

Organic & Biomolecular Chemistry

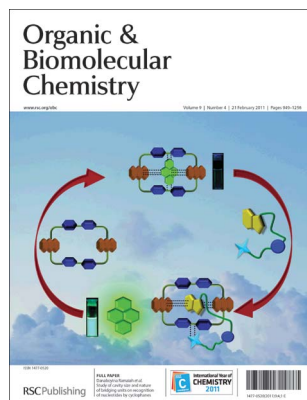
An international journal of synthetic, physical and biomolecular organic chemistry

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IN THIS ISSUE

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Cover

See Danaboyina Ramaiah *et al.*, pp. 1021–1029.

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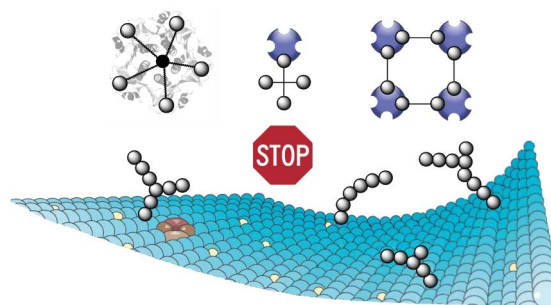
PERSPECTIVE

966

Insights in the rational design of synthetic multivalent glycoconjugates as lectin ligands

David Deniaud, Karine Julienne and Sébastien G. Gouin*

This perspective article presents the important structural features of synthetic multivalent ligands for a tight binding with specific lectins.



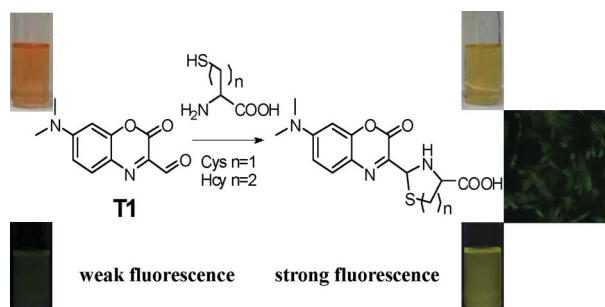
COMMUNICATIONS

980

Fluorescent chemodosimeter for Cys/Hcy with a large absorption shift and imaging in living cells

Mingming Hu, Jiangli Fan,* Honglin Li, Kedong Song, Song Wang, Guanghui Cheng and Xiaojun Peng*

T1 exhibited enhanced fluorescence intensity and absorption peak shift after addition of Cys/Hcy. It can be used for bioimaging and detection in human plasma by visual color change.



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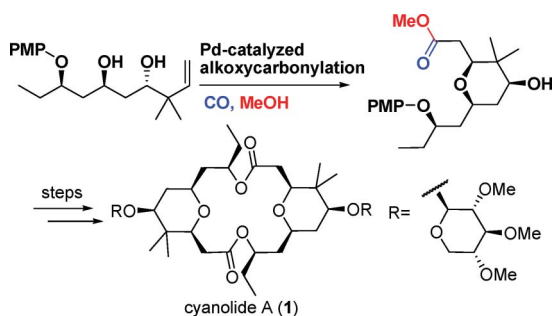
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984

Total synthesis of cyanolide A

Zhen Yang, Xingang Xie, Peng Jing, Gaoyuan Zhao, Jiyue Zheng, Changui Zhao and Xuegong She*

The total synthesis of cyanolide A has been achieved in 14 steps from commercially available (*S*)-2-ethylloxirane, exploiting the palladium-catalyzed intramolecular alkoxy carbonylation as the key step to construct the tetrasubstituted *cis*-tetrahydropyran ring with high stereoselectivity.

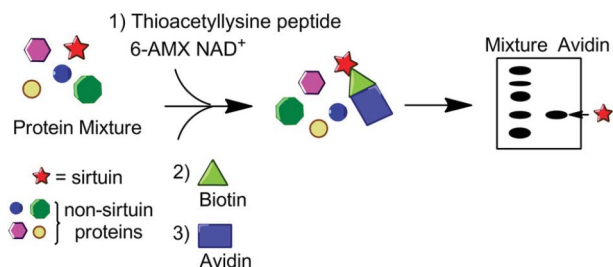


987

Mechanism-based affinity capture of sirtuins

Yana Cen, Jessica N. Falco, Ping Xu, Dou Yeon Youn and Anthony A. Sauve*

The novel NAD⁺ analog “6-AMX-NAD⁺” when combined with a thioacetyllysine peptide pan-sirtuin inhibitor forms a temporally stable complex on sirtuin active sites that can be conjugated to biotin and avidin, accomplishing “sirtuin capture” from protein mixtures.

