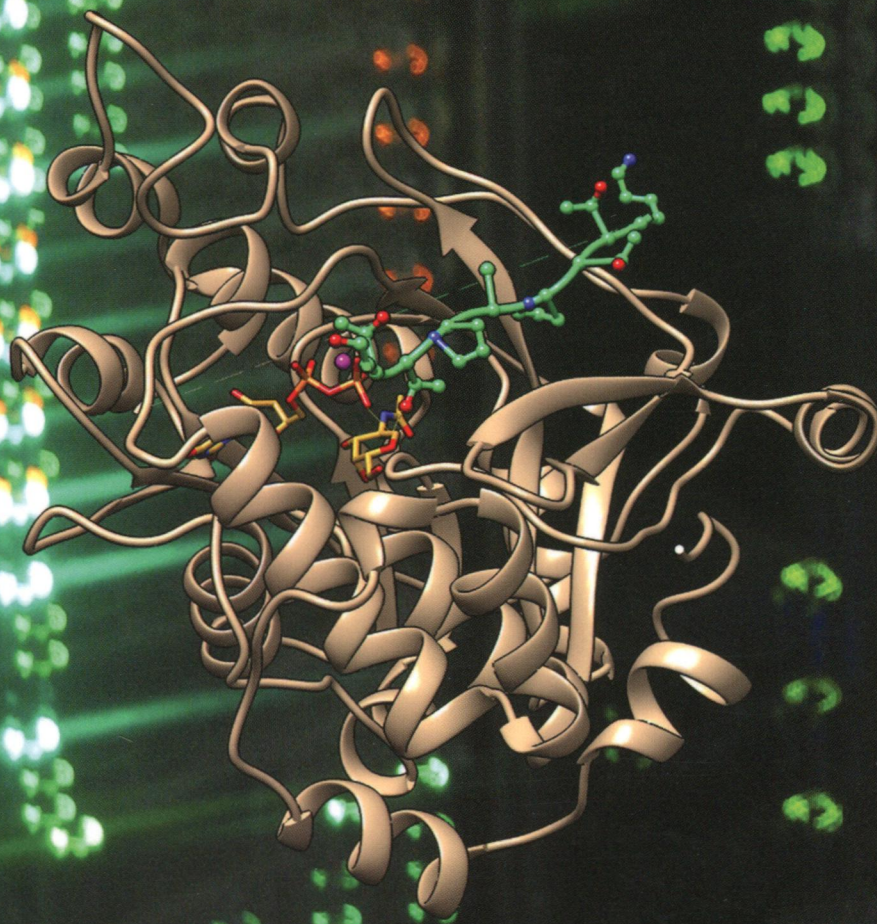


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Organic & Biomolecular Chemistry

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PAPER

Lawrence A. Tabak, Laura Masgrau *et al.*
A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2

Organic & Biomolecular Chemistry

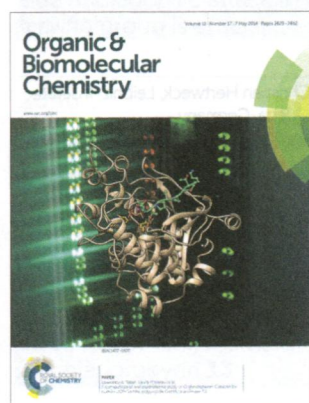
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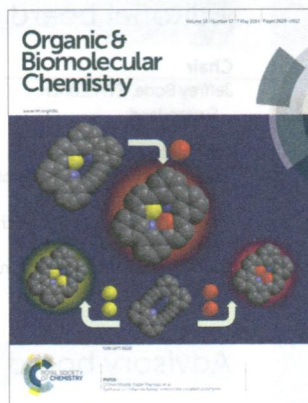
ISSN 1477-0520 CODEN OBCRAK 12(17) 2629–2812 (2014)



Cover

See Lawrence A. Tabak,
Laura Masgrau *et al.*,
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Inside cover

See Chihiro Maeda,
Naoki Yoshioka *et al.*,
pp. 2656–2662.

