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PAPER

Huidong Yu, Yong Huang *et al.*

Directed arene/alkyne annulation reactions *via* aerobic copper catalysis

Organic & Biomolecular Chemistry

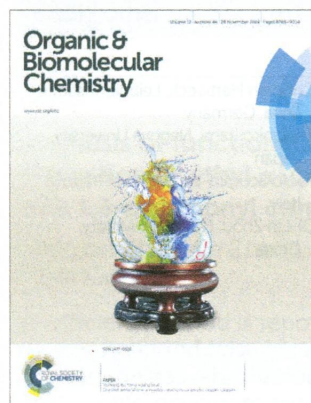
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Cover

See Huidong Yu,
Yong Huang *et al.*,
pp. 8844–8850.

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2014, **12**, 8844.

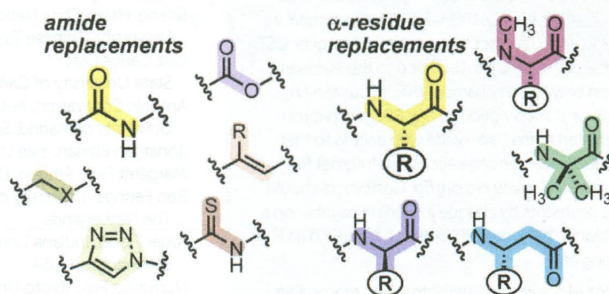
PERSPECTIVE

8796

Protein backbone engineering as a strategy to advance foldamers toward the frontier of protein-like tertiary structure

Zachary E. Reinert and W. Seth Horne*

This Perspective surveys work on protein backbone engineering and its recent application to design heterogeneous backbones that adopt complex tertiary folds.



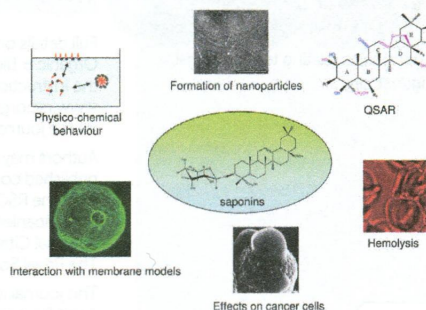
REVIEW

8803

The amphiphilic nature of saponins and their effects on artificial and biological membranes and potential consequences for red blood and cancer cells

Joseph H. Lorent,* Joëlle Quetin-Leclercq and Marie-Paule Mingeot-Leclercq

Saponins, amphiphiles of natural origin with numerous biological activities, are widely used in research, the cosmetic and pharmaceutical industry.

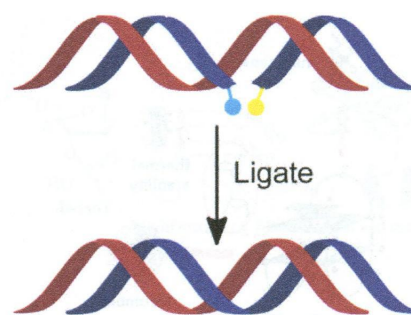


8823

Templated DNA ligation with thiol chemistry

Dadong Li, Xiaojian Wang, Fubo Shi, Ruojie Sha, Nadrian C. Seeman* and James W. Canary*

Templated DNA ligation reactions are useful in a variety of contexts and have drawn much attention recently. Herein we describe two different DNA-templated ligation systems based on thiols and thiol-mediated chemistry. One system follows the principle of native chemical ligation reaction, and the other utilizes a thiol-disulfide exchange reaction.

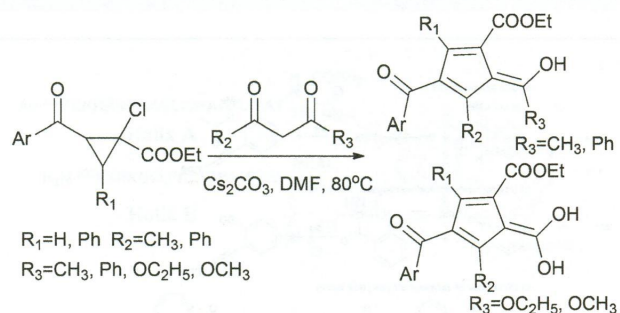


8828

Synthesis of functionalized fulvenes: [3 + 2] annulation of ethyl α -chlorocyclopropaneformates with 1,3-dicarbonyl compounds

Yuequan Zhu, Min Zhang, Hongling Yuan and Yuefa Gong*

An efficient method is reported to produce acidic multi-substituted fulvenes at high yields (up to 94%) through the base-promoted [3 + 2] annulation reaction of ethyl α -chlorocyclopropaneformates with 1,3-dicarbonyl compounds.

