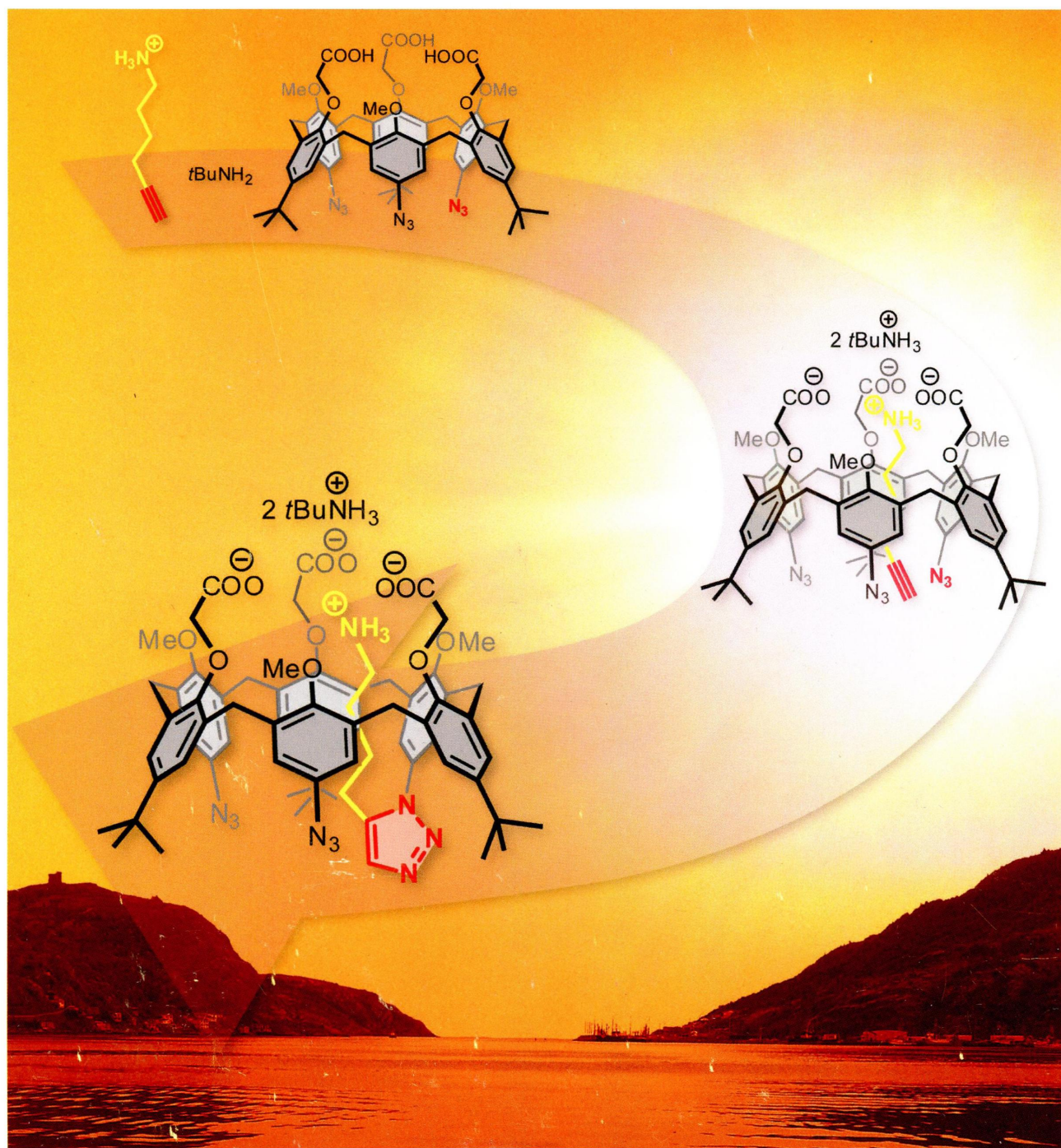


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# JOC

The Journal of Organic Chemistry

MARCH 7, 2014 VOLUME 79, NUMBER 5 [pubs.acs.org/joc](http://pubs.acs.org/joc)



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**ON THE COVER:** Illustrated is the selective monofunctionalization of a calix[6]arene through an intramolecular thermal Huisgen reaction with a guest accommodated into the cavity. This supramolecular approach can be used as a general tool for the selective functionalization of molecular receptors. The background image is the bay of St. John's (Newfoundland and Labrador) where the 12th International Conference on Calixarenes (Calix 2013) was held. See Jabin and co-workers, p 1913.

