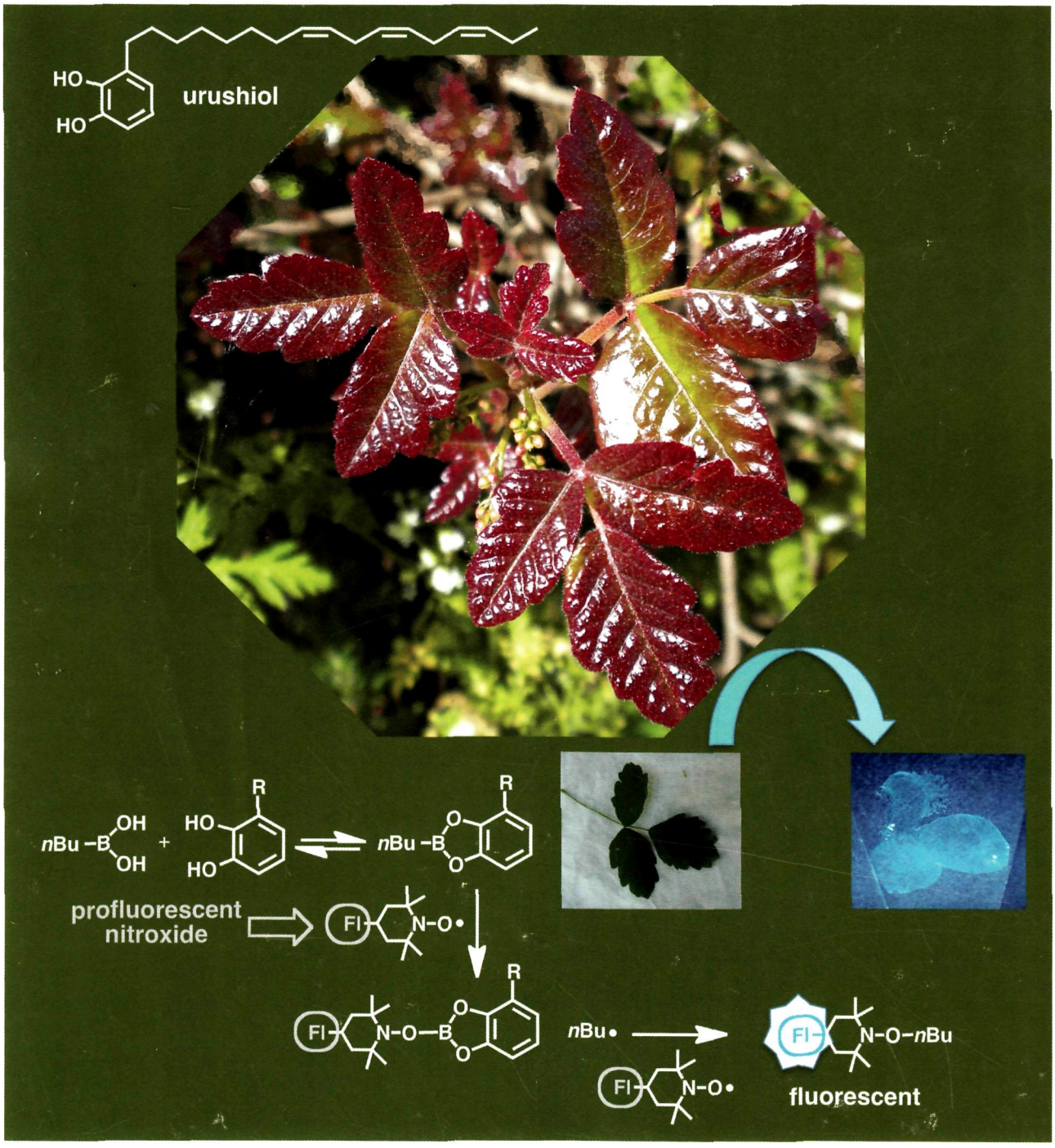
JOC

The Journal of Organic Chemistry

JANUARY 18, 2013 VOLUME 78, NUMBER 2 pubs.acs.org/joc



JOC The Journal of Organic Chemistry

JANUARY 18, 2013
VOLUME 78 ISSUE 2
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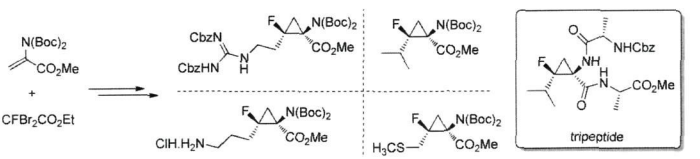
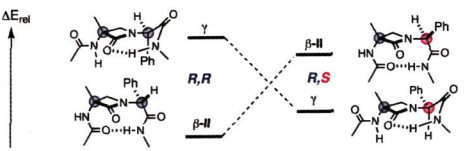
ON THE COVER: Urushiol, the causative agent of contact dermatitis from poison oak, ivy, and sumac, reacts with an alkylboronic acid and a profluorescent nitroxide to form a highly fluorescent alkoxyamine. This reaction sequence is depicted with a photograph of *Toxicodendron diversilobum*: western or pacific poison oak (*Rhus diversiloba*). The fluorescence serves to reveal the location of urushiol contamination. The oily sheen seen on the leaves is urushiol. See Braslau and co-workers, p 238.

Editorial

Featured Articles

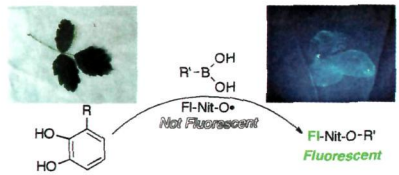




238 dx.doi.org/10.1021/jo301135m

Urushiol Detection using a Profluorescent Nitroxide

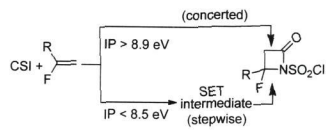
