

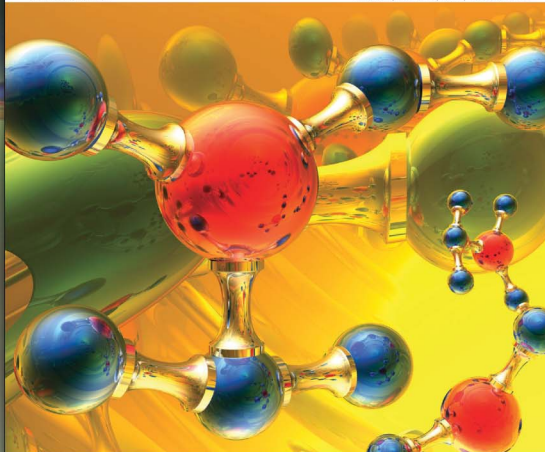


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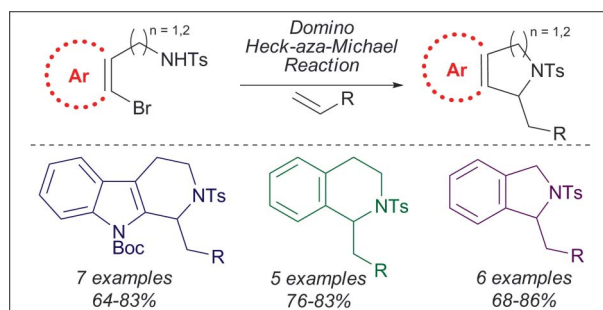
Registered Charity Number 207890

1508

A general approach to *N*-heterocyclic scaffolds using domino Heck–aza-Michael reactions

Daniel L. Priebbenow, Scott G. Stewart and Frederick M. Pfeffer*

Domino Heck–aza-Michael reactions have been developed for the synthesis of C1-substituted tetrahydro- β -carbolines, tetrahydroisoquinolines and isoindolines.

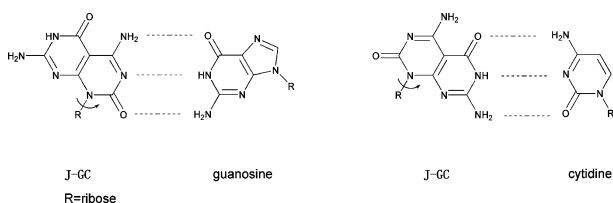


1516

Synthesis of Janus type nucleoside analogues and their preliminary bioactivity

Hao-Zhe Yang, Mei-Ying Pan, Da-Wei Jiang and Yang He*

Novel Janus type nucleosides J-GC and J-HC which have dual Watson–Crick hydrogen bond faces have been synthesized and J-GC exhibits a preliminary bioactivity.

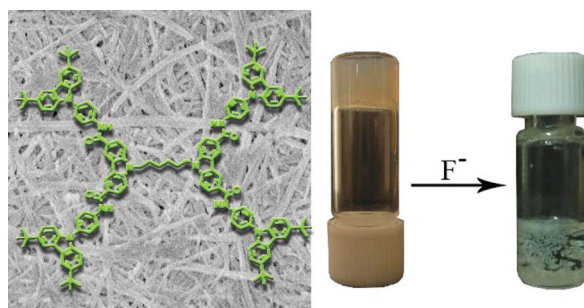


1523

New dendritic gelator bearing carbazole in each branching unit: selected response to fluoride ion in gel phase

Defang Xu, Xingliang Liu, Ran Lu,* Pengchong Xue, Xiaofei Zhang, Huipeng Zhou and Junhui Jia

Dendritic oligocarbazole-based organogel with aggregation-induced emission has been prepared for detecting F^- .