## Featured Articles

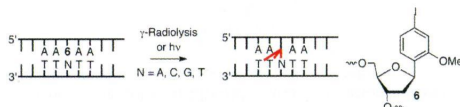
1877

5

[dx.doi.org/10.1021/jo4028227](http://dx.doi.org/10.1021/jo4028227)

**DNA Interstrand Cross-Linking upon Irradiation of Aryl Halide C-Nucleotides**

Dianjie Hou and Marc M. Greenberg\*



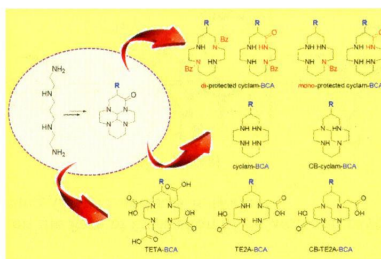
1885

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[dx.doi.org/10.1021/jo4028566](http://dx.doi.org/10.1021/jo4028566)

**Full Control of the Regiospecific *N*-Functionalization of *C*-Functionalized Cyclam Bisaminal Derivatives and Application to the Synthesis of their TETA, TE2A, and CB-TE2A Analogues**

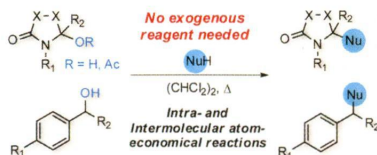
Nathalie Camus, Zakaria Halime, Nathalie Le Bris, H el ene Bernard, Carlos Platas-Iglesias, and Rapha el Tripier\*



1900 **5**

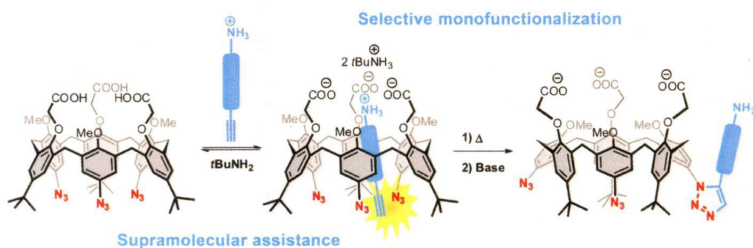
dx.doi.org/10.1021/jo4015886

**Intra- and Intermolecular Alkylation of *N,O*-Acetals and  $\pi$ -Activated Alcohols Catalyzed by in Situ Generated Acid**  
 Mélanie Hamon, Niall Dickinson, Alice Devineau, David Bolién, Marie-José Tranchant, Catherine Taillier, Ivan Jabin, David C. Harrowven, Richard J. Whitby, A. Ganesan, and Vincent Dalla\*

1913 **5**

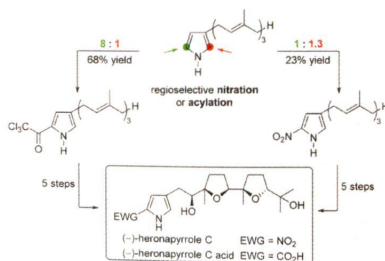
dx.doi.org/10.1021/jo402080d

**Supramolecular Assistance for the Selective Monofunctionalization of a Calix[6]arene Tris-carboxylic Acid-Based Receptor**  
 Alex Inthasot, Minh-Dung Dang Thy, Manuel Lejeune, Luca Fusaro, Olivia Reinaud, Michel Luhmer,\* Benoit Colasson,\* and Ivan Jabin\*

1920 **5**

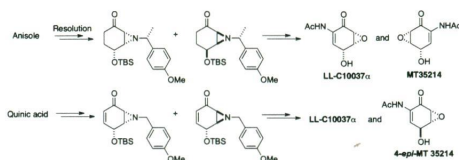
dx.doi.org/10.1021/jo402240g

**Synthetic Endeavors toward 2-Nitro-4-Alkylpyrroles in the Context of the Total Synthesis of Heronapyrrole C and Preparation of a Carboxylate Natural Product Analogue**  
 Jens Schmidt and Christian B. W. Stark\*