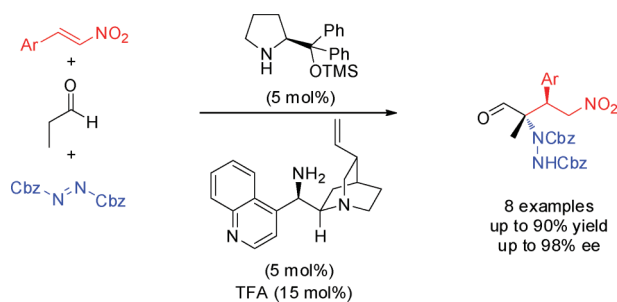


994

Asymmetric organocatalytic Michael– α -amination sequence for the construction of a quaternary stereocenter

Alaric Desmarchelier, Jérôme Marrot, Xavier Moreau* and Christine Greck*

Combination of secondary and primary amine-catalyzed Michael– α -amination sequence is described. α -Hydrazino aldehydes bearing a quaternary stereocenter are obtained with high yields and excellent stereoselectivities.

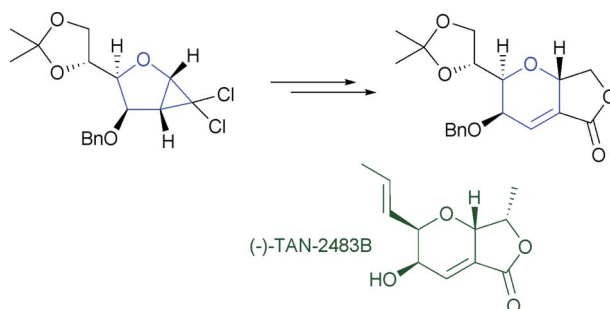


998

Synthesis of the (–)-TAN-2483B ring system via a D-mannose-derived cyclopropane

Russell J. Hewitt and Joanne E. Harvey*

The ring system of the fungal metabolite (–)-TAN-2483B has been synthesised by ring expansion of a D-mannose-derived cyclopropane.



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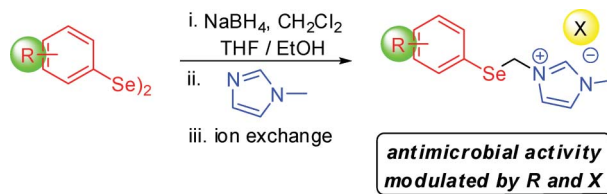
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1001

Imidazolium ionic liquids containing selenium: synthesis and antimicrobial activity

Eduardo E. Alberto, Luana L. Rossato, Sydney Hartz Alves, Diego Alves and Antonio L. Braga*

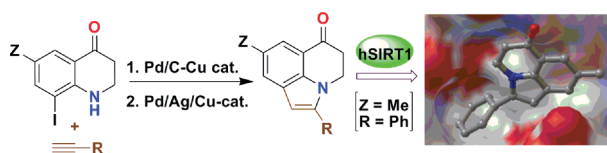
The synthesis and antimicrobial profile of imidazolium ionic liquids containing selenium are described.



1004

Transition metal mediated construction of pyrrole ring on 2,3-dihydroquinolin-4(1H)-one: synthesis and pharmacological evaluation of novel tricyclic heteroarenes

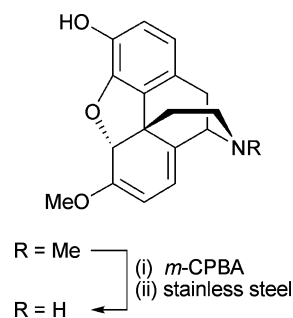
Mohosin Layek, Appi Reddy M., A. V. Dhanunjaya Rao, Mallika Alvala, M. K. Arunasree, Aminul Islam, K. Mukkanti, Javed Iqbal* and Manojit Pal*

Novel tricyclic heteroarenes were synthesized *via* transition metal mediated coupling-cyclization strategy and evaluated for SIRT1 activation *in vitro*.

1008

Further investigations into the *N*-demethylation of oripavine using iron and stainless steel

Gaik B. Kok and Peter J. Scammells*

Further investigations into the direct synthesis of *N*-nororipavine from oripavine using iron powder under non-classical Polonovski conditions have been conducted. The stoichiometry, solvents and iron oxidation rates were found to have a dramatic effect on the rate of *N*-demethylation as well as product yield. Herein, we also present high-yield access to the *N*-demethylated product simply by employing stainless steel rather than iron powder as redox catalyst.