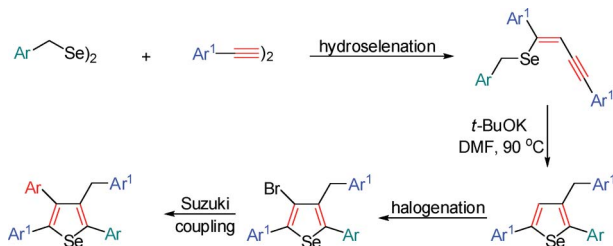


1529

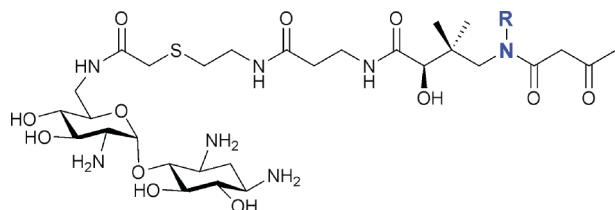
Selective base-promoted synthesis of substituted selenophenes by carbocyclization of (*Z*)-benzylselenoenynes

Daniela A. Barancelli, Carmine I. Acker, Paulo H. Menezes and Gilson Zeni*

The synthesis of 3-benzyl-2,5-diarylselenophenes *via* carbocyclization reactions is described.



1538

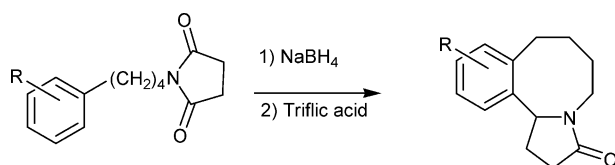


Synthesis of 4'-aminopantetheine and derivatives to probe aminoglycoside *N*-6'-acetyltransferase

Xuxu Yan, T. Olukayode Akinnusi, Aaron T. Larsen and Karine Auclair*

The first synthesis of 4'-aminopantetheine and derivatization to probe aminoglycoside resistance

1547

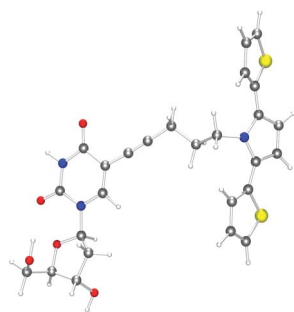


A novel synthesis of (di)-benzazocinones *via* an endocyclic *N*-acyliminium ion cyclisation

Frank D. King,* Abil E. Aliev, Stephen Caddick and D. A. Tocher

The reduction and triflic acid-mediated cyclisation of *N*-(4-arylbutyl)imides provides a novel synthesis of various (di)-benzazocin-5-ones.

1555

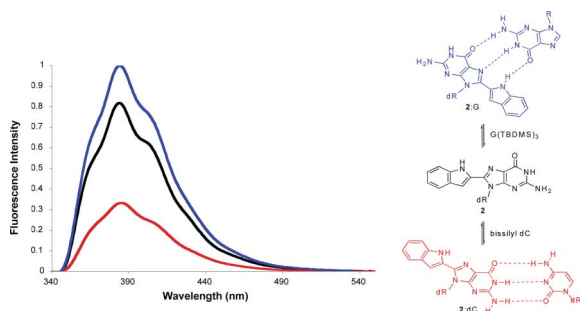


Pyrrolyl-, 2-(2-thienyl)pyrrolyl- and 2,5-bis(2-thienyl)pyrrolyl-nucleosides: synthesis, molecular and electronic structure, and redox behaviour of C5-thymidine derivatives

Miguel A. Galindo, Jennifer Hannant, Ross W. Harrington, William Clegg, Benjamin R. Horrocks, Andrew R. Pike and Andrew Houlton*

A series of C5-modified thymidine nucleosides has been prepared with alkyne-alkyl linked pyrrolyl-based units capable of forming conducting polymers upon oxidation.

1565



An indole-linked C⁸-deoxyguanosine nucleoside acts as a fluorescent reporter of Watson–Crick *versus* Hoogsteen base pairing

Katherine M. Schlitt, Andrea L. Millen, Stacey D. Wetmore* and Richard A. Manderville*

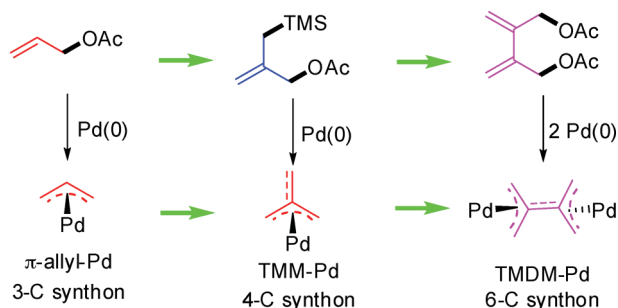
A fluorescent indole-linked C⁸-deoxyguanosine acts as a reporter of H-bonding specificity by exhibiting enhanced emission upon Hoogsteen H-bonding and quenched emission upon Watson–Crick H-bonding.