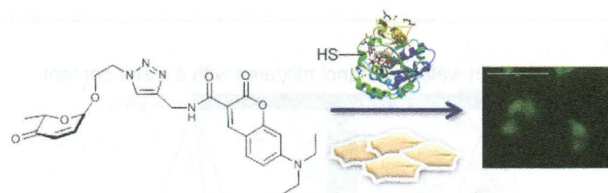


8832

Chemical and biological evaluation of unusual sugars, α -aculosides, as novel Michael acceptors

Hiromasa Ikeda, Erika Kaneko, Shunsuke Okuzawa, Daisuke Takahashi and Kazunobu Toshima*

Unusual sugars, α -aculosides, were found to be novel and selective Michael acceptors to a thiol function of cysteine residues of proteins in living cells.

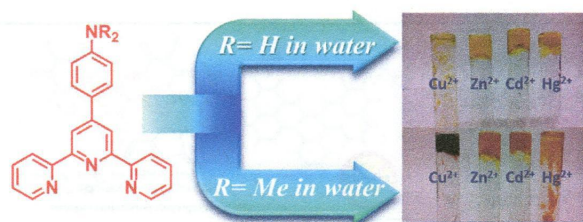


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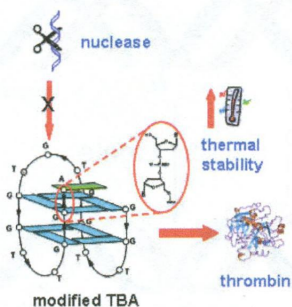
Transition metal ion induced hydrogelation by amino-terpyridine ligands

Sandip Bhowmik, Biswa Nath Ghosh and Kari Rissanen*

Hydrogelation behavior of a new class of terpyridine based metallogelators are explored. The gelation and the gel morphology was found to be critically dependent on divalent metal ions, anions and on subtle structural changes on the gelator molecule.



8840



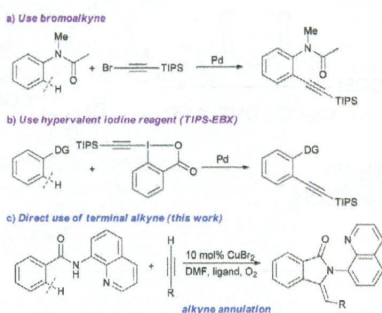
A straightforward modification in the thrombin binding aptamer improving the stability, affinity to thrombin and nuclease resistance

Veronica Esposito, Maria Scuotto, Antonella Capuozzo, Rita Santamaria, Michela Varra, Luciano Mayol, Antonella Virgilio* and Aldo Galeone*

Introduction of inversion of polarity sites at the 5'- and/or 3'-end in the thrombin binding aptamer is a simple modification able to improve, at the same time, thermal stability, affinity to thrombin and nuclease resistance.

PAPERS

8844



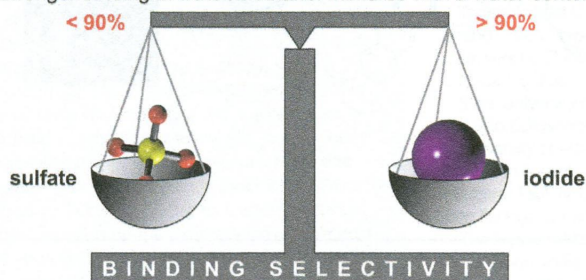
Directed arene/alkyne annulation reactions via aerobic copper catalysis

Yi Zhang, Qian Wang, Huidong Yu* and Yong Huang*

We describe a straightforward protocol for a smooth dehydrogenative annulation reaction between various arenes and terminal alkynes using a catalytic amount of CuBr_2 and molecular oxygen.