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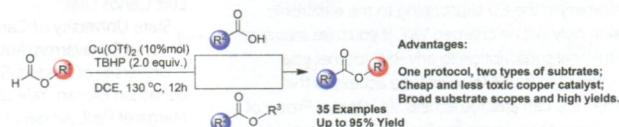
COMMUNICATIONS

2637

Copper-catalyzed highly efficient ester formation from carboxylic acids/esters and formates

Jun Liu, Changdong Shao, Yanghui Zhang,*
Guangfa Shi and Shulei Pan

Copper-catalyzed ester formation from carboxylic acids/esters and formates has been developed with high efficiency and broad substrate scopes.

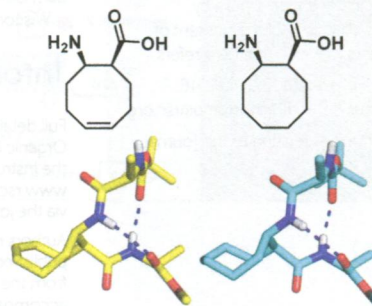


2641

Helical folding of α/β -peptides containing β -amino acids with an eight-membered ring constraint

Woohyung Lee, Sunmi Kwon, Philjae Kang, Iliia A. Guzei and Soo Hyuk Choi*

Cyclic β -amino acid that contains a cyclooctane or a cyclooctene ring promotes 11/9-helical folding of α/β -peptides.



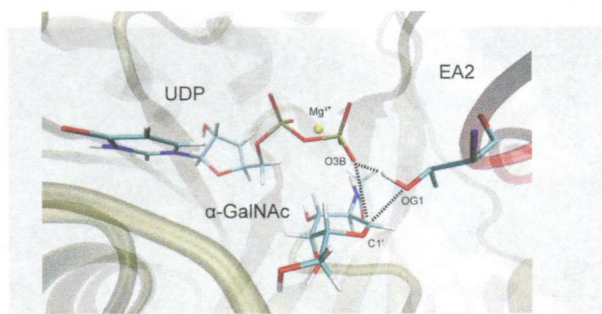
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Центральная научная библиотека
Уральского отделения
Российской академии наук (ЦНБ УрО РАН)

2645

A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2

Hansel Gómez, Raúl Rojas, Divya Patel, Lawrence A. Tabak,* José M. Lluch and Laura Masgrau*

GalNAc-T2 catalyses GalNAc O-glycosylation *via* a front-side nucleophilic attack in which stabilization of the UDP leaving group is crucial.

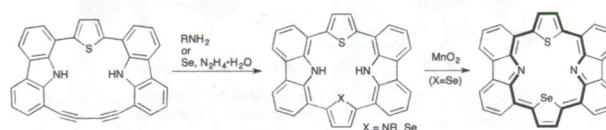


2656

Synthesis of carbazole-based hetero-core-modified porphyrins

Chihiro Maeda,* Motoki Masuda and Naoki Yoshioka*

Annulation reaction of a 1,1'-(1,3-butadiene)-8,8'-(2,5-thiophene)-bridged carbazole dimer **10** provided the carbazole-based isophlorines **11a–11c** and **12**. The oxidation of **12** generated the corresponding 21-selena-23-thiaporphyrin **13**.

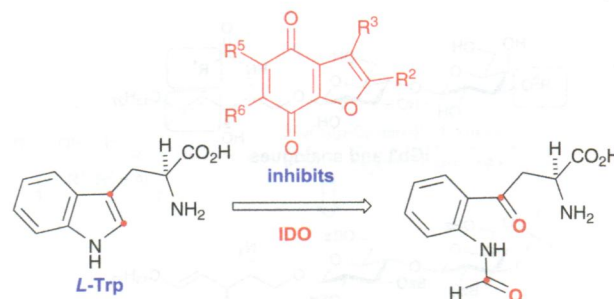


2663

Benzofuranquinones as inhibitors of indoleamine 2,3-dioxygenase (IDO). Synthesis and biological evaluation

Catarina Carvalho, David Siegel, Martyn Inman, Rui Xiong, David Ross and Christopher J. Moody*

Benzofuran- and benzimidazole-quinones are effective inhibitors of the tryptophan metabolizing enzyme indoleamine-2,3-dioxygenase (IDO).