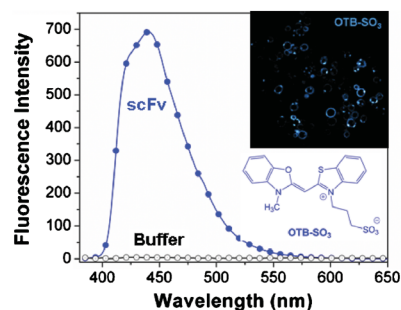
PAPERS

1012

Blue fluorescent dye-protein complexes based on fluorogenic cyanine dyes and single chain antibody fragments

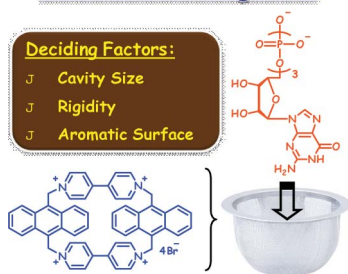
Kimberly J. Zanotti, Gloria L. Silva, Yehuda Creeger, Kelly L. Robertson, Alan S. Waggoner, Peter B. Berget and Bruce A. Armitage*

Dye-protein complexes that emit intense blue fluorescence have been created from fluorogenic cyanine dyes and single chain antibody fragments.



1021

Nucleotide Recognition

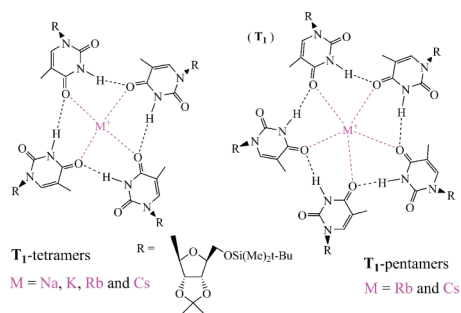


Study of cavity size and nature of bridging units on recognition of nucleotides by cyclophanes

Prakash P. Neelakandan, Paramjyothi C. Nandajan, Baby Subymol and Danaboyina Ramaiah*

The biomolecular recognition properties of cyclophanes reveal that these systems undergo selective encapsulation with nucleotides involving electrostatic, π - π stacking and hydrophobic interactions.

1030

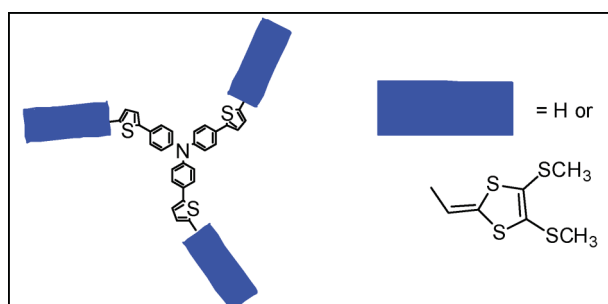


The formation of thymidine-based T-tetramers with remarkable structural and metal ion size effects

Qun Luo, Dayong Wu, Shixiong Liu, Daihua Tang,* Yong Huang, Xinhou Liu, Fuyi Wang,* Ruiyao Wang and Gang Wu*

We present direct ESI Q-TOF MS and X-ray evidence for remarkable structural and metal ion size effects on the formation of thymidine-based T-tetramers.

1034

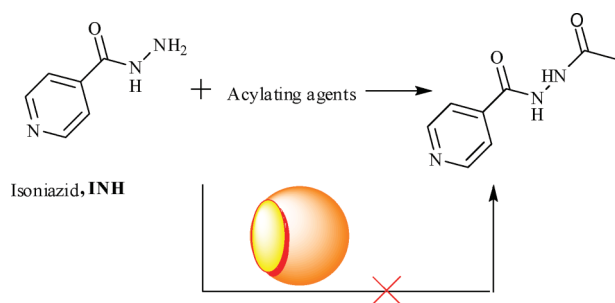


Trithienylphenylamine – extended dithiafulvene hybrids as bifunctional electroactive species

Emilie Ripaud, Philippe Leriche,* Nicolas Cocherel, Thomas Cauchy, Pierre Frère and Jean Roncali

The syntheses, electrochemical and spectroscopic properties of several trithienylphenylamine – dithiafulvene hybrids are presented.

1041



Cucurbituril-resisted acylation of the anti-tuberculosis drug isoniazid *via* a supramolecular strategy

Hang Cong, Chun-Rong Li, Sai-Feng Xue, Zhu Tao,* Qian-Jiang Zhu and Gang Wei*

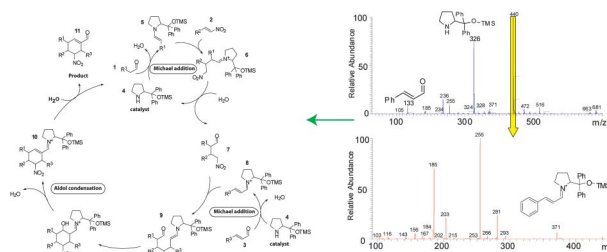
A chemical investigation into resistance *via* cucurbituril-induced acylation of isoniazid, revealed cucurbiturils can be used as potential drug-carriers of isoniazid.