8851

stronger binding in water/methanol mixtures with a water content

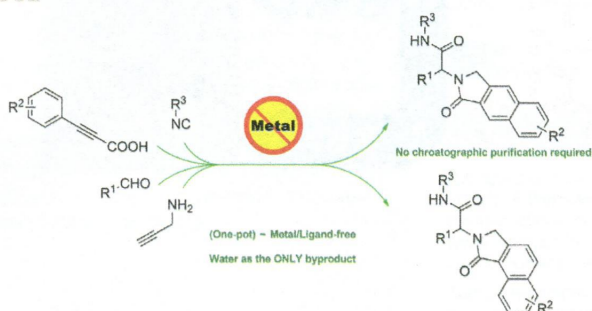


Anion binding of a neutral bis(cyclopeptide) in water–methanol mixtures containing up to 95% water

Fabian Sommer and Stefan Kubik*

Selectivity of a synthetic anion receptor reverses from strongly coordinating sulfate to weakly coordinating iodide anions upon increasing the water content of the solution.

8861



Solvent switchable cycloaddition: a (one-pot) metal-free approach towards *N*-substituted benzo[e]- or [f]isoindolones via C_{sp^2} -H functionalization

Pratik A. Ambasana, Dipak D. Vachhani,* Marzia Galli, Jeroen Jacobs, Luc Van Meervelt, Anamik K. Shah and Erik V. Van der Eycken*

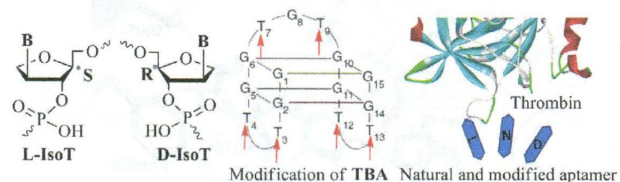
Solvent steers the selectivity: Green and practical C_{sp^2} -H functionalization towards *N*-substituted benzo[e]- or [f]isoindolones.

8866

Stability and bioactivity of thrombin binding aptamers modified with D-/L-isothymidine in the loop regions

Baobin Cai, Xiantao Yang, Lidan Sun, Xinmeng Fan, Liyu Li, Hongwei Jin, Yun Wu, Zhu Guan, Liangren Zhang, Lihe Zhang and Zhenjun Yang*

D-/L-IsoT were used to modify the loop regions of TBA and greatly improved its bioactivity as well as stability.

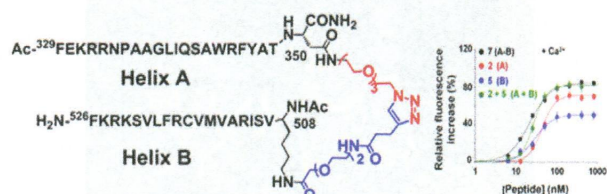


8877

Clicked bis-PEG-peptide conjugates for studying calmodulin-Kv7.2 channel binding

M. Angeles Bonache, Alessandro Alaimo, Covadonga Malo, Oscar Millet, Alvaro Villaruel and Rosario González-Muñiz*

Small bis-conjugates helix A³²⁹⁻³⁵⁰-PEG-triazole-PEG-helix B⁵⁰⁸⁻⁵²⁶ (41 residues), prepared through click chemistry of PEGylated peptide derivatives, bind to CaM with nanomolar affinity, behaving as mimics of the Kv7.2 native fragment (239 residues).

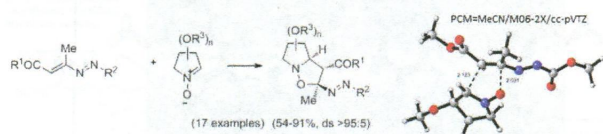


8888

Highly diastereoselective 1,3-dipolar cycloadditions of chiral non-racemic nitrones to 1,2-diaza-1,3-dienes: an experimental and computational investigation

Roberta Majer, Olga Konechnaya, Ignacio Delso, Tomas Tejero, Orazio A. Attanasi,* Stefania Santeusano and Pedro Merino*

Asymmetric 1,3-dipolar cycloadditions between 1,2-diaza-1,3-dienes and chiral non-racemic nitrones to give 3-substituted-5-diazenyl isoxazolidines were studied.