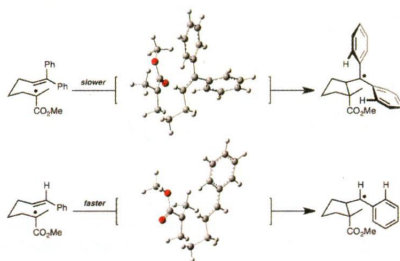


Use of Aziridines for the Stereocontrolled Synthesis of (–)-LL-C10037 $\alpha$ , (+)-MT35214, and (+)-4-epi-MT35214

Christopher D. Maycock,\* Paula Rodrigues, and M. Rita Ventura

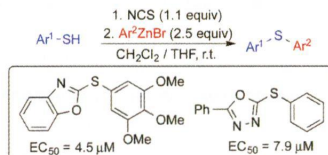
Effect of Double-Bond Substituents on the Rate of Cyclization of  $\alpha$ -Carbomethoxyhex-5-enyl Radicals

Arthur Han, Tudor Spataru, John Hartung, Gang Li, and Jack R. Norton\*



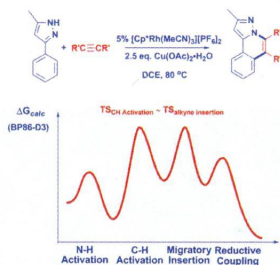
## Diaryl and Heteroaryl Sulfides: Synthesis via Sulfenyl Chlorides and Evaluation as Selective Anti-Breast-Cancer Agents

Ivelina M. Yonova, Charlotte A. Osborne, Naomi S. Morrisette, and Elizabeth R. Jarvo\*



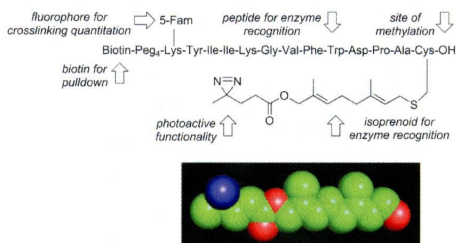
### Combined Experimental and Computational Investigations of Rhodium- and Ruthenium-Catalyzed C–H Functionalization of Pyrazoles with Alkynes

Andrés G. Algarra, Warren B. Cross,\* David L. Davies,\* Qudsia Khamker, Stuart A. Macgregor,\* Claire L. McMullin, and Kuldip Singh



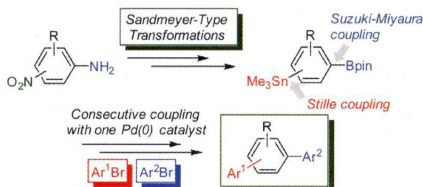
### Diazirine-Containing Photoactivatable Isoprenoid: Synthesis and Application in Studies with Isoprenylcysteine Carboxyl Methyltransferase

Jeffrey S. Vervacke, Amy L. Funk, Yen-Chih Wang, Mark Strom, Christine A. Hrycyna,\* and Mark D. Distefano\*



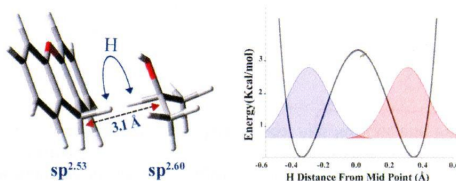
### Synthesis of Trimethylstannyl Arylboronate Compounds by Sandmeyer-Type Transformations and Their Applications in Chemoselective Cross-Coupling Reactions

Di Qiu, Shuai Wang, Shengbo Tang, He Meng, Liang Jin, Fanyang Mo, Yan Zhang, and Jianbo Wang\*



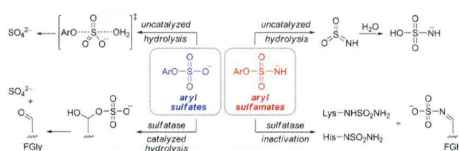
### Computational Replication of the Abnormal Secondary Kinetic Isotope Effects in a Hydride Transfer Reaction in Solution with a Motion Assisted H-Tunneling Model

Sadra Kashefolgheta, Mortezaali Razzaghi, Blake Hammann, James Eilers, Daniel Roston, and Yun Lu\*