1047

Electrospray mass spectrometry for detailed mechanistic studies of a complex organocatalyzed triple cascade reaction

M. Wasim Alachraf, Peni P. Handayani, Matthias R. M. Hüttl, Christoph Grondal, Dieter Enders and Wolfgang Schrader*

Electrospray mass spectrometry (ESI-MS) was used to conduct detailed studies of a complex organocatalytic triple cascade reaction for the synthesis of tetra-substituted cyclohexene carbaldehydes.

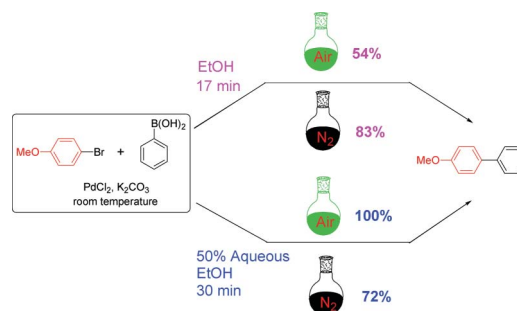


1054

Oxygen-promoted PdCl₂-catalyzed ligand-free Suzuki reaction in aqueous media

Chun Liu,* Qijian Ni, Pingping Hu and Jieshan Qiu

A systematic investigation of the effects of atmospheres in different solvents revealed that an aerobic atmosphere could accelerate the Suzuki reaction in aqueous media.

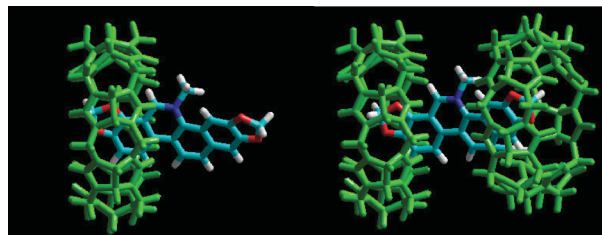


1061

Inclusion complex formation of sanguinarine alkaloid with cucurbit[7]uril: inhibition of nucleophilic attack and photooxidation

Zsombor Miskolczy, Mónika Megyesi, Gábor Tárkányi, Réka Mizsei and László Biczók*

The 1 : 1 and 1 : 2 inclusion complex formation with cucurbit[7]uril not only protects sanguinarine against nucleophilic addition and photodegradation, but also can be utilized for pH-controlled drug release.

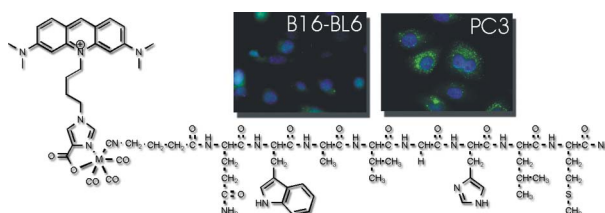


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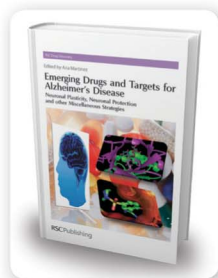
Trifunctional ^{99m}Tc based radiopharmaceuticals: metal-mediated conjugation of a peptide with a nucleus targeting intercalator

Karel Zelenka, Lubor Borsig and Roger Alberto*

The combination of a receptor specific peptide (BBN 7-14), a fluorescence marker (acridine orange) and a rhenium or ^{99m}Tc complex fragment yields trifunctional conjugates. This design is the base for future cell specific, nuclear targeting compounds.



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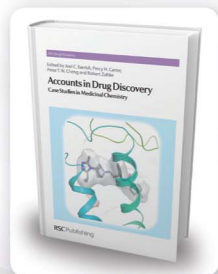
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1079

On the enantioselectivity of aziridination of styrene catalysed by copper triflate and copper-exchanged zeolite Y: consequences of the phase behaviour of enantiomeric mixtures of *N*-arene-sulfonyl-2-phenylaziridines

Laura Jeffs, Damien Arquier, Benson Kariuki, Donald Bethell, Philip C. Bulman Page and Graham J. Hutchings

The enantioselectivity of the aziridination of styrene catalysed by copper with a chiral bis-oxazoline ligand has been re-examined.