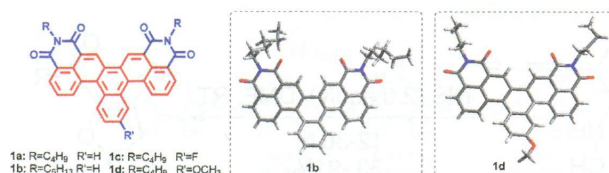


8902

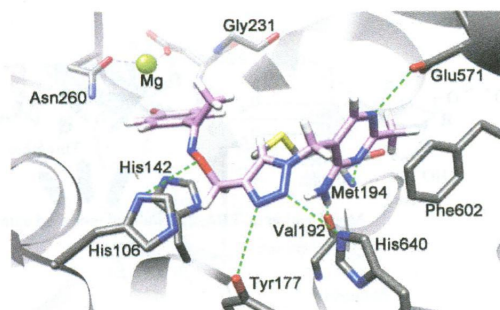
Imides modified benzopicenenes: synthesis, solid structure and optoelectronic properties

Di Wu, Haojie Ge, Zhao Chen, Jinhua Liang, Jie Huang, Yufeng Zhang, Xiaoqiang Chen, Xianggao Meng, Sheng Hua Liu* and Jun Yin*

Imide-modified polycyclic aromatic hydrocarbons can be widely applied in the field of optoelectronic materials.



8911

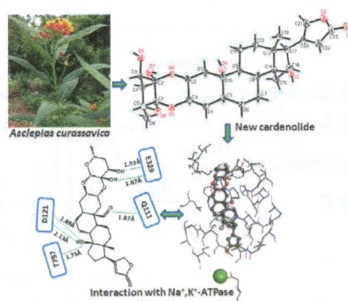


The design, synthesis and biological evaluation of novel thiamin diphosphate analog inhibitors against the pyruvate dehydrogenase multienzyme complex E1 from *Escherichia coli*

Lingling Feng, Junbo He, Haifeng He, Lulu Zhao, Lingfu Deng, Li Zhang, Lin Zhang, Yanliang Ren, Jian Wan* and Hongwu He*

Optimal binding mode for the novel potent inhibitor **4j** against PDHc-E1 from *E. coli*.

8919

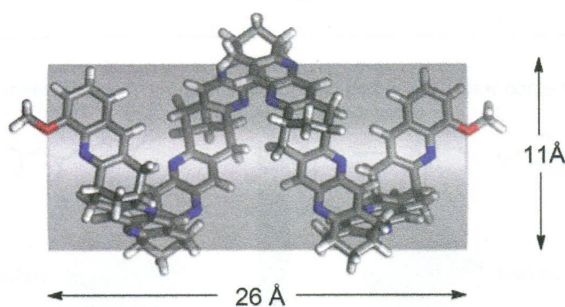


Structures, chemotaxonomic significance, cytotoxic and Na⁺,K⁺-ATPase inhibitory activities of new cardenolides from *Asclepias curassavica*

Rong-Rong Zhang, Hai-Yan Tian, Ya-Fang Tan, Tse-Yu Chung, Xiao-Hui Sun, Xue Xia, Wen-Cai Ye, David A. Middleton, Natalya Fedosova, Mikael Esmann,* Jason T. C. Tzen* and Ren-Wang Jiang*

New cardenolides with potent cytotoxic and Na⁺,K⁺-ATPase inhibitory activities were isolated from the ornamental milkweed *Asclepias curassavica*.

8930

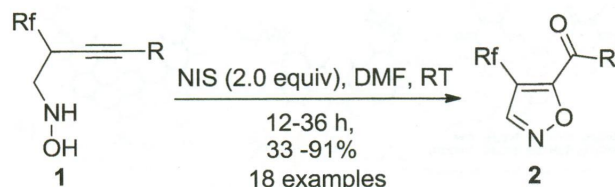


A short designed semi-aromatic organic nanotube – synthesis, chiroptical characterization, and host properties

Torbjörn Wixe, Niels Johan Christensen, Sven Lidin, Peter Fristrup and Kenneth Wärnmark*

A short helical nanotube having its aromatic system perpendicular to its axis of propagation was synthesized and its properties were studied.