Rebecca Braslau,* Frank Rivera III, Erin Lilie, and MariEllen Cottman



246 dx.doi.org/10.1021/jo3016488

Kinetic Studies on the Reaction of Chlorosulfonyl Isocyanate with Monofluoroalkenes: Experimental Evidence for Both Stepwise and Concerted Mechanisms and a Pre-equilibrium Complex on the Reaction Pathway

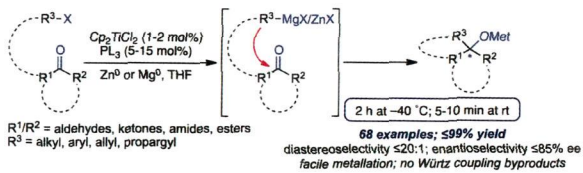
Dale F. Shellhamer,* Summer A. Bunting, Kelli R. Hickle, Parker C. Horn, Jacob C. Milligan, Danielle E. Shipowick, Lincoln B. Smith, David J. Vandenbroek, Marc C. Perry, and Jerry A. Boatz



253 dx.doi.org/10.1021/jo301726v

Cooperative Titanocene and Phosphine Catalysis: Accelerated C–X Activation for the Generation of Reactive Organometallics

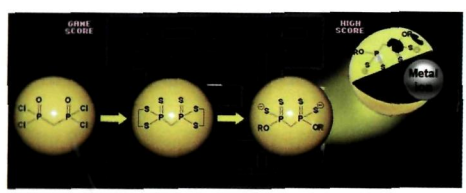
Lauren M. Fleury, Andrew D. Kosal, James T. Masters, and Brandon L. Ashfeld*



270 dx.doi.org/10.1021/jo301786m

O,O′-Diester Methylenediphosphonotetrathioate: Synthesis, Characterization, and Potential Applications

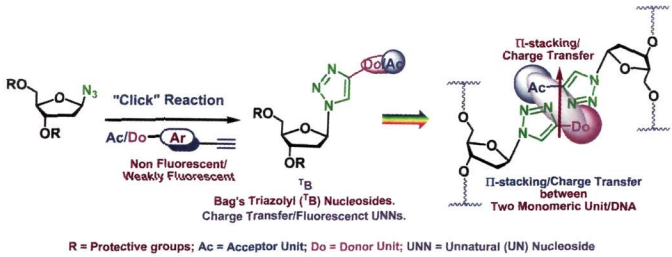
Aviran Amir, Alon H. Sayer, Rostislav Zagalsky, Linda J. W. Shimon, and Bilha Fischer*