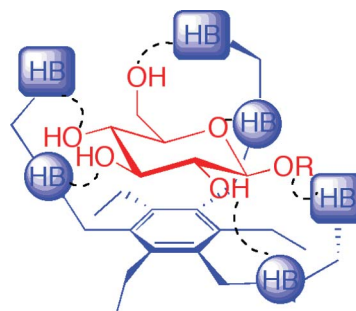


1085

Pyrrolic tripodal receptors for carbohydrates. Role of functional groups and binding geometry on carbohydrate recognition

Martina Cacciarini,* Cristina Nativi, Martina Norcini, Samuele Staderini, Oscar Francesconi and Stefano Roelens*

What are the essential requirements for carbohydrate recognition? The synthesis of a set of benzene-based tripodal receptors has been developed to investigate the contribution from several H-bonding groups (HB) and the impact of geometric requirements.

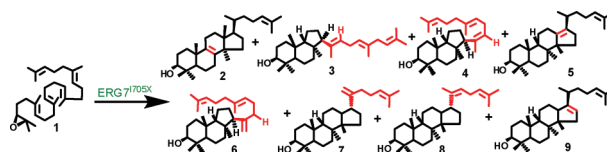


1092

Mutation of isoleucine 705 of the oxidosqualene-lanosterol cyclase from *Saccharomyces cerevisiae* affects lanosterol's C/D-ring cyclization and 17 α / β -exocyclic side chain stereochemistry

Tung-Kung Wu,* Yi-Chun Chang, Yuan-Ting Liu, Cheng-Hsiang Chang, Hao-Yu Wen, Wen-Hsuan Li and Wen-Shiang Shie

Product profiles of ERG7^{I705X} site-saturated and ERG7^{F699X/I705F} double mutation experiments unravel catalytic role of the second-tier Ile705 within oxidosqualene-lanosterol cyclase.

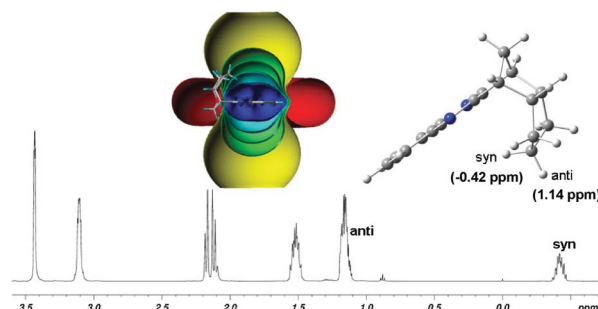


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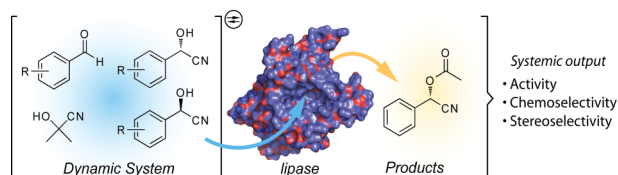
The anisotropic effect of functional groups in ¹H NMR spectra is the molecular response property of spatial nucleus independent chemical shifts (NICS)—Conformational equilibria of *exo/endo* tetrahydrodicyclopentadiene derivatives

Erich Kleinpeter,* Anica Lämmermann and Heiner Kühn

Five-membered ring inversion of TH-DCPD derivatives is studied by v.t. NMR and preferred conformers assigned by quantifying anisotropic effects of functional groups.



1112

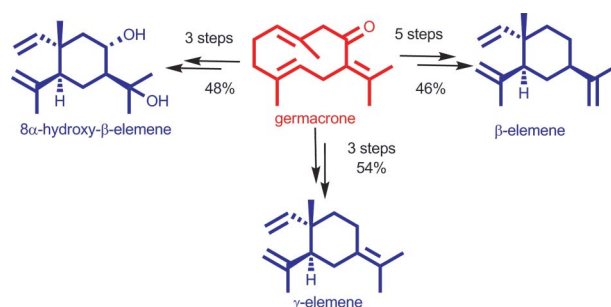


In Situ Evaluation of Lipase Performances Through Dynamic Asymmetric Cyanohydrin Resolution

Morakot Sakulsombat, Pornrapee Vongvilai and Olof Ramström*

Dynamic cyanohydrin systems resolved by lipase-mediated transesterification resulted in efficient evaluation of complex lipase performances in asymmetric cyanohydrin synthesis.

1118

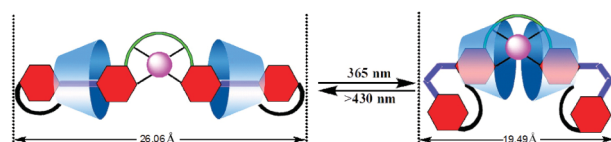


Efficient synthesis of the anticancer β -elemene and other bioactive elemenes from sustainable germacrone

Alejandro F. Barrero,* M. Mar Herrador,* José F. Quílez del Moral, Pilar Arteaga, Niklas Meine, M. Carmen Pérez-Morales and Julieta V. Catalán

Synthesis of anticancer elemenes.

