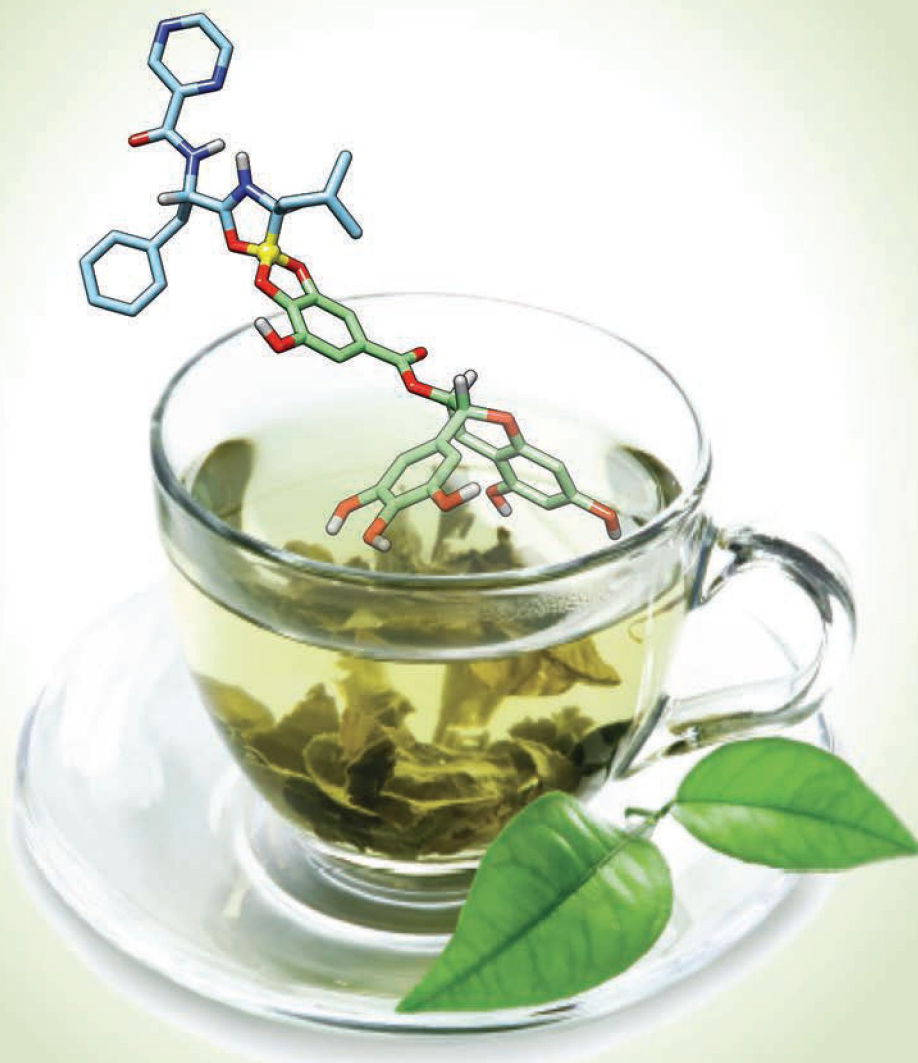


Organic & Biomolecular Chemistry

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PAPER

Nicos A. Petasis *et al.*

Molecular characterization of the boron adducts of the proteasome inhibitor bortezomib with epigallocatechin-3-gallate and related polyphenols

Organic & Biomolecular Chemistry

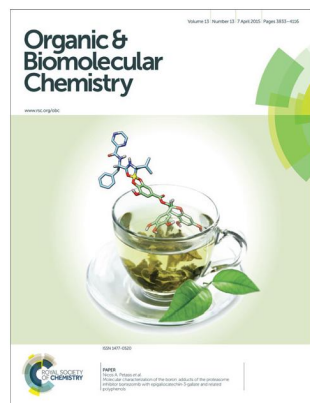
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IN THIS ISSUE

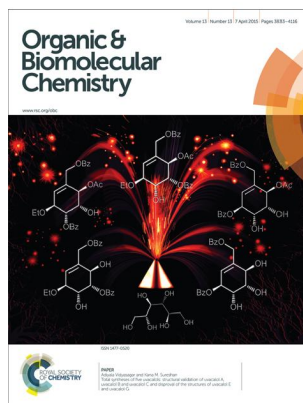
ISSN 1477-0520 CODEN OBCRAK 13(13) 3833–4116 (2015)



Cover

See Nicos A. Petasis *et al.*, pp. 3887–3899.

