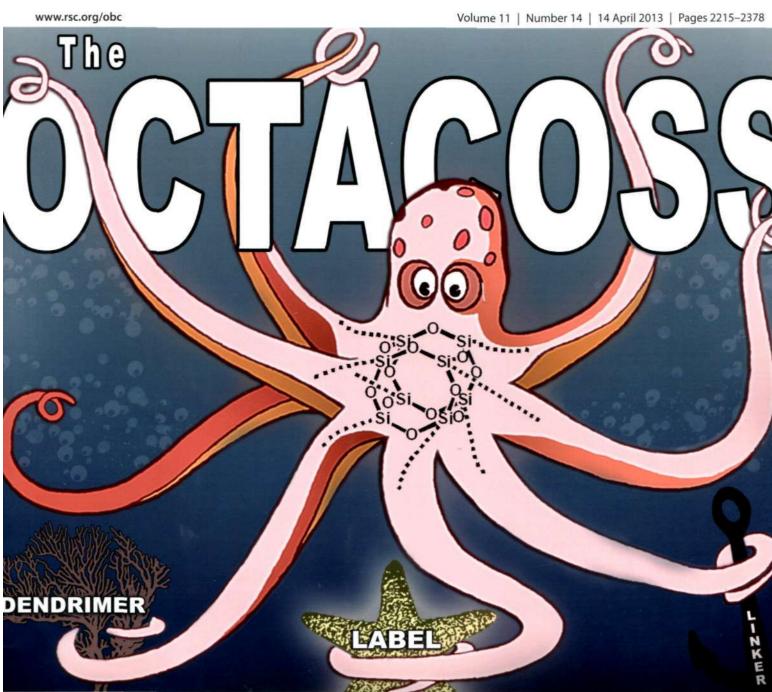
Organic & Biomolecular Chemistry



ISSN 1477-0520



Bioconiugation on cube-octameric silsesquioxanes

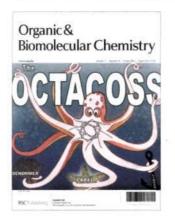
Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry www.rsc.org/obc

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org

IN THIS ISSUE

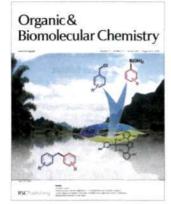
ISSN 1477-0520 CODEN OBCRAK 11(14) 2215-2378 (2013)



Cover

See Sebastian Fabritz et al., pp. 2224-2236.

Image reproduced by permission of Harald Kolmar from Org. Biomol. Chem., 2013, 11, 2224.



Inside cover

See Jian-Mei Lu et al., pp. 2266-2272.

Image reproduced by permission of Jian-Mei Lu from Org. Biomol. Chem., 2013, 11, 2266.

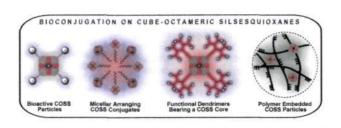
PERSPECTIVE

2224

Bioconjugation on cube-octameric silsesquioxanes

Sebastian Fabritz,* Sebastian Hörner, Olga Avrutina and Harald Kolmar

Bioconjugation on cube-octameric silsesquioxanes (COSS) is reviewed. Important characteristics of COSS scaffolds, the expanded arsenal of conjugation methods and application of resulted conjugates to biosystems are critically discussed.



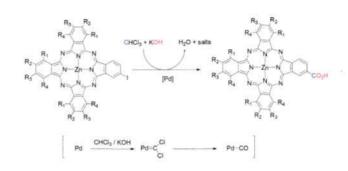
COMMUNICATIONS

2237

Synthesis of unsymmetrical carboxyphthalocyanines by palladium-catalyzed hydroxycarbonylation of iodo-substituted precursors

Íñigo Aguirre de Carcer García, Altug Mert Sevim, Andrés de la Escosura and Tomás Torres*

A mild and efficient one-step palladium-catalyzed reaction allows the straightforward synthesis of unsymmetrical carboxyphthalocyanines by hydroxycarbonylation of iodo-substituted precursors.