1126

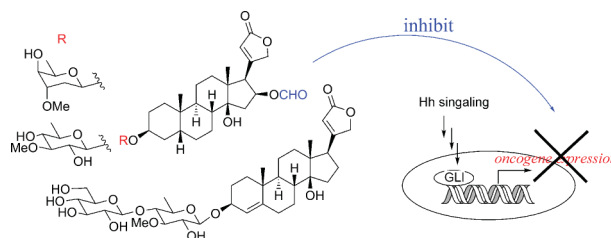


A light-powered stretch-contraction supramolecular system based on cobalt coordinated [1]rotaxane

Chao Gao, Xiang Ma, Qiong Zhang, Qiaochun Wang, Dahui Qu and He Tian*

A novel light-powered supramolecular system based on cobalt coordinated [1]rotaxane could contract and stretch reversibly by different UV irradiations, accompanying with obvious ICD signal variance.

1133



New hedgehog/GLI-signaling inhibitors from *Adenium obesum*

Midori A. Arai,* Chikashi Tateno, Takashi Koyano, Thaworn Kowithayakorn, Seiichiro Kawabe and Masami Ishibashi*

17 cardiac glycosides, including 3 new compounds, were isolated as new hedgehog (Hh)/GLI signaling pathway inhibitors. These compounds inhibited GLI-related protein expression and mRNA expression in human pancreatic cancer cells (PANC1), which express Hh/GLI components aberrantly.

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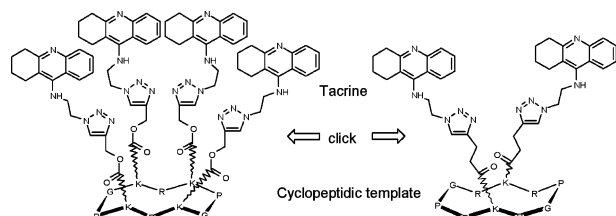
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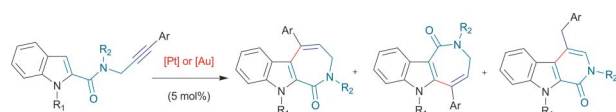


Clicked tacrine conjugates as acetylcholinesterase and β -amyloid directed compounds

Myriam Ouberaï, Kristoffer Brannstrom, Monika Vestling, Anders Olofsson, Pascal Dumy, Sabine Chierici* and Julian Garcia*

Synergetic effect of the known AChE inhibitor “tacrine” in a cyclic peptide hybrid as an amyloid beta aggregation inhibitor.

1148

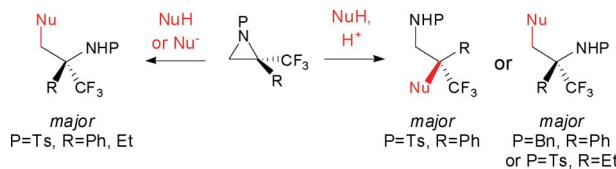


Platinum-catalyzed cyclization reaction of alkynes: synthesis of azepero[3,4-*b*]indol-1-ones

Marina Gruit, Anahit Pews-Davtyan and Matthias Beller*

Novel azepero[3,4-*b*]indol-1-ones were synthesized from alkyne-substituted indole-2-carboxamides by catalytic intramolecular cyclization in the presence of PtCl_2 in up to 80% yield.

1160

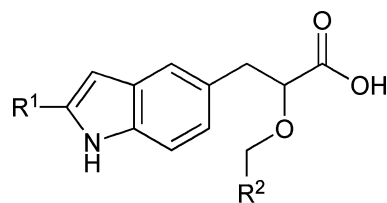


Enantiomerically pure 2-aryl(alkyl)-2-trifluoromethylaziridines: synthesis and ring opening with selected *O*- and *N*-nucleophiles

Fabienne Grellepois,* Jean Nonnenmacher, Fabien Lachaud and Charles Portella

The stereoselective synthesis of enantiopure 2,2-disubstituted 2-trifluoromethylaziridines and their use as precursors of β -amino alcohols and β -diamines bearing a quaternary trifluoromethyl group.