278 dx.doi.org/10.1021/jo302033f

Triazolyl Donor/Acceptor Chromophore Decorated Unnatural Nucleosides and Oligonucleotides with Duplex Stability Comparable to That of a Natural Adenine/Thymine Pair

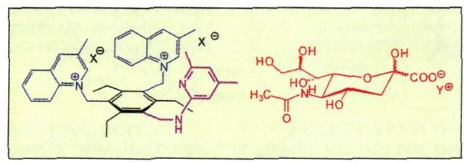
Subhendu Sekhar Bag,* Sangita Talukdar, Katsuhiko Matsumoto, and Rajen Kundu



292 dx.doi.org/10.1021/jo301966z

Molecular Recognition of *N*-Acetylneuraminic Acid by Acyclic Pyridinium- and Quinolinium-Based Receptors in Aqueous Media: Recognition through Combination of Cationic and Neutral Recognition Sites

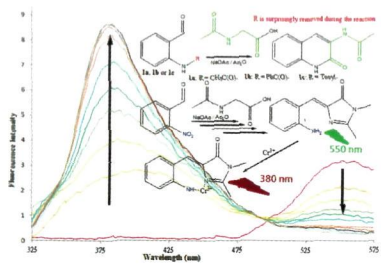
Christoph Geffert, Matthias Kuschel, and Monika Mazik*



301 dx.doi.org/10.1021/jo302050y

Synthesis, Photophysical Properties, and Application of *o*- and *p*-Amino Green Fluorescence Protein Synthetic Chromophores

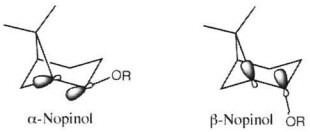
Yi-Hui Chen, Wei-Jen Lo, and Kuangsen Sung*



311 S dx.doi.org/10.1021/jo3020243

Hyperconjugation Involving Strained Carbon–Carbon Bonds. Structural Analysis of Ester and Ether Derivatives and One-Bond $^{13}C–^{13}C$ Coupling Constants of α- and β-Nopinol

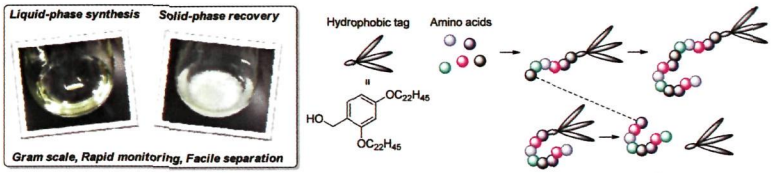
Shinn Dee Yeoh, Colin E. Skene, and Jonathan M. White*



320 S dx.doi.org/10.1021/jo302127d

Tag-Assisted Liquid-Phase Peptide Synthesis Using Hydrophobic Benzyl Alcohols as Supports

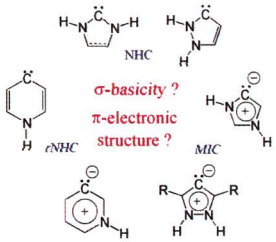
Yohei Okada, Hideaki Suzuki, Takashi Nakae, Shuji Fujita, Hitoshi Abe, Kazuo Nagano, Toshihide Yamada, Nobuyoshi Ebata, Shokaku Kim, and Kazuhiro Chiba*



328 S dx.doi.org/10.1021/jo302080c

Electronic Structural Trends in Divalent Carbon Compounds

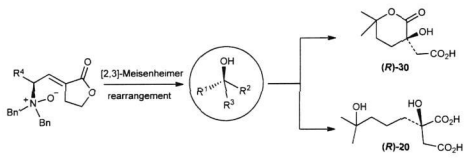
Han Vinh Huynh and Gilles Frison*



339 S dx.doi.org/10.1021/jo302203g

Construction of Chiral Tertiary Alcohol Stereocenters via the [2,3]- Meisenheimer Rearrangement: Enantioselective Synthesis of the Side-Chain Acids of Homoharringtonine and Harringtonine

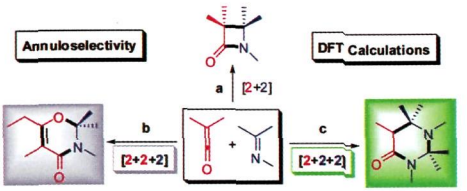
Hua Yang,* Moran Sun, Shuguang Zhao, Ming Zhu, Yangla Xie, Changling Niu, and Chunlin Li