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Inside cover

See Adiyala Vidyasagar and Kana M. Sureshan, pp. 3900–3910.

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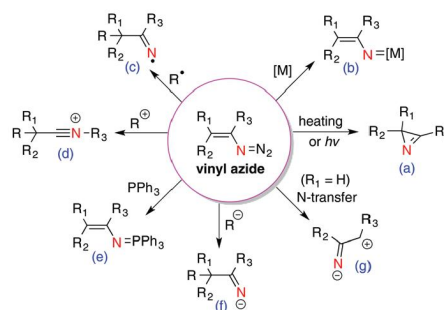
REVIEW

3844

Reactivities of vinyl azides and their recent applications in nitrogen heterocycle synthesis

Bao Hu* and Stephen G. DiMaggio

This review categorizes the active intermediates generated from denitrogenation of vinyl azides under different reaction conditions, and highlights newly discovered transformations of vinyl azides that lead to convenient syntheses of N-heterocycles.



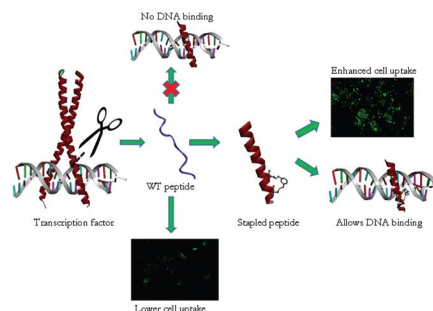
COMMUNICATIONS

3856

Stapling monomeric GCN4 peptides allows for DNA binding and enhanced cellular uptake

Abhishek Iyer, Dorien Van Lysebetten, Yara Ruiz García, Benoit Louage, Bruno G. De Geest and Annemieke Madder*

Facile synthesis of DNA binding stapled peptides which show enhanced cellular uptake is described considering the GCN4 transcription factor as a model protein.



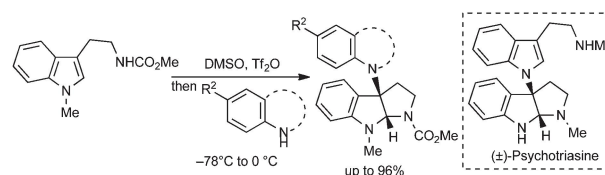
COMMUNICATIONS

3863

DMSO/Tf₂O-mediated cross-coupling of tryptamine with substituted aniline to access C3a–N1'-linked pyrroloindoline alkaloids

Masanori Tayu, Takako Ishizaki, Kazuhiro Higuchi* and Tomomi Kawasaki*

The cross-coupling of tryptamine with substituted aniline to C3a–nitrogen-linked pyrroloindolines has been developed *via* the consecutive cyclization of tryptamine with DMSO/Tf₂O and the substitution of 3a-pyrroloindolythionium intermediate with aniline.

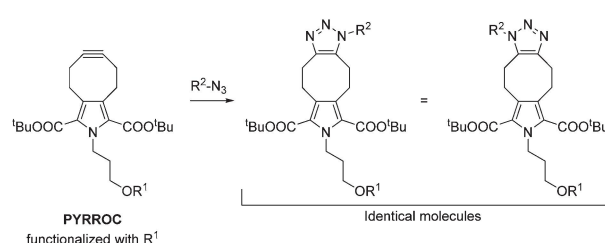


3866

PYRROC: the first functionalized cycloalkyne that facilitates isomer-free generation of organic molecules by SPAAC

Corinna Gröst and Thorsten Berg*

PYRROC is the first functionalized cycloalkyne which cannot form isomers in the strain-promoted cycloaddition with azides, and displays unprecedented rate accelerations and rate constants in aqueous buffer.