1169



$R^1 = \text{H}; \text{benzyl}; \text{naphthylmethyl}$

$R^2 = \text{CH}_3; \text{CF}_3$

Synthesis of novel PPAR α / γ dual agonists as potential drugs for the treatment of the metabolic syndrome and diabetes type II designed using a new *de novo* design program PROTOBUILD

Yushma Bhurruth-Alcor, Therese Røst, Michael R. Jorgensen, Christos Kontogiorgis, Jon Skorve, Robert G. Cooper, Joseph M. Sheridan, William D. O. Hamilton, Jonathan R. Heal, Rolf K. Berge and Andrew D. Miller*

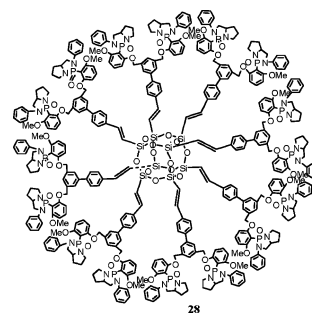
Proof of concept application of *de novo* design program PROTOBUILD.

1189

Synthesis of hybrid dendritic molecules with diazaphospholidine oxide grafted at the surface of octavinylsilsesquioxane (OVS)

Ge Cheng, Alexandra M. Z. Slawin, Nicolas R. Vautravers, Pascal André, Russell E. Morris, Ifor D. W. Samuel and David Cole-Hamilton*

Grubbs metathesis has been used to anchor SEMI-ESPHOS groups to octavinylsilsesquioxane cores. Full functionalisation of the core has been achieved

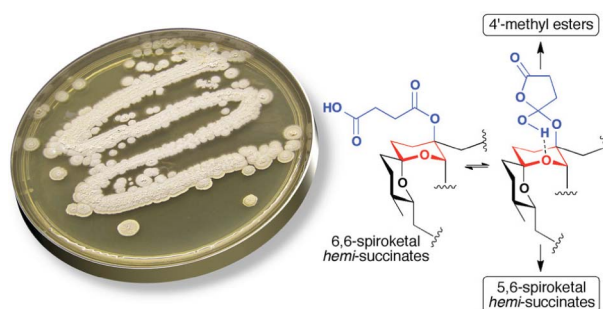


1201

Reveromycins Revealed: New polyketide spiroketals from Australian marine-derived and terrestrial *Streptomyces* spp. A case of natural products vs. artifacts

Leith Fremlin, Michelle Farrugia, Andrew M. Piggott, Zeinab Khalil, Ernest Lacey and Robert J. Capon*

Australian *Streptomyces* spp. yielded sixteen examples of the rare reveromycin class of polyketide, and disclosed an unprecedented ketal-succinyl equilibrium that revealed the presence of artifacts and informed a plausible biosynthesis.

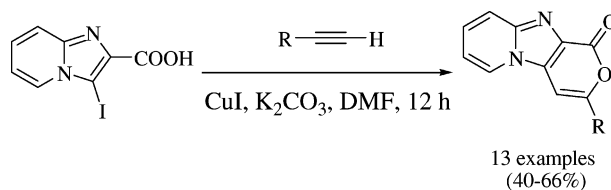


1212

Copper(I)-mediated preparation of new pyrano[3',4':4,5]imidazo[1,2-*a*]-pyridin-1-one compounds under mild palladium-free conditions

Zineb Bahlaouan, Mohamed Abarbri,* Alain Duchêne, Jérôme Thibonnet, Nicolas Henry, Cécile Enguehard-Gueiffier and Alain Gueiffier

A general and efficient Cu(I)-mediated cross-coupling and heterocyclization reaction of 3-iodoimidazo[1,2-*a*]pyridine-2-carboxylic acid, and terminal alkynes was developed under very mild conditions.

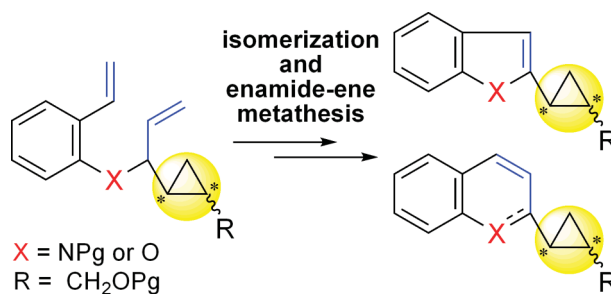


1219

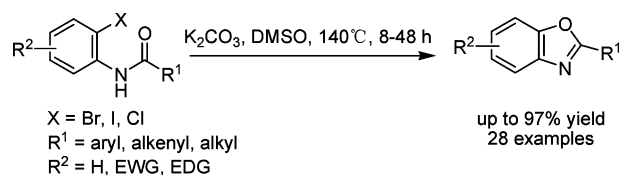
Alkene isomerization/enamide-ene and diene metathesis for the construction of indoles, quinolines, benzofurans and chromenes with a chiral cyclopropane substituent

Takaaki Kobayashi, Mitsuhiro Arisawa* and Satoshi Shuto*

A synthetic method for bicyclic heterocycles, such as indole, benzofuran and chromene derivatives bearing a chiral cyclopropane at the 2-position, was established using isomerization of a terminal olefin and enamide-ene or diene metathesis.