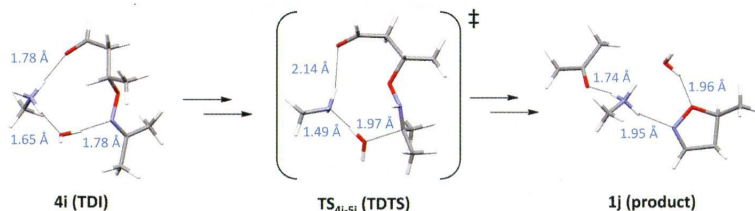
### Experimental and Theoretical Insights into the Mechanisms of Sulfate and Sulfamate Ester Hydrolysis and the End Products of Type I Sulfatase Inactivation by Aryl Sulfamates

Spencer J. Williams,\* Emma Denehy, and Elizabeth H. Krenske\*



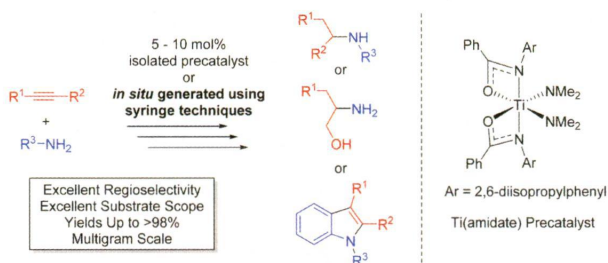
### Reaction Mechanism of an Intramolecular Oxime Transfer Reaction: A Computational Study

Jani Moilanen,\* Antti Neuvonen, and Petri Pihko\*

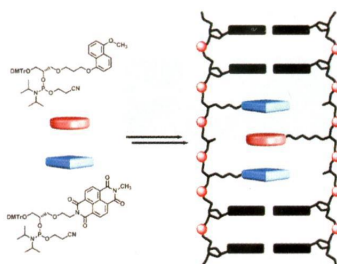


**Bis(amidate)bis(amido) Titanium Complex: A Regioselective Intermolecular Alkyne Hydroamination Catalyst**

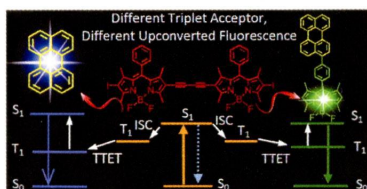
Jacky C.-H. Yim, Jason A. Bexrud, Rashidat O. Ayinla, David C. Leitch, and Laurel L. Schafer\*

**NDI and DAN DNA: Nucleic Acid-Directed Assembly of NDI and DAN**

Brian A. Ikkanda, Stevan A. Samuel, and Brent L. Iverson\*

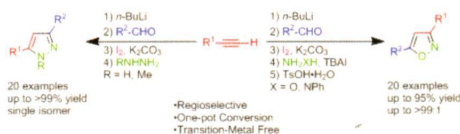
**Perylene-Derived Triplet Acceptors with Optimized Excited State Energy Levels for Triplet–Triplet Annihilation Assisted Upconversion**

Xiaoneng Cui, Azzam Charaf-Eddin, Junsu Wang, Boris Le Guennic, Jianzhang Zhao,\* and Denis Jacquemin\*



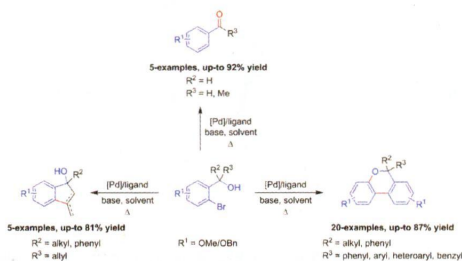
### Preparation of 3,5-Disubstituted Pyrazoles and Isoxazoles from Terminal Alkynes, Aldehydes, Hydrazines, and Hydroxylamine

Ryo Harigae, Katsuhiko Moriyama, and Hideo Togo\*



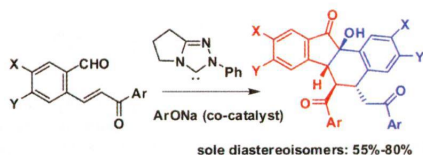
### Substitution Controlled Functionalization of *ortho*-Bromobenzyl Alcohols via Palladium Catalysis: Synthesis of Chromenes and Indenols