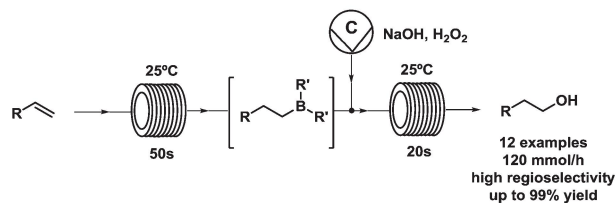


3871

Development of a flow method for the hydroboration/oxidation of olefins

José A. Souto,* Robert A. Stockman and Steven V. Ley

A method for the continuous preparation of alcohols by hydroboration/oxidation of olefins using flow techniques is described.

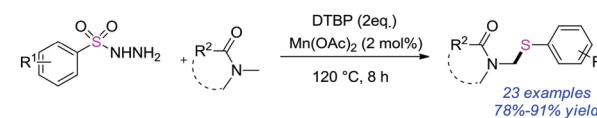


3878

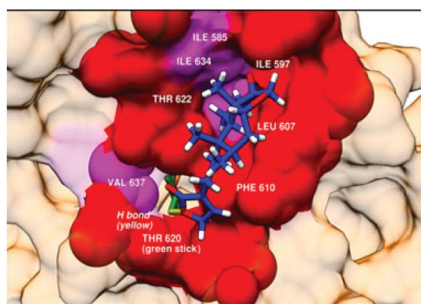
Manganese catalysed sulfenylation of N-methyl amides with arenesulfonyl hydrazides

Jinwei Sun, Yi Wang* and Yi Pan

A convenient oxidative sulfenylation method for the formation of various sulfonyl amides has been reported.



3882



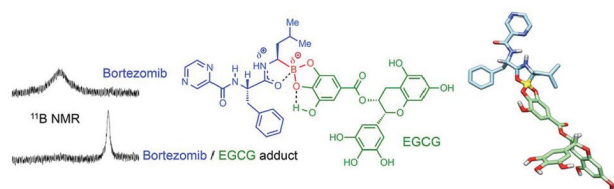
Crispene E, a *cis*-clerodane diterpene inhibits STAT3 dimerization in breast cancer cells

Julia Mantaj, S. M. Abdur Rahman,* Bishwajit Bokshi, Choudhury M. Hasan, Paul J. M. Jackson, Richard B. Parsons and Khondaker M. Rahman*

Crispene E inhibited STAT3 dimerization in a cell-free fluorescent polarization assay and was found to have significant toxicity against STAT3-dependent MDA-MB 231 breast cancer cell line and selectively inhibited the expression of STAT3 and STAT3 target genes.

PAPERS

3887



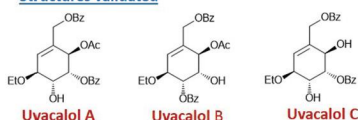
Molecular characterization of the boron adducts of the proteasome inhibitor bortezomib with epigallocatechin-3-gallate and related polyphenols

Stephen J. Glynn, Kevin J. Gaffney, Marcos A. Sainz, Stan G. Louie and Nicos A. Petasis*

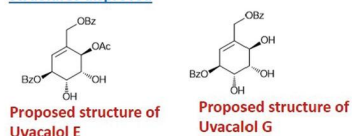
Green tea polyphenol EGCG antagonizes Bortezomib's anticancer activity through a stable intramolecular cyclic borate adduct involving the adjacent amide bond.

3900

Structures validated



Structures disproved

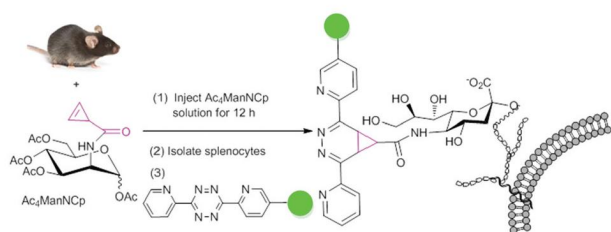


Total syntheses of five uvacalols: structural validation of uvacalol A, uvacalol B and uvacalol C and disproval of the structures of uvacalol E and uvacalol G

Adiyala Vidyasagar and Kana M. Sureshan*

The first total syntheses of five uvacalols have been achieved from chiral pool starting material D-mannitol. This study validates the structures of uvacalol A, B and C, it also disproves the structures of uvacalol E and G.