347 S dx.doi.org/10.1021/jo302216d

Annuloselectivity in Cycloadditions of Ketenes with Imines: A DFT Study

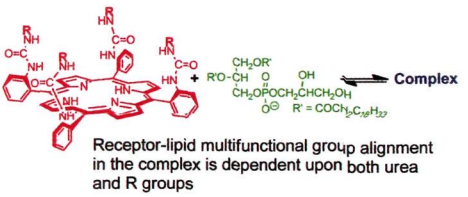
Xinyao Li and Jiaxi Xu*



356 S dx.doi.org/10.1021/jo302228w

Synthesis and Characterization of Picket Porphyrin Receptors That Bind Phosphatidylglycerol, an Anionic Phospholipid Found in Bacterial Membranes

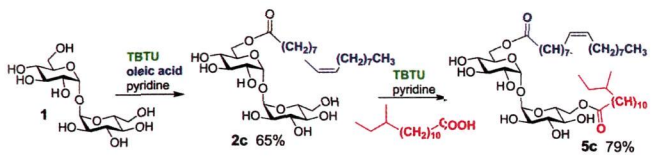
Amanda Alliband, Frederick A. Meece, Champika Jayasinghe, and Dennis H. Burns*



363 S dx.doi.org/10.1021/jo302231v

Direct Synthesis of Maradolipids and Other Trehalose 6-Monoesters and 6,6′-Diesters

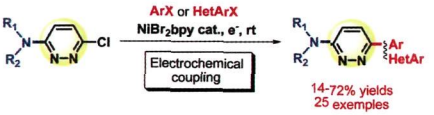
Nawal K. Paul, Jean-d'Amour K. Twibanire, and T. Bruce Grindley*



370 S dx.doi.org/10.1021/jo3022428

An Electrochemical Nickel-Catalyzed Arylation of 3-Amino-6-Chloropyridazines

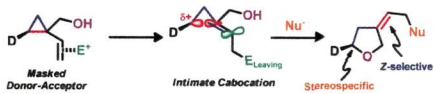
Stéphane Sengmany, Arnaud Vitu-Thiebaud, Erwan Le Gall, Sylvie Condon, Eric Léonel,* Christine Thobie-Gautier, Muriel Pipelier, Jacques Lebreton, and Didier Dubreuil



380 S dx.doi.org/10.1021/jo302204k

Electrophile-Induced C–C Bond Activation of Vinylcyclopropanes for the Synthesis of *Z*-Alkylidenetetrahydrofurans

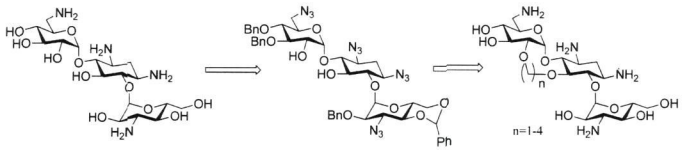
Venkataraman Ganesh, Taraknath Kundu, and Srinivasan Chandrasekaran*



400 S dx.doi.org/10.1021/jo302247x

Design, Synthesis, and Antibacterial Activities of Conformationally Constrained Kanamycin A Derivatives

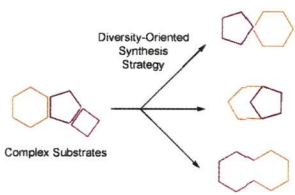
Wenxuan Zhang, Ying Chen, Qingzhao Liang, Hui Li, Hongwei Jin, Liangren Zhang, Xiangbao Meng,* and Zhongjun Li*



410 S dx.doi.org/10.1021/jo302211f

Molecular Library Synthesis Using Complex Substrates: Expanding the Framework of Triterpenoids

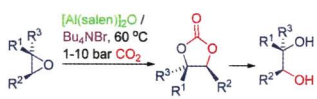
Vasily A. Ignatenko, Yong Han, and Gregory P. Tochtrop*



419 S dx.doi.org/10.1021/jo302317w

Influence of Temperature and Pressure on Cyclic Carbonate Synthesis Catalyzed by Bimetallic Aluminum Complexes and Application to Overall *syn*-Bis-hydroxylation of Alkenes