In vitro evolution of a Friedel-Crafts deoxyribozyme

Utpal Mohan, Ritwik Burai and Brian R. McNaughton*

We report the in vitro selection of a single-stranded 72-nucleotide DNA enzyme (deoxyribozyme) that catalyzes a Friedel-Crafts reaction between an indole and acyl imidazole in good yield and in aqueous solvent.

2245

Synthesis of green and blue fluorescent ladder-type conjugated imidazolium compounds

Koji Takagi,* Yohei Ito, Kazuma Kusafuka and Masanori Sakaida

The synthetic route to green and blue fluorescent ladder-type conjugated imidazolium compounds was developed.

$$\begin{array}{c} C_8H_{17} \\ H_{-N} \\ N \\ Br \end{array}$$

$$R$$

$$A = CI \text{ and } (CF_3SO_2)_2N$$

$$Wavelength/nm$$

$$Wavelength/nm$$

$$Wavelength/nm$$

2249

Synthesis of imidazo and benzimidazo[2,1-a]isoquinolines by rhodium-catalyzed intramolecular double C-H bond activation

Vutukuri Prakash Reddy, Takanori Iwasaki and Nobuaki Kambe*

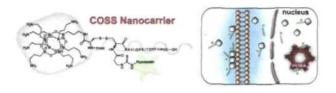
The rhodium-catalyzed intramolecular direct arylation of imidazole and benzimidazole derivatives via double C-H bond cleavage was developed.

2254

A naked-eye chemosensor for fluoride ions: a selective easy-to-prepare test paper

Xue Yong, Minjian Su, Wen Wang, Yichen Yan, Jinging Qu* and Ruiyuan Liu*

A new naked-eye chromogenic chemosensor based on 2-thiohydantoin shows high selectivity for fluoride ions and is used to develop a test paper for detection of fluoride ions in the solid state.



Cube-octameric silsesquioxane-mediated cargo peptide delivery into living cancer cells

Sebastian Hörner, Sebastian Fabritz, Henry D. Herce,* Olga Avrutina, Christian Dietz, Robert W. Stark, M. Cristina Cardoso and Harald Kolmar*

Cube-octameric sislesquioxane (COSS) delivery system allows for drug targeting in living cancer cells.

2266 B(OH)₂ NHC-Pd(II)-Im 1 (1.5 mol%) KOH, H₂O, 60 °C, 12 h NHC-Pd(II)-Im 1: NHC-Pd(II)-Im

N-Heterocyclic carbene-palladium(II)1-methylimidazole complex catalyzed SuzukiMiyaura coupling of benzylic chlorides with
arylboronic acids or potassium
phenyltrifluoroborate in neat water

Yun Zhang, Meng-Ting Feng and Jian-Mei Lu*

NHC-Pd(II)-Im complex catalyzed Suzuki-Miyaura coupling of benzylic chlorides in neat water.

2273

 $R^1 = iso$ propyl, $R^2 = Ac$ $IC_{50} = 3.8$ nM

 $R^1 = isopropyl$, $R^2 = MOM IC_{50} = 22 nM$

 R^1 = aryl or cyclohexyl or R^2 = benzoyl INACTIVE

Synthesis and structure–activity relationship studies of novel tubulysin U analogues – effect on cytotoxicity of structural variations in the tubuvaline fragment

Sreejith P. Shankar, Monika Jagodzinska, Luciana Malpezzi, Paolo Lazzari, Ilaria Manca, Jain R. Greig, Monica Sani* and Matteo Zanda*

A scalable synthesis of several tubulysin analogues modified at the tubuvaline fragment was developed.

2288

Synthetic and mechanistic insight into nosylation of glycine residues

Nicolai Stuhr-Hansen,* Theis Ivan Sølling and Kristian Strømgaard

The glycine residue is the only primary amine moiety undergoing bis-nosylation upon reaction with an excess of

A study on the substituent effects of norbornadiene derivatives in iridium-catalyzed asymmetric [2 + 2] cycloaddition reactions

Jun Hu, Qingjing Yang, Lu Yu, Jianbin Xu, Shanshan Liu, Chao Huang, Lin Wang, Yongyun Zhou and Baomin Fan*

Employing a series of norbornadiene derivatives as substrates, the effects of various substituents on the Ir-catalyzed asymmetric [2 + 2] cycloaddition reactions with arylacetylenes were studied.