3911



Rapid probing of sialylated glycoproteins *in vitro* and *in vivo* via metabolic oligosaccharide engineering of a minimal cyclopropene reporter

De-Cai Xiong, Jingjing Zhu, Ming-Jie Han, Hui-Xin Luo, Cong Wang, Yang Yu, Yuqian Ye, Guihua Tai and Xin-Shan Ye*

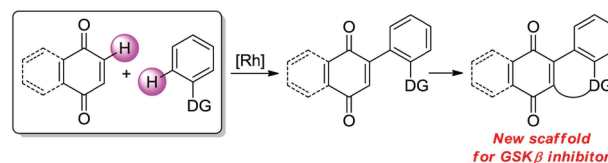
A minimal and efficient cyclopropene chemical handle was identified both *in vitro* and *in vivo*.

3918

Rh(III)-catalyzed direct C–H/C–H cross-coupling of quinones with arenes assisted by a directing group: identification of carbazole quinones as GSK β inhibitors

Youngtaek Moon, Yujeong Jeong, Daehyuk Kook and Sungwoo Hong*

Rh-catalyzed direct cross-coupling of various (hetero)-arenes with quinones is developed. This protocol is effective for a broad range of substrates and a wide range of directing groups.

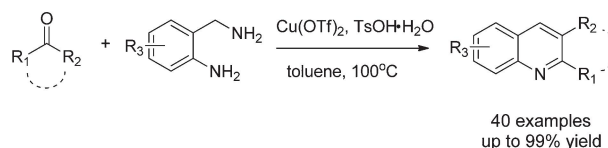


3924

An efficient synthesis of quinolines via copper-catalyzed C–N cleavage

Long-Yi Xi, Ruo-Yi Zhang, Lei Zhang, Shan-Yong Chen* and Xiao-Qi Yu*

An efficient method to synthesize substituted quinolines from ketones and 2-amino benzylamines is described.

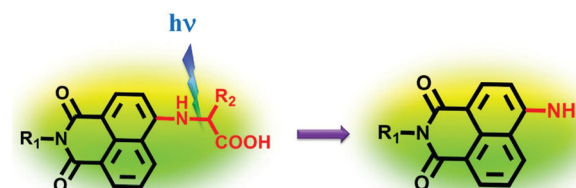


3931

Visible-light-induced cleavage of 4- α -amino acid substituted naphthalimides and its application in DNA photocleavage

Jin Zhou, Canliang Fang, Ying Liu, Yao Zhao, Nan Zhang, Xiangjun Liu, Fuyi Wang and Dihua Shangguan*

4- α -Amino acid substituted naphthalimides can be photocleaved at the C–N bond between the 4-amino and the amino acid residue under visible light irradiation, releasing a fluorophore, 4-aminonaphthalimide.

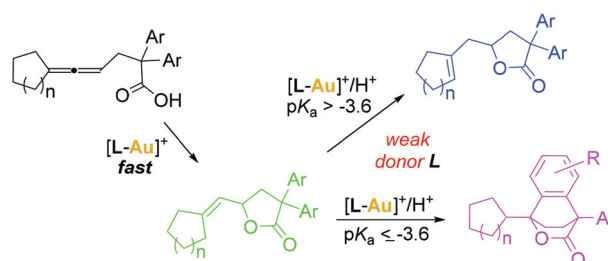


3936

Ligand- and Brønsted acid/base-switchable reaction pathways in gold(I)-catalyzed cycloisomerizations of allenic acids

Sachin Handa, Sri S. Subramaniam, Aaron A. Ruch, Joseph M. Tanski and LeGrande M. Slaughter*

Competing gold-catalyzed cycloisomerizations of γ -allenic acids are optimized through ligand and Brønsted acid/base effects, affording three distinct classes of lactones.



3950

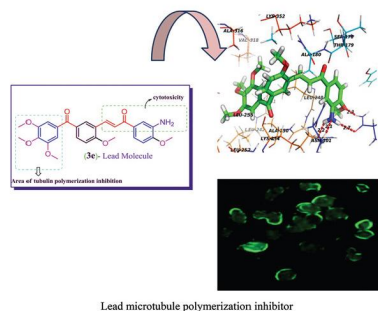


Sulfonate derived phosphoramidates as active intermediates in the enzymatic primer-extension of DNA

S. De, E. Groaz, L. Margamuljana, M. Abramov, P. Marlière and P. Herdewijn*

The incorporation and extension of synthetically unprecedented nucleoside phosphoramidate sulfonates is demonstrated using thermophilic and mesophilic microbial polymerases.