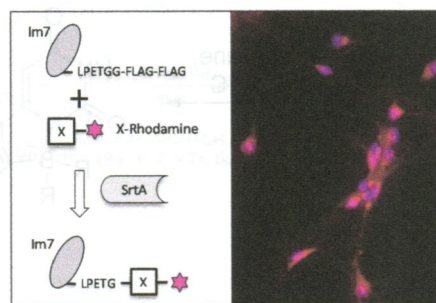


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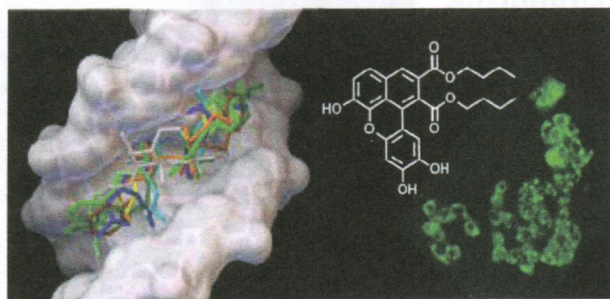
Comparison of alternative nucleophiles for Sortase A-mediated bioconjugation and application in neuronal cell labelling

Samuel Baer, Julie Nigro, Mariusz P. Madej, Rebecca M. Nisbet, Randy Suryadinata, Gregory Coia, Lisa P. T. Hong, Timothy E. Adams, Charlotte C. Williams* and Stewart D. Nuttall

Sortase A-mediated conjugation reactions were performed with a number of different nucleophiles. A peptide-Im7-labelled conjugate was used to image neuronal cells.



2686

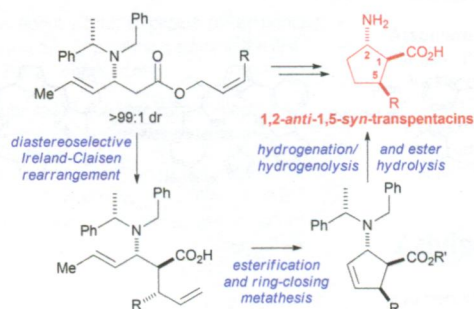


Bio-inspired benzo[*k,l*]xanthene lignans: synthesis, DNA-interaction and antiproliferative properties

Carmela Spatafora, Vincenza Barresi, Vedamurthy M. Bhusainahalli, Simone Di Micco, Nicolò Musso, Raffaele Riccio, Giuseppe Bifulco, Daniele Condorelli and Corrado Tringali*

Twelve benzo[*k,l*]xanthene lignans were synthesized by biomimetic oxidative coupling of caffeic esters and amides. Their antiproliferative activity was evaluated on a panel of six tumor cell lines.

2702

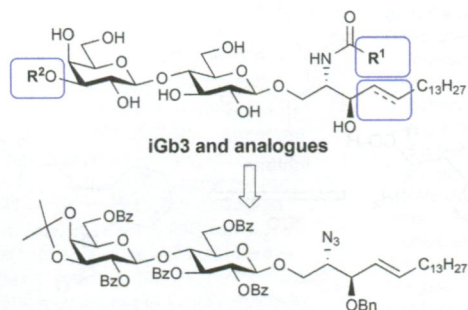


Diastereoselective Ireland–Claisen rearrangements of substituted allyl β -amino esters: applications in the asymmetric synthesis of C(5)-substituted transpentacins

Stephen G. Davies,* Ai M. Fletcher, James A. Lee, Paul M. Roberts, Myriam Y. Souleymanou, James E. Thomson and Charlotte M. Zammit

The Ireland–Claisen rearrangements of substituted allyl β -amino esters were evaluated, and subsequently employed in syntheses of C(5)-substituted transpentacins.