Lodi Mahendar and Gedu Satyanarayana\*



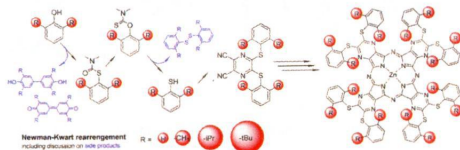
### Changing the Reaction Pathway by NHC/Bronsted Base Cooperative Catalysis: Highly Stereoselective Synthesis of Multifunctional Benzo[*a*]fluoren-11-ones from the Dimerization of 2-(ArOylvinyl)arylaldehydes

Yuan-feng Tong, Jian-hui Mao, Song Wu, Yuan Zhao, and Ying Cheng\*



### Role of Steric Hindrance in the Newman-Kwart Rearrangement and in the Synthesis and Photophysical Properties of Arylsulfanyl Tetrapyrroloporphyrazines

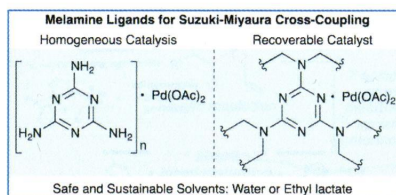
Veronika Novakova,\* Miroslav Miletin, Tereza Filandrová, Juraj Lenčo, Aleš Růžička, and Petr Zimčík\*





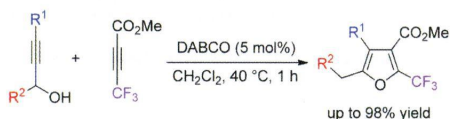
### Melamine and Melamine-Formaldehyde Polymers as Ligands for Palladium and Application to Suzuki–Miyaura Cross-Coupling Reactions in Sustainable Solvents

Grant A. Edwards, Mitchell A. Trafford, Alaina E. Hamilton, Audrey M. Buxton, Matthew C. Bardeaux, and Justin M. Chalker\*



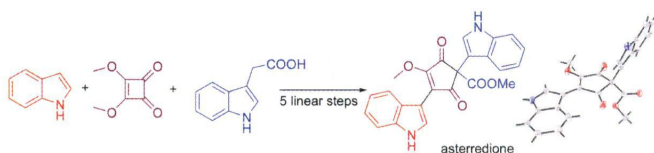
### DABCO-Catalyzed Synthesis of Trifluoromethylated Furans from Propargyl Alcohols and Methyl 2-Perfluoroalkynoate

Qinglei Chong, Xiaoyi Xin, Chunxiang Wang, Fan Wu, Haolong Wang, Ji-cheng Shi,\* and Boshun Wan\*



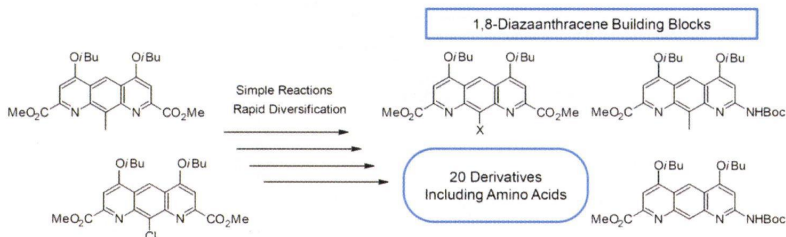
### Total Synthesis of Asterredione

Sinan Gai, Qing Zhang, and Xiangdong Hu\*



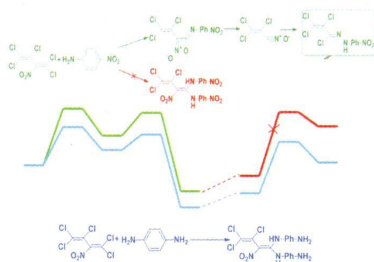
### Synthesis of 1,8-Diazaanthracenes as Building Blocks for Internally Functionalized Aromatic Oligoamide Foldamers

Michael L. Singleton, Nicola Castellucci, Stéphane Massip, Brice Kauffmann, Yann Ferrand, and Ivan Huc\*