3963

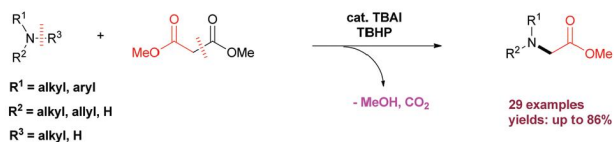


Synthesis of phenstatin/isocombretastatin–chalcone conjugates as potent tubulin polymerization inhibitors and mitochondrial apoptotic inducers

Ahmed Kamal,* G. Bharath Kumar, M. V. P. S. Vishnuvardhan, Anver Basha Shaik, Vangala Santhosh Reddy, Rasala Mahesh, Ibrahim Bin Sayeeda and Jeevak Sopanrao Kapure

A series of phenstatin/isocombretastatin–chalcones were synthesized and screened for their cytotoxic activity.

3982

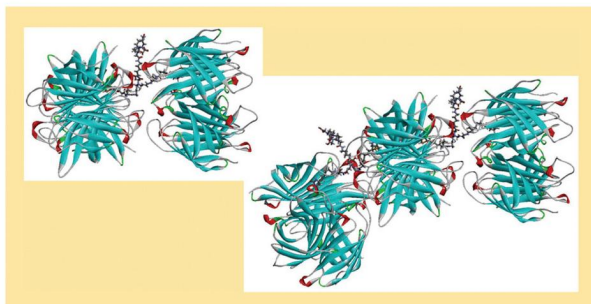


Transition-metal-free decarboxylation of dimethyl malonate: an efficient construction of α -amino acid esters using TBAI/TBHP

Jie Zhang, Ying Shao,* Yaxiong Wang, Huihuang Li, Dongmei Xu* and Xiaobing Wan*

A new strategy has been developed for the synthesis of α -amino acid esters *via* a tandem hydrolysis/ decarboxylation/nucleophilic substitution using TBAI/ TBHP.

3988



Design and solid phase synthesis of new DOTA conjugated (+)-biotin dimers planned to develop molecular weight-tuned avidin oligomers

Alessandro Pratesi, Mauro Ginanneschi, Fabrizio Melani, Marco Chinol, Angela Carollo, Giovanni Paganelli, Marco Lumini, Mattia Bartoli, Marco Frediani, Luca Rosi, Giorgio Petrucci, Luigi Messori and Anna Maria Papini*

Oligomeric architectures of avidin generated by a new class of bis-biotins.

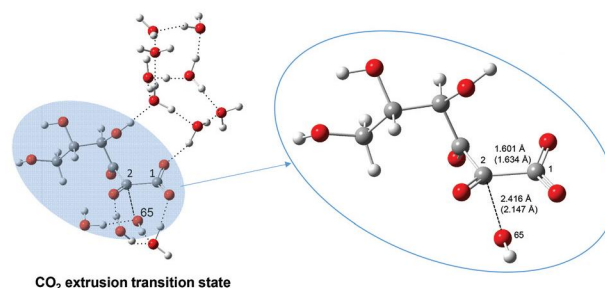
PAPERS

4002

Frontier orbitals and transition states in the oxidation and degradation of L-ascorbic acid: a DFT study

Shinichi Yamabe,* Noriko Tsuchida, Shoko Yamazaki and Shigeyoshi Sakaki

DFT calculations were carried out to investigate reaction paths of L-ascorbic acid, hydroxyl radicals and water clusters up to threonic, oxalic, xylonic and lyxonic acids.

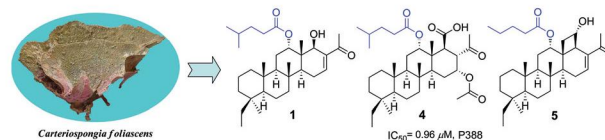


4016

Cytotoxic scalarane sesterterpenoids from the South China Sea sponge *Carteriospongia foliascens*

Fei Cao, Ze-Hong Wu, Chang-Lun Shao, Sen Pang, Xiao-Yan Liang, Nicole J. de Voogd and Chang-Yun Wang*

Cytotoxic scalarane sesterterpenoids from the sponge *Carteriospongia foliascens* collected from the South China Sea.