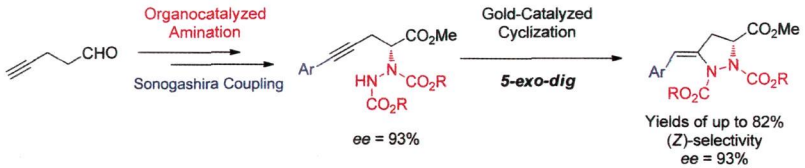
Christopher Beattie, Michael North,* Pedro Villuendas, and Carl Young



427 Ⓢ dx.doi.org/10.1021/jo302320v

Synthesis of Enantioenriched Aza-Proline Derivatives through Gold(I)-Catalyzed Cyclization of Chiral α-Hydrazino Esters

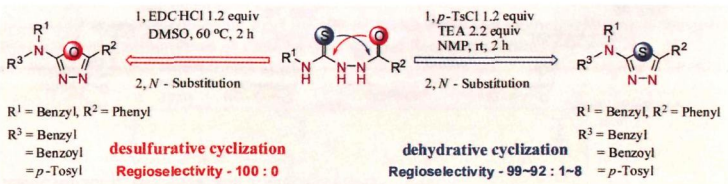
Sébastien Bouvet, Xavier Moreau, Vincent Coeffard,* and Christine Greck*



438 Ⓢ dx.doi.org/10.1021/jo302324r

Regioselective Synthesis of 2-Amino-Substituted 1,3,4-Oxadiazole and 1,3,4-Thiadiazole Derivatives via Reagent-Based Cyclization of Thiosemicarbazide Intermediate

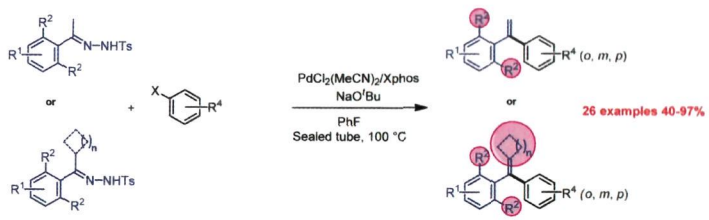
Seung-Ju Yang, Seok-Hyeong Lee, Hyun-Jung Kwak, and Young-Dae Gong*



445 Ⓢ dx.doi.org/10.1021/jo3023268

Synthesis of *Ortho*/*Ortho*′-Substituted 1,1-Diarylethylenes through Cross-Coupling Reactions of Sterically Encumbered Hydrazones and Aryl Halides

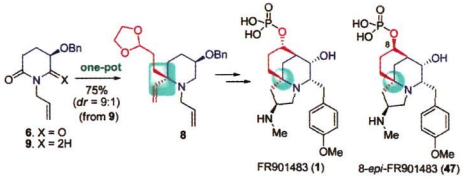
Maxime Roche, Abdallah Hamze,* Olivier Provot, Jean-Daniel Brion, and Mouad Alami*



455 S dx.doi.org/10.1021/jo302362b

Enantioselective Total Syntheses of (−)-FR901483 and (+)-8-*epi*-FR901483

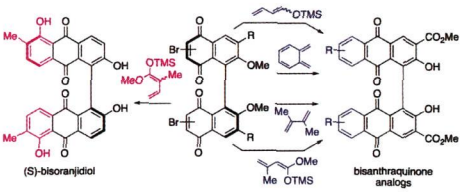
Hao-Hua Huo, Xiao-Er Xia, Hong-Kui Zhang,* and Pei-Qiang Huang*



466 S dx.doi.org/10.1021/jo302364h

Divergent Approach to the Bisanthraquinone Natural Products: Total Synthesis of (*S*)-Bisoranjidiol and Derivatives from Binaphtho-*para*-quinones

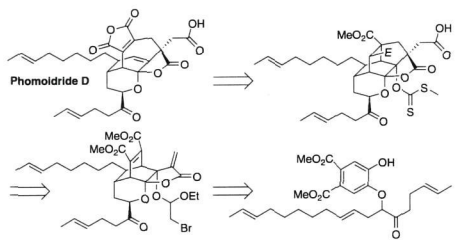
Erin E. Podlesny and Marisa C. Kozlowski*