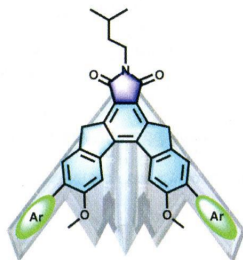
### Mechanisms of the Reaction between Polyhalogenated Nitrobutadienes and Electron-Deficient Anilines: Computational Modeling

Ozlem Sari, Safiye Sağ Erdem,\* and Dieter E. Kaufmann



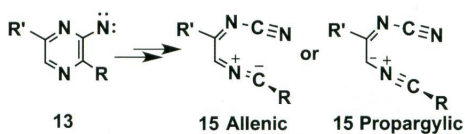
### Dihydroindeno[2,1-c]fluorene-Based Imide Dyes: Synthesis, Structures, Photophysical and Electrochemical Properties

Yang-Yang Li, Hai-Yan Lu,\* Meng Li, Xiao-Jun Li, and Chuan-Feng Chen\*



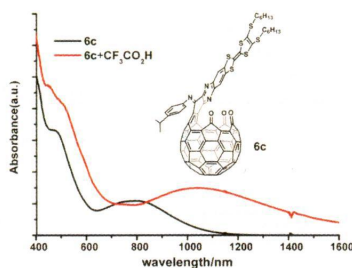
### Nitrile Ylides: Allenic and Propargylic Structures from Pyrazinylnitrenes. Experimental and Theoretical Characterization

Didier Bégué,\* Chris Addicott, Riko Burgard, Pawel Bednarek, Emilie Guille, Isabelle Baraille, and Curt Wentrup\*

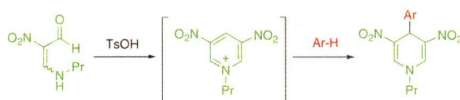


Near-Infrared Absorbing Compounds Based on  $\pi$ -Extended Tetrathiafulvalene Open-Cage Fullerenes

Yuming Yu, Liang Xu, Xincheng Huang, and Liangbing Gan\*

Synthesis of 4-Substituted 3,5-Dinitro-1,4-dihydropyridines by the Self-Condensation of  $\beta$ -Formyl- $\beta$ -nitroenamine

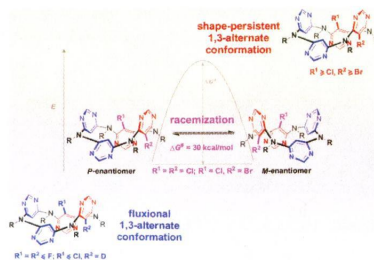
Yumi Nakaïke, Nagatoshi Nishiwaki,\* Masahiro Ariga, and Yoshito Tobe\*

Ruthenium-Catalyzed Oxidation of Allyl Alcohols with Intermolecular Hydrogen Transfer: Synthesis of  $\alpha,\beta$ -Unsaturated Carbonyl Compounds

Kai Ren, Bei Hu, Mengmeng Zhao, Yahui Tu, Xiaomin Xie, and Zhaoguo Zhang\*

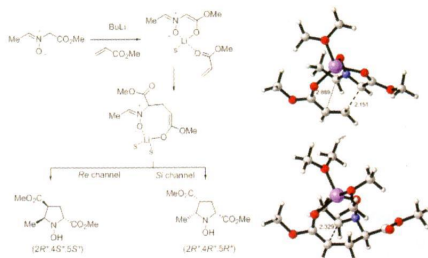
## Synthesis, Resolution, Structure, and Racemization of Inherently Chiral 1,3-Alternate Azacalix[4]pyrimidines: Quantification of Conformation Mobility

Jiang-Tao Li, Li-Xia Wang, De-Xian Wang, Liang Zhao, and Mei-Xiang Wang\*



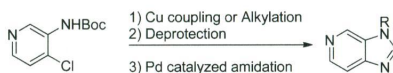
### Theoretical Elucidation of the Mechanism of the Cycloaddition between Nitron Ylides and Electron-Deficient Alkenes