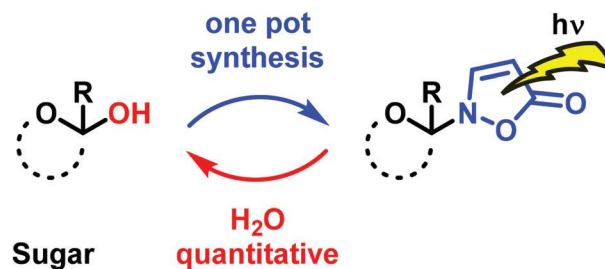


4025

Synthesis and photosensitivity of isoxazolin-5-one glycosides

Tobias Becker, Prashant Kartikeya, Christian Paetz, Stephan H. von Reuß and Wilhelm Boland*

An improved synthetic protocol is described, allowing the synthesis of novel and naturally occurring isoxazolin-5-one glycosides. The photohydrolysis efficiency and pH stability of the obtained isoxazolin-5-one glycosides was studied.

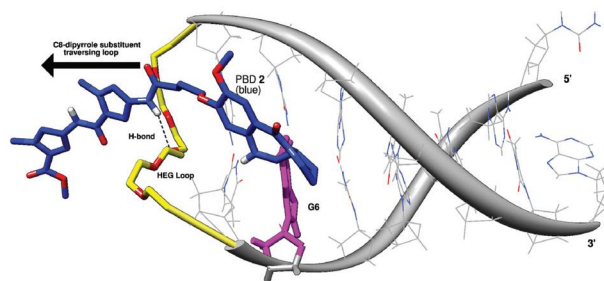


4031

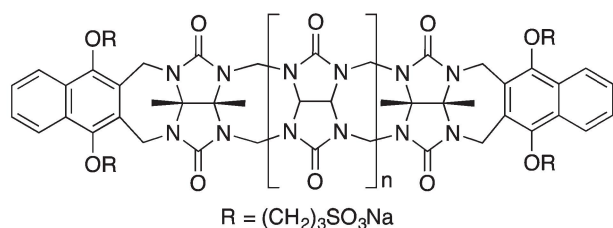
Effect of hairpin loop structure on reactivity, sequence preference and adduct orientation of a DNA-interactive pyrrolo[2,1-c][1,4]benzodiazepine (PBD) antitumour agent

David E. Thurston,* Higia Vassoler, Paul J. M. Jackson, Colin H. James and Khondaker M. Rahman*

Pyrrolobenzodiazepine (PBD) monomer GWL-78 reacts faster with DNA hairpins containing a hexaethylene glycol (HEG) loop compared to hairpins containing a TTT loop due to the greater structural flexibility of the HEG.



4041

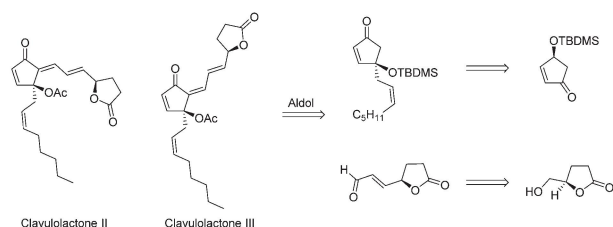


Acyclic cucurbit[n]uril-type molecular containers: influence of glycoluril oligomer length on their function as solubilizing agents

Laura Gilberg, Ben Zhang, Peter Y. Zavalij, Vladimir Sindelar* and Lyle Isaacs*

A series of glycoluril molecular clips and acyclic CB[n]-type receptors are tested as solubilizing agents for insoluble drugs.

4051

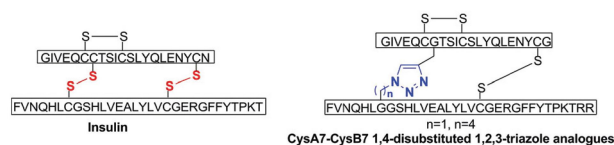


First total synthesis of the marine natural products clavulolactones II and III

Charlotte M. Miller, Tore Benneche* and Marcus A. Tius

The first total synthesis of the marine prostanoids clavulolactones II and III is presented from an easily accessible chiral, non-racemic cyclopentenone intermediate.