8942



NIS-mediated oxidative cyclization of *N*-(2-trifluoromethyl-3-alkynyl) hydroxylamines: a facile access to 4-trifluoromethyl-5-acylisoxazoles

Li Zhang, Qin Zeng, Ao Mao, Ziang Wu, Tian Luo, Yuanjing Xiao* and Junliang Zhang*

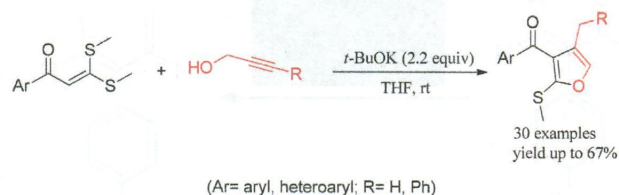
A NIS mediated sequential procedure involving oxidation and electrophilic cycloisomerization of *N*-(2-trifluoromethyl-3-alkynyl) hydroxylamines for 4-trifluoromethyl-5-acylisoxazole synthesis is developed.

8947

A convenient base-mediated synthesis of 3-aryl-4-methyl (or benzyl)-2-methylthio furans from α -oxo ketene dithioacetals and propargyl alcohols via domino coupling/annulations

Xiaobing Yang, Fangzhong Hu,* Hongjing Di, Xinxin Cheng, Dan Li, Xiaoli Kan, Xiaomao Zou and Qichun Zhang*

A convenient base-mediated synthesis of 3-aryl-4-methyl (or benzyl)-2-methylthio furans **2** has been developed through the domino coupling/annulations from α -oxo ketene dithioacetals **1** and propargyl alcohols.

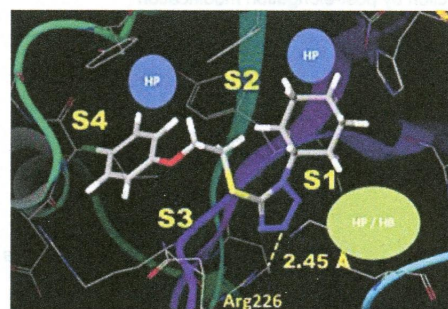


8952

Approaches to design non-covalent inhibitors for human granzyme B (hGrB)

Mi-Sun Kim, Lauriane A. Buisson, Dean A. Heathcote, Haipeng Hu, D. Christopher Braddock, Anthony G. M. Barrett, Philip G. Ashton-Rickardt and James P. Snyder*

A structure-based design campaign for non-covalent small molecule inhibitors of hGrB was carried out by virtual screening employing three constraints and probe site-mapping with FTMAP to identify ligand "hot spots".

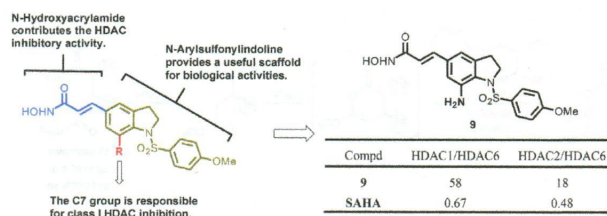


8966

Effect of C7-substitution of 1-arylsulfonyl-5-(N-hydroxyacrylamide)indolines on the selectivity towards a subclass of histone deacetylases

Hsueh-Yun Lee, Li-Ting Wang, Yu-Hsuan Li, Shioh-Lin Pan, Yi-Lin Chen, Che-Ming Teng and Jing-Ping Liou*

This study focused on the substitution effect at position C7 of 1-arylsulfonyl-5-(N-hydroxyacrylamide)indolines.