P. Merino,\* T. Tejero, and A. Díez-Martínez



### Copper- and Palladium-Catalyzed Amidation Reactions for the Synthesis of Substituted Imidazo[4,5-c]pyridines

Robert J. Wilson, Adam J. Rosenberg, Lauren Kaminsky, and Daniel A. Clark\*



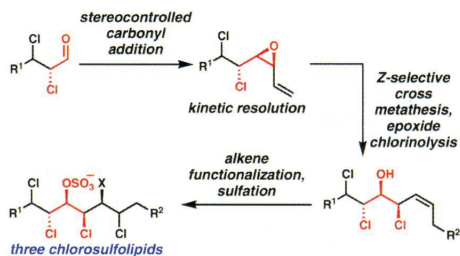
### Synthesis of Pyrrolidine-Fused 1,3-Dithiolane Oligomers by the Cycloaddition of Polycyclic Dithiolethiones to Maleimides and Evaluation as Mercury(II) Indicators

Pedro Fuertes, María García-Valverde, José V. Cuevas, Borja Díaz de Greñu, Teresa Rodríguez, Josefa Rojo, and Tomás Torroba\*



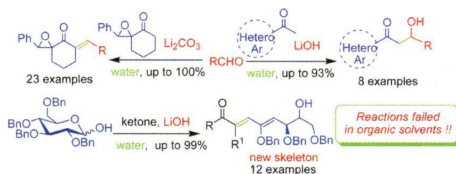
### General Approach to the Synthesis of the Chlorosulfolipids Danicalipin A, Mytilipin A, and Malhamensilipin A in Enantioenriched Form

Won-jin Chung, Joseph S. Carlson, and Christopher D. Vanderwal\*



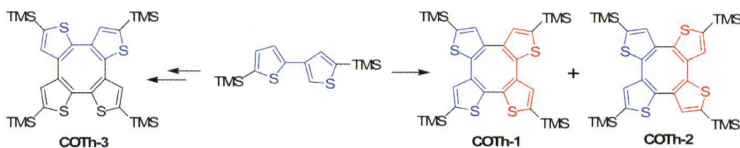
### Neighboring Heteroatom Effect Unique to Aqueous Aldol Reactions of Water-Insoluble Substrates

Bo Li and Chunbao Li\*



### Synthesis and Characterization of Cyclooctatetriaphenes with Different Connection Sequences

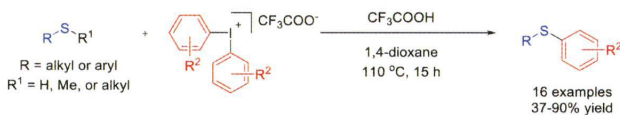
Yong Wang, Jinsheng Song,\* Li Xu, Yuhe Kan,\* Jianwu Shi, and Hua Wang\*



## Notes

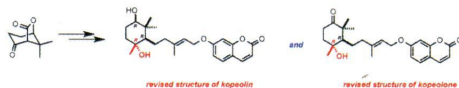
### Transition-Metal-Free Acid-Mediated Synthesis of Aryl Sulfides from Thiols and Thioethers

Anna M. Wagner and Melanie S. Sanford\*



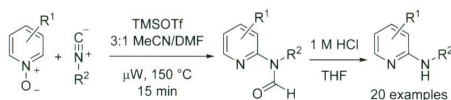
### Revised Structure, Total Synthesis, and Absolute Configuration of Kopeolin and Kopeolone

Stéphanie Miquet, Paul Brémond,\* Benjamin Ayela, Sylvain R. A. Marque, and Gérard Audran\*



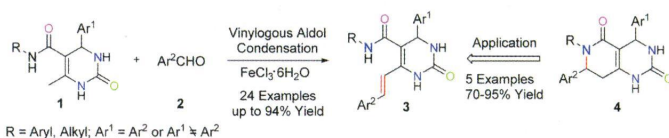
### 2-Aminopyridines via Reaction of Pyridine *N*-Oxides and Activated Isocyanides

Mitchell Vamos and Nicholas D. P. Cosford\*



### Iron-Catalyzed Vinylous Aldol Condensation of Biginelli Products and Its Application toward Pyrido[4,3-*d*]pyrimidinones

Lianqiang Zhang, Zhiguo Zhang,\* Qingfeng Liu, Tongxin Liu, and Guisheng Zhang\*



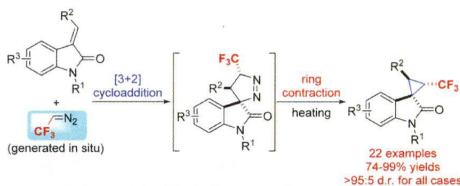
### Prins Cascade Cyclization for the Synthesis of 1,9-Dioxo-4-azaspiro[5.5]undecane Derivatives