4059

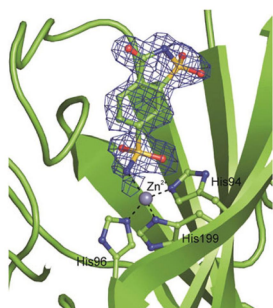


Replacement of the CysA7–CysB7 disulfide bond with a 1,2,3-triazole linker causes unfolding in insulin glargine

Geoffrey M. Williams, Kathryn Lee, Xun Li, Garth J. S. Cooper and Margaret A. Brimble*

Two analogues of insulin glargine containing a 1,4-disubstituted 1,2,3-triazole group in place of the CysA7–CysB7 disulfide bond were prepared using CuAAC click chemistry to efficiently join the peptide chains.

4064



X-ray crystallographic and kinetic investigations of 6-sulfamoyl-saccharin as a carbonic anhydrase inhibitor

V. Alterio, M. Tanc, J. Ivanova, R. Zalubovskis, I. Vozny, S. M. Monti, A. Di Fiore, G. De Simone and C. T. Supuran*

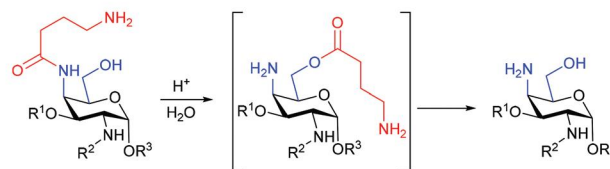
Sulfamoylated saccharin binds to human carbonic anhydrase II through the SO_2NH_2 and not CONHSO_2 moiety.

4070

Investigations into the decomposition of aminoacyl-substituted monosaccharide scaffolds from a drug discovery library

Q. Q. He, N. Wimmer, G. Verquin, W. Meutermans and V. Ferro*

Decomposition of aminoacyl-substituted D-galactoside scaffolds under acidic conditions is dependent on the length of the side chain and is accelerated by the presence of a free hydroxyl group at C-6. In the latter case, evidence is provided that the reaction occurs *via* an N- to O-acyl transfer.

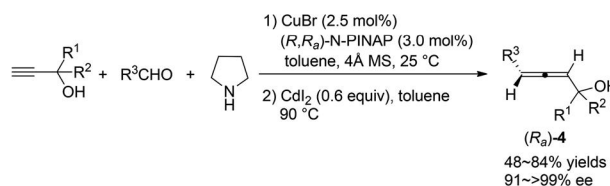


4080

Harmony of Cdl₂ with CuBr for the one-pot synthesis of optically active α-allenols

Jiasheng Zhang, Juntao Ye and Shengming Ma*

A highly efficient one-pot synthesis of chiral α-allenols from propargylic alcohols, aldehydes and pyrrolidine induced by CuBr and (*R,R*)-N-PINAP or (*R,S*)-N-PINAP and Cdl₂ has been developed.

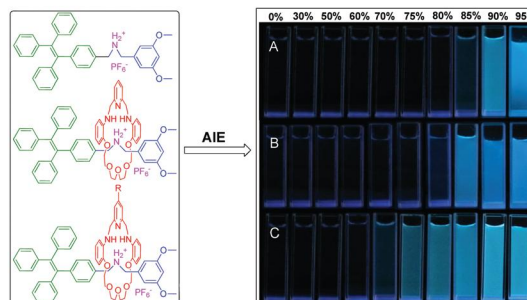


4090

Tetraphenylethene modified [n]rotaxanes: synthesis, characterization and aggregation-induced emission behavior

Guoxing Liu, Di Wu, Jinhua Liang, Xie Han, Sheng Hua Liu and Jun Yin*

A series of novel [n]rotaxanes based on a tetraphenylethene (TPE) backbone were constructed by a template-directed clipping approach and their structures were well-characterized.



4101

N-(1-Oxy-2-picolylo)oxalamic acids as a new type of O,O-ligands for the Cu-catalyzed N-arylation of azoles with aryl halides in water or organic solvent

Yongbin Wang, Yu Zhang, Beibei Yang, Ao Zhang* and Qizheng Yao*

A new type of chelators was identified as efficient ligands for promoting Cu-catalyzed N-arylation of azoles with applicability to different solvents.