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.

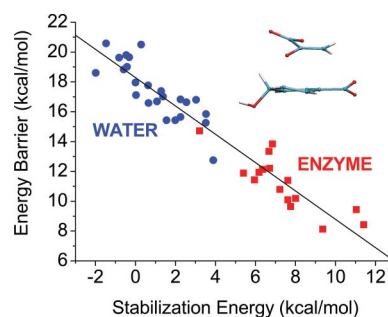


1578

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

Frederik Claeysens, 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.

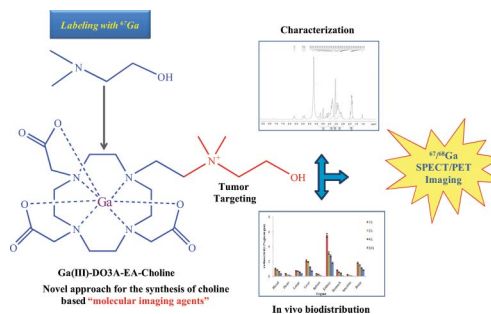


1591

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.

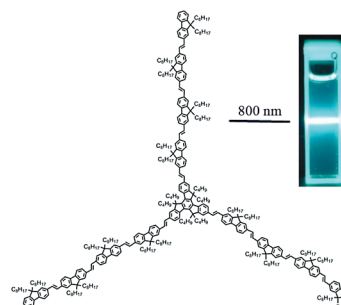


1600

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.



A decorative graphic at the top of the page featuring a network of glowing blue lines and nodes on a dark blue background, resembling a molecular or digital network structure.

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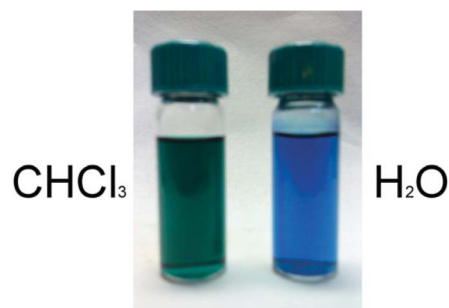
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1608

Synthesis and NLO properties of new *trans* 2-(thiophen-2-yl)vinyl heteroaromatic iodides

Cosimo Gianluca Fortuna,* Carmela Bonaccorso, Fadi Qamar, Anu Anu, Isabelle Ledoux and Giuseppe Musumarra

The synthesis and characterisation of new *trans* 2-(thiophen-2-yl)vinyl pyridinium, imidazolium and quinoilinium iodides is reported together with their solvatochromic shifts and EFISH characterization.

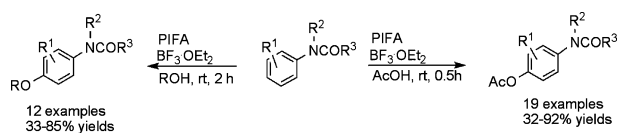


1614

Direct acetoxylation and etherification of anilides using phenyliodine bis(trifluoroacetate)

Huan Liu, Xuemin Wang and Yonghong Gu*

The direct acetoxylation and etherification of anilides induced by phenyliodine bis(trifluoroacetate) has been developed to produce the corresponding oxygenated anilides with high regioselectivity in good to excellent yields.

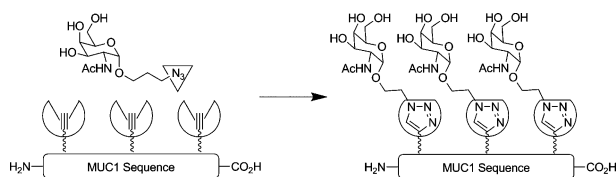


1621

Synthesis of MUC1 Neoglycopeptides using efficient microwave-enhanced chaotrope-assisted click chemistry

Dong Jun Lee, Paul W. R. Harris and Margaret A. Brimble*

The first synthesis of click neoglycopeptide analogues of the biologically relevant MUC1 sequence is reported using microwave-enhanced chaotrope-assisted click reaction conditions.