477 S dx.doi.org/10.1021/jo302353g

Toward the Synthesis of Phomoidride *D*

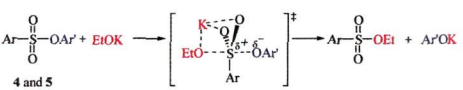
Graham K. Murphy, Tatsuya Shirahata, Naoto Hama, Aaron Bedermann, Ping Dong, Travis C. McMahon, Barry M. Twenter, David A. Spiegel, Ivar M. McDonald, Nobuaki Taniguchi, Munenori Inoue, and John L. Wood*



490 S dx.doi.org/10.1021/jo302373y

A Kinetic Study on Nucleophilic Displacement Reactions of Aryl Benzenesulfonates with Potassium Ethoxide: Role of K^+ Ion and Reaction Mechanism Deduced from Analyses of LFERs and Activation Parameters

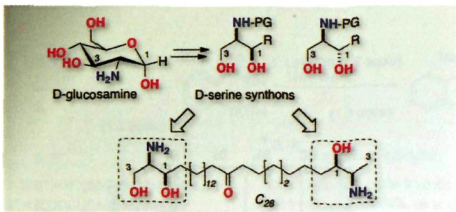
Ik-Hwan Um,* Ji-Sun Kang, Young-Hee Shin, and Erwin Buncel



498 S dx.doi.org/10.1021/jo302355t

d-Glucosamine-Derived Synthons for Assembly of l-*threo*-Sphingoid Bases. Total Synthesis of Rhizochalinin C

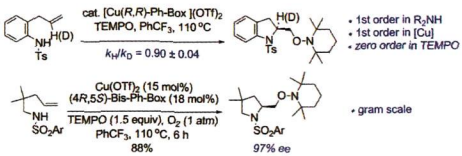
Jaeyoung Ko and Tadeusz F. Molinski*



506 S dx.doi.org/10.1021/jo3023632

Mechanistic Analysis and Optimization of the Copper-Catalyzed Enantioselective Intramolecular Alkene Aminooxygenation

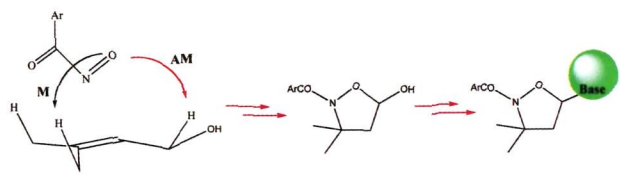
Monissa C. Paderes, Jerome B. Keister, and Sherry R. Chemler*



516 S dx.doi.org/10.1021/jo302346a

***N,O*-Nucleosides from Ene Reactions of Nitrosocarbonyl Intermediates with the 3-Methyl-2-buten-1-ol**

Paolo Quadrelli,* Mariella Mella, Serena Carosso, and Bruna Bovio

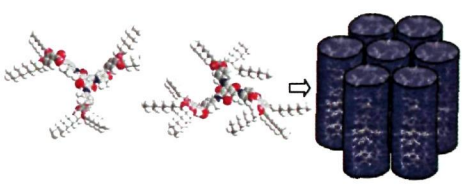


Ar	Markovnikov path (M)	Anti-Markovnikov path (AM)
Ph	60	0
Mes	50	25
Anthra	27	52

527 S dx.doi.org/10.1021/jo302332u

Self-Assembly of Hekates-Tris(*N*-salicylideneaniline)s into Columnar Structures: Synthesis and Characterization

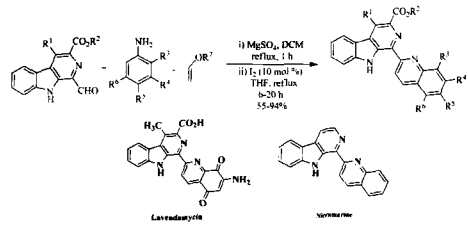
Ammathnadu S. Achalkumar, Uma S. Hiremath, D. S. Shankar Rao, S. Krishna Prasad, and Channabasaveshwar V. Yelamaggad*



545 S dx.doi.org/10.1021/jo302389s

A Formal Synthesis of Lavendamycin Methyl Ester, Nitramarine, and Their Analogues: A Povarov Approach