2729

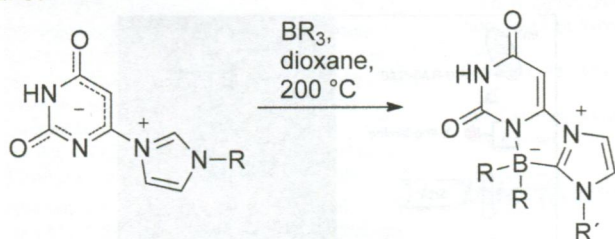


A divergent approach to the synthesis of iGb3 sugar and lipid analogues via a lactosyl 2-azido-sphingosine intermediate

Janice M. H. Cheng, Emma M. Dangerfield, Mattie S. M. Timmer* and Bridget L. Stocker*

Isoglobotrihexosylceramide (iGb3, **1**) is an immunomodulatory glycolipid that binds to CD1d and is presented to the T-cell receptor (TCR) of invariant natural killer T (iNKT) cells.

2737



Zwitterionic borane adducts of N-heterocyclic carbenes from mesomeric betaines of uracil

Jiayi Zhang, Nazar Pidlynyi, Martin Nieger, Jan C. Namyslo and Andreas Schmidt*

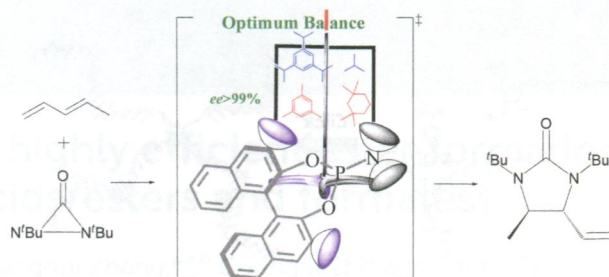
Imidazolium-substituted uracil-anions are in equilibrium with their N-heterocyclic carbenes which can be trapped as cyclic borane adducts.

2745

Rational design of catalysts for asymmetric diamination reaction using transition state modeling

Garima Jindal and Raghavan B. Sunoj*

DFT calculations have been used to design chiral phosphoramidite ligands for the asymmetric diamination of vicinal diamines. The substituents at both the 3,3' positions of the binol framework and the amido nitrogen play a vital role in the stereochemical outcome.

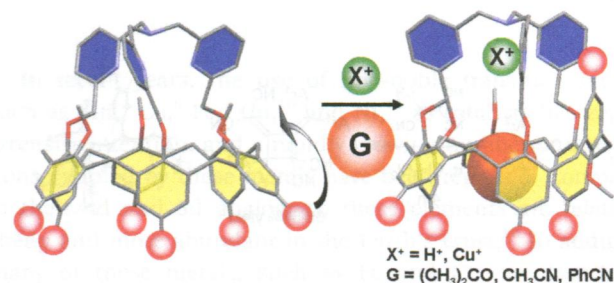


2754

An induced-fit process through mechanical pivoting of aromatic walls in host-guest chemistry of calix[6]arene aza-cryptands

Andrea Brugnara, Luca Fusaro, Michel Luhmer, Thierry Prangé, Benoit Colasson* and Olivia Reinaud*

A rigid calix[6]arene-based receptor can be fully *ipso*-nitrated. The nitrated receptor exhibits a new adaptive behavior upon cation and/or guest encapsulation.

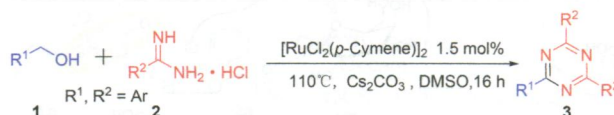


2761

An efficient ruthenium-catalyzed dehydrogenative synthesis of 2,4,6-triaryl-1,3,5-triazines from aryl methanols and amidines

Feng Xie, Mengmeng Chen, Xiaoting Wang, Huanfeng Jiang and Min Zhang*

An efficient ruthenium-catalyzed dehydrogenative synthesis of 2,4,6-triaryl-1,3,5-triazines from aryl methanols and amidines has been demonstrated.