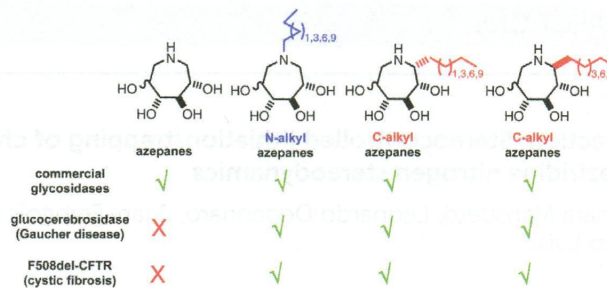


8977

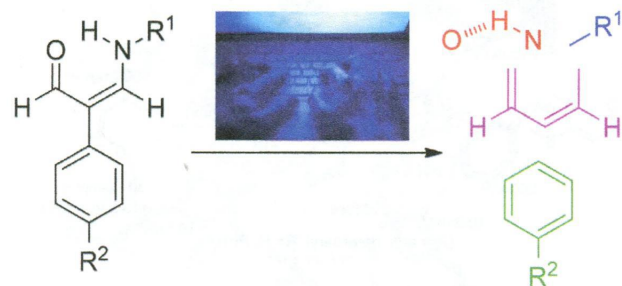
N- and C-alkylation of seven-membered iminosugars generates potent glucocerebrosidase inhibitors and F508del-CFTR correctors

J. Désiré,* M. Mondon, N. Fontelle, S. Nakagawa, Y. Hirokami, I. Adachi, R. Iwaki, G. W. J. Fleet, D. S. Alonzi, G. Twigg, T. D. Butters, J. Bertrand, V. Cendret, F. Becq, C. Norez, J. Marrot, A. Kato* and Y. Blériot*

The synthesis and biological evaluation of a library of novel seven-membered iminosugars is reported.



8997

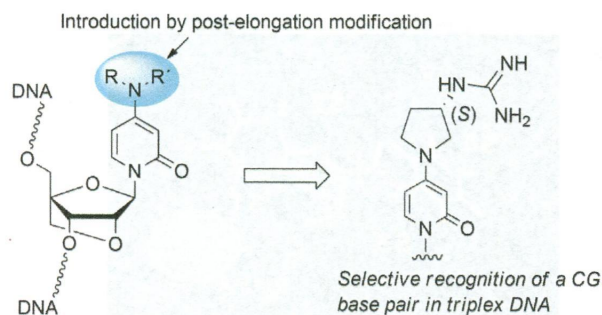


Pseudo-cyclic structures of mono- and di-azaderivatives of malondialdehydes. Synthesis and conformational disentangling by computational analyses

María P. Romero-Fernández,* Martín Ávalos, Reyes Babiano, Pedro Cintas,* José L. Jiménez, Mark E. Light and Juan C. Palacios

Aminoacroleins and vinamidines are structures featuring H-bonding and complex conformational and tautomeric equilibria, which have been dissected by computation.

9011

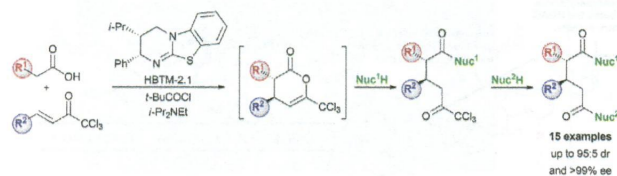


Synthesis of oligonucleotides containing *N,N*-disubstituted 3-deazacytosine nucleobases by post-elongation modification and their triplex-forming ability with double-stranded DNA

Masaaki Akabane-Nakata, Satoshi Obika* and Yoshiyuki Hari*

A post-elongation modification for construction of *N,N*-disubstituted 3-deazacytosines was developed, and a 2'-*O*,4'-*C*-methylene-bridged 3-deazacytidine analog was found for recognition of a CG base pair in triplex DNA.

9016



Organocatalytic Michael addition–lactonisation of carboxylic acids using α,β -unsaturated trichloromethyl ketones as α,β -unsaturated ester equivalents

L. C. Morrill, D. G. Stark, J. E. Taylor, S. R. Smith, J. A. Squires, A. C. A. D'Hollander, C. Simal, P. Shapland, T. J. C. O'Riordan and A. D. Smith*

Isothiourea HBTM-2.1 catalyses the Michael addition–lactonisation of 2-aryl and 2-alkenylacetic acids and α,β -unsaturated trichloromethyl ketones.

CORRECTIONS

9028

Correction: Stereocontrolled lithiation/trapping of chiral 2-alkylideneaziridines: investigation into the role of the aziridine nitrogen stereodynamics

Rosmara Mansueto, Leonardo Degennaro, Jean-François Brière, Karen Griffin, Michael Shipman, Saverio Florio and Renzo Luisi*

Correction: Non-isoprenoid polyene natural products – structures and synthetic strategies

Katrina S. Madden, Fathia A. Mosa and Andrew Whiting*