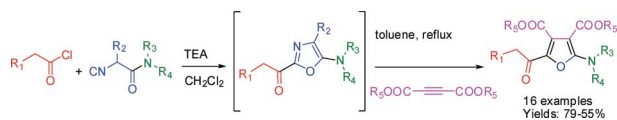


1627

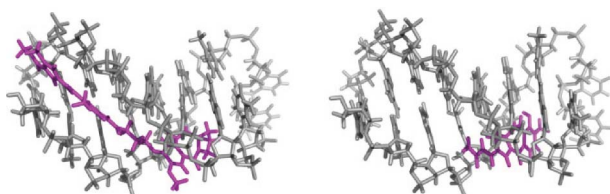
A novel α -isocyanoacetamide-based three-component reaction for the synthesis of dialkyl 2-acyl-5-aminofuran-3,4-dicarboxylates

Riccardo Mossetti, Diego Caprioglio, Giampiero Colombano, Gian Cesare Tron and Tracey Pirali*

α -Isocyanoacetamides, acyl chlorides and dialkylacetylenedicarboxylates undergo a smooth multicomponent reaction to produce dialkyl 2-acyl-5-aminofuran-3,4-dicarboxylates in good yield. The scope and mechanism of this new multicomponent transformation are discussed.



1632

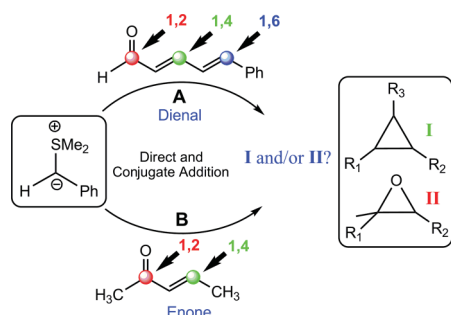


Observation of the reversibility of a covalent pyrrolobenzodiazepine (PBD) DNA adduct by HPLC/MS and CD spectroscopy

Khondaker M. Rahman, Colin H. James and David E. Thurston*

Using HPLC/MS and Circular Dichroism (CD) methodologies, it has been established for the first time that the aminal bond formed between pyrrolobenzodiazepine (PBD) molecules and DNA can be reversible.

1642

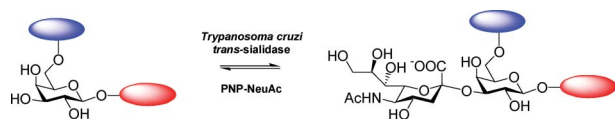


Chemo-, regio-, and diastereoselectivity preferences in the reaction of a sulfur ylide with a dienal and an enone

Deepa Janardanan and Raghavan B. Sunoj*

The chemo-, regio-, and diastereoselectivities in the addition of a sulfur ylide to a dienal and a dienone is described using DFT computation.

1653



Probing the acceptor substrate binding site of *Trypanosoma cruzi* trans-sialidase with systematically modified substrates and glycoside libraries

Jennifer A. Harrison, K. P. Ravindranathan Kartha, Eric J. L. Fournier, Todd L. Lowary, Carles Malet, Ulf J. Nilsson, Ole Hindsgaul, Sergio Schenkman, James H. Naismith and Robert A. Field*

Trypanosoma cruzi trans-sialidase is a versatile catalyst for enzymatic α -2,3-sialylation reactions.

1661



Peptidomimetic bond formation by DNA-templated acyl transfer

Mireya L. McKee, Amanda C. Evans, Simon R. Gerrard, Rachel K. O'Reilly,* Andrew J. Turberfield* and Eugen Stulz*

The efficiencies of DNA-templated acyl transfer reactions between thioester modified oligonucleotides and a series of amine and thiol based DNA-nucleophiles are directly compared; stable peptide-like bond formation can be achieved under physiological conditions by careful optimisation of the system.