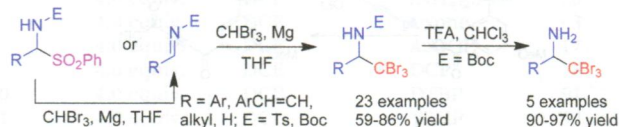


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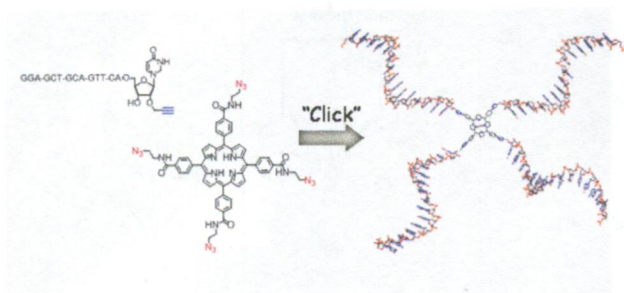
Synthesis of α -tribromomethylamines via Mg-mediated addition of bromoform to imines

Elumalai Gopi and Irishi N. N. Namboothiri*

N-Sulfonyl- and *N*-Boc-imines undergo facile addition of bromoform in the presence of Mg to afford α -tribromomethyl *N*-sulfonyl- and *N*-Boc-amines.



2778

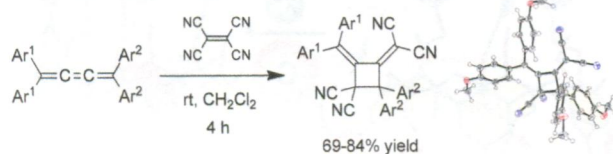


Synthesis of a multibranching porphyrin-oligonucleotide scaffold for the construction of DNA-based nano-architectures

Guillaume Clavé, Grégory Chatelain, Arianna Filoramo, Didier Gasparutto, Christine Saint-Pierre, Eric Le Cam, Olivier Piétremont, Vincent Guérineau and Stéphane Campidelli*

A multiclick-based approach was used to build DNA-porphyrin hybrid platforms.

2784

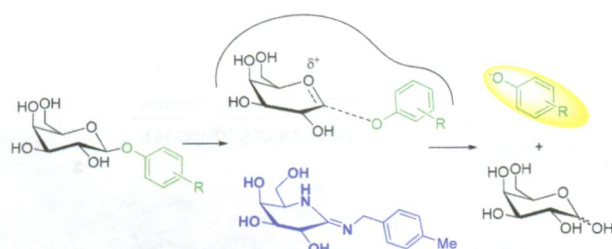


Regioisomeric allene dimer formation by the reaction of tetraarylbutatrienes with tetracyanoethene

Shoko Ueta,* Kazuo Hida, Masaki Nishiuchi and Yasuhiko Kawamura*

Title reactions formed head-to-tail unsymmetrically substituted diaryllallene dimers possessing four cyano groups in appreciably high yield at room temperature.

2792

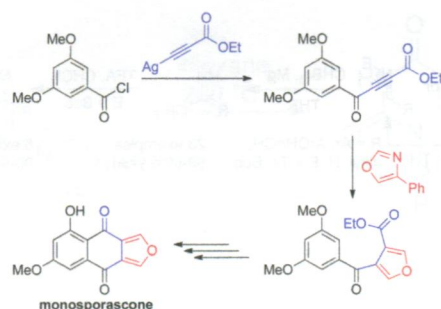


Evaluating *N*-benzylgalactonoamidines as putative transition state analogs for β -galactoside hydrolysis

Qiu-Hua Fan, Susanne Striegler,* Rebekah G. Langston and James D. Barnett

The kinetic evaluation of several *N*-benzylgalactonoamidines identified *p*-methylbenzylgalactonoamidinium as a putative transition state analog for the enzymatic hydrolysis of β -galactopyranosides by β -galactosidase (*A. oryzae*).

2801



Total synthesis of monosporascone and dihydromonosporascone

Kathryn A. Punch and Matthew J. Piggott*

The first synthesis of monosporascone has been achieved in five steps and 57% overall yield.