1225

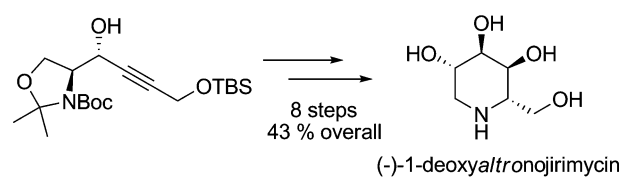


Direct transition-metal-free intramolecular C–O bond formation: synthesis of benzoxazole derivatives

Jinsong Peng,* Cuijuan Zong, Min Ye, Tonghui Chen, Dewei Gao, Yufeng Wang and Chunxia Chen*

A direct base-mediated intramolecular carbon-oxygen bond formation has been developed without a transition-metal catalyst.

1231



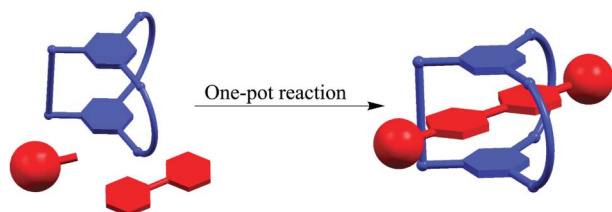
Only two chromatographic purifications

Rapid and practical synthesis of (-)-1-deoxyaltronojirimycin

Oskari K. Karjalainen and Ari M. P. Koskinen*

An efficient (43% overall) and rapid access to (-)-deoxyaltronojirimycin requiring minimal amount of purifications is described.

1237

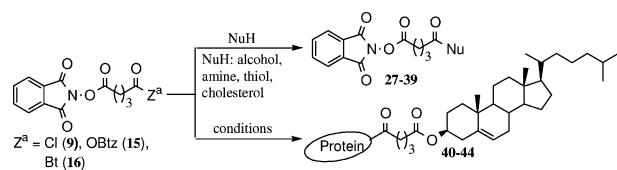


One-pot synthesis of donor–acceptor [2]rotaxanes based on cryptand–paraquat recognition motif

Zhikai Xu, Lasheng Jiang,* Yahui Feng, Suhui Zhang, Jidong Liang, Shaowu Pan, Yu Yang, Dengke Yang and Yuepeng Cai

Cryptand-based [2]rotaxanes can be easily prepared by one-pot reactions of three nonionic starting materials.

1244

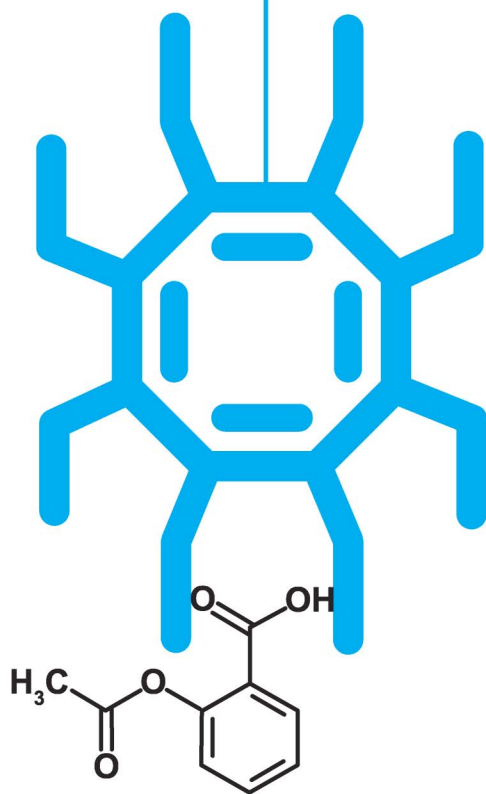


Syntheses and reactivities of non-symmetrical “active ester” bi-dentate cross-linking reagents having a phthalimidoyl and acid chloride, 2-benzothiazole, or 1-benzotriazole group

Md. Chanmiya Sheikh,* Shunsuke Takagi, Mebumi Sakai, Tasuya Mori, Naoto Hayashi, Tetsuo Fujie, Shin Ono, Toshiaki Yoshimura* and Hiroyuki Morita*

Non-symmetrical cross-linking reagents were synthesized and studied their reactivities toward nucleophiles for easy chemical modification of sugar derivatives and proteins

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