more than 21 successful examples X = O. 89-99 % ee X = NR, 90-95 % ee X = CH2, 69-80 % ee X = CR2, no reaction

2302

Specific nucleophile-electrophile interactions in nucleophilic aromatic substitutions

Rodrigo Ormazábal-Toledo,* Renato Contreras, Ricardo A. Tapia and Paola R. Campodónico

In S_NAr reactions the hydrogen bond interaction along the reaction coordinate enhances the reactivity of both the nucleophile and the electrophile moieties by inducing a redistribution of their electronic density. In this type of reaction, the alpha effect is promoted by an additional hydrogen bond.



2310

Specific recognition of cytosine by hypoxanthine in pyrrolidinyl peptide nucleic acid

Chotima Vilaivan, Wimonmas Srinarang, Nattawut Yotapan, Woraluk Mansawat, Chalothorn Boonlua, Junji Kawakami, Yoshie Yamaguchi, Yuko Tanaka and Tirayut Vilaivan*

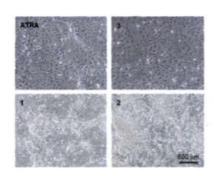
DNA binding studies revealed a remarkable preference for hypoxanthine in acpcPNA to pair with dC in DNA.

2318

Broadening the catalyst and reaction scope of regio- and chemoselective C-H oxygenation: a convenient and scalable approach to 2-acylphenols by intriguing Rh(II) and Ru(II) catalysis

Gang Shan, Xuesong Han, Yun Lin, Shanyou Yu and Yu Rao*

Intriguing Rh(II) and Ru(II) catalysis for regio- and chemoselective C-H oxygenation.



Synthesis and applications of 2,4-disubstituted thiazole derivatives as small molecule modulators of cellular development

Garr-Layy Zhou, Daniel M. Tams, Todd B. Marder,* Roy Valentine, Andrew Whiting* and Stefan A. Przyborski*

Understanding how the structure of molecules relates to their function and biological activity is essential in the development of new analogues with targeted activity.

2335

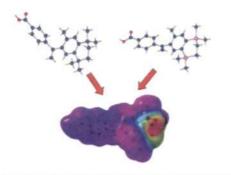


Regioselective C2-arylation of imidazo[4,5-b]-pyridines

Jonathan Macdonald, Victoria Oldfield, Vassilios Bavetsias and Julian Blagg*

We show that N3-protected imidazo[4,5-b]pyridines undergo selective C2-arylation facilitating the divergent synthesis of substituted variants of this purine isostere.

2348

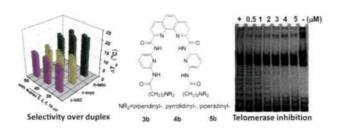


Electron densities of bexarotene and disilabexarotene from invariom application: a comparative study

Peter Luger,* Manuela Weber, Christian Hübschle and Reinhold Tacke*

The electrostatic difference potential (center) illustrates where the electronic structures of bexarotene (left) and disila-bexarotene (right) differ.

2355



Synthesis and binding studies of novel disubstituted phenanthroline compounds with genomic promoter and human telomeric DNA G-quadruplexes

Chunying Wei,* Yanbo Wang and Meiying Zhang

A new class of potent and selective stabilizers of *h*-telo, c-kit2, and c-myc G-quadruplexes and telomerase inhibitors.

Fluoride as an inducible DNA cross-linking agent for new antitumor prodrug

Jun Wu, Rong Huang, Tianlu Wang, Xi Zhao, Wanyi Zhang, Xiaocheng Weng, Tian Tian and Xiang Zhou*

Two new small compounds, which undergo fluoridemediated self rearrangement, produce active nitrogen mustard finally leading to cell death.

2370

Microwave-assisted synthesis of difficult sequencecontaining peptides using the isopeptide method

Waleed M. Hussein, Tzu-Yu Liu, Istvan Toth* and Mariusz Skwarczynski*

Microwave-assisted Fmoc solid phase peptide synthesis (SPPS) was applied in combination with the isopeptide strategy to establish a new method for the rapid synthesis of difficult sequence-containing peptides.