B. V. Subba Reddy,\* Durgaprasad Medaboina, B. Sridhar, and Kiran Kumar Singarapu



### Synthesis of CF<sub>3</sub>-Containing 3,3'-Cyclopropyl Spirooxindoles by Sequential [3 + 2] Cycloaddition/Ring Contraction of Ylideneoxindoles with 2,2,2-Trifluorodiazaoethane

Tian-Ren Li, Shu-Wen Duan, Wei Ding, Yi-Yin Liu, Jia-Rong Chen, Liang-Qiu Lu,\* and Wen-Jing Xiao\*

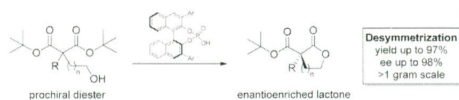


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## Enantioselective Desymmetrization of Diesters

Jennifer Wilent and Kimberly S. Petersen\*

dx.doi.org/10.1021/jo402853v

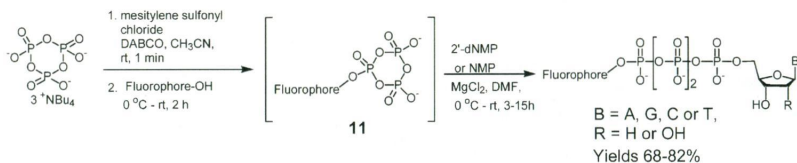


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## Synthesis of Nucleoside 5'-Tetraphosphates Containing Terminal Fluorescent Labels via Activated Cyclic Trimetaphosphate

Samy Mohamady and Scott D. Taylor\*

dx.doi.org/10.1021/jo500051y

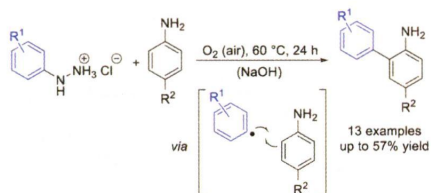


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## Oxidative Radical Arylation of Anilines with Arylhydrazines and Dioxygen from Air

Josefa Hofmann, Hannelore Jasch, and Markus R. Heinrich\*

dx.doi.org/10.1021/jo500063r

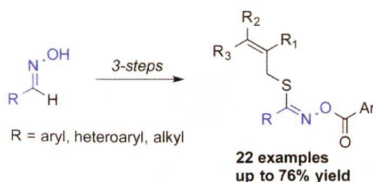


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## Synthesis of Thiohydroxamic Acids and Thiohydroxamic Acid Derivatives

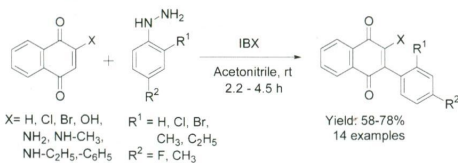
Bérénice C. Lemerrier and Joshua G. Pierce\*

dx.doi.org/10.1021/jo500080x



### Aryl-Free Radical-Mediated Oxidative Arylation of Naphthoquinones Using *o*-Iodoxybenzoic Acid and Phenylhydrazines and Its Application toward the Synthesis of Benzocarbazoledione

Pravin Patil, Abhay Nimonkar, and Krishnacharya G. Akamanchi\*



## Additions and Corrections

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dx.doi.org/10.1021/jo500315m

### Correction to Synthesis and Characterization of Glycoconjugated Porphyrin Triphenylamine Hybrids for Targeted Two-Photon Photodynamic Therapy

Fabien Hammerer, Guillaume Garcia, Su Chen, Florent Poyer, Sylvain Achelle, Céline Fiorini-Debuisschert, Marie-Paule Teulade-Fichou, and Philippe Maillard\*

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dx.doi.org/10.1021/jo500386r

### Correction to Gold(I)-Catalyzed Regioselective Inter-/Intramolecular Addition Cascade of Di- and Triynes for Direct Construction of Substituted Naphthalenes

Saori Naoe, Yamato Suzuki, Kimio Hirano, Yusuke Inaba, Shinya Oishi, Nobutaka Fujii,\* and Hiroaki Ohno\*