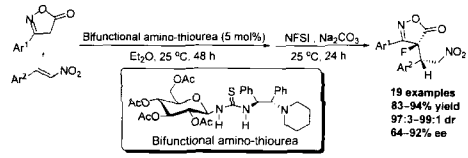
Subburethinam Ramesh and Rajagopal Nagarajan*



559 S dx.doi.org/10.1021/jo302419e

Organocatalytic Asymmetric One-Pot Sequential Conjugate Addition/Dearomative Fluorination: Synthesis of Chiral Fluorinated Isoxazol-5(4*H*)-ones

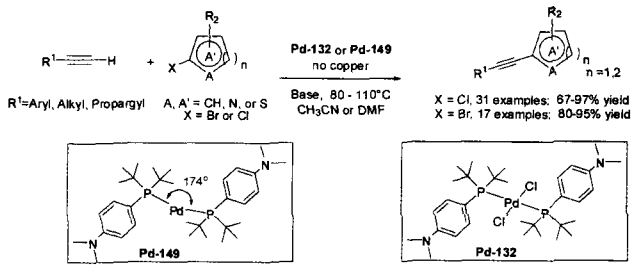
Wen-Ting Meng, Yan Zheng, Jing Nie, Heng-Ying Xiong, and Jun-An Ma*



568 S dx.doi.org/10.1021/jo302195y

Heck Alkynylation (Copper-Free Sonogashira Coupling) of Aryl and Heteroaryl Chlorides, Using Pd Complexes of t-Bu$_2$(*p*-NMe$_2$C$_6$H$_4$)P: Understanding the Structure–Activity Relationships and Copper Effects

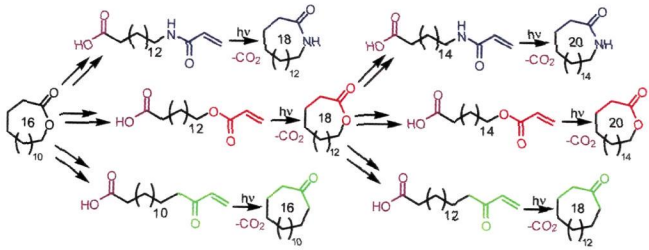
Xiaotao Pu, Hongbo Li, and Thomas J. Colacot*



582 dx.doi.org/10.1021/jo3024126

Radical Photocyclization Route for Macrocyclic Lactone Ring Expansion and Conversion to Macrocyclic Lactams and Ketones

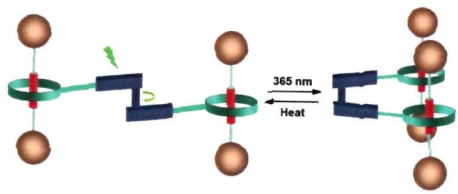
Keisuke Nishikawa, Yasuharu Yoshimi,* Kousuke Maeda, Toshio Morita, Ichiro Takahashi, Tatsuya Itou, Sho Inagaki, and Minoru Hatanaka



590 dx.doi.org/10.1021/jo302426c

Photodriven Clamlike Motion in a [3]Rotaxane with Two [2]Rotaxane Arms Bridged by an Overcrowded Alkene Switch

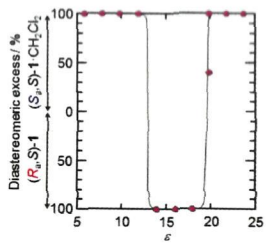
Wei Zhou, Ya-Jing Guo, and Da-Hui Qu*



597 dx.doi.org/10.1021/jo3024285

Switching of the Diastereomer Deposited during the Crystallization of *N*-[(*S*)-1-Phenylethyl]-2′-carbamoyl-1,1′-binaphthalene-2-carboxylic Acid: Investigation of the Mechanism of Dielectrically Controlled Resolution

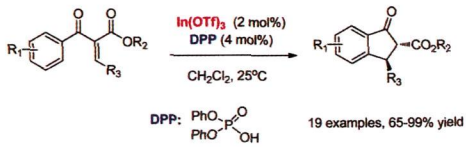
Yuichi Kitamoto, Kazumi Suzuki, Naoya Morohashi, Kenichi Sakai, and Tetsutaro Hattori*



606 S dx.doi.org/10.1021/jo302451b

Catalytic Nazarov Reaction of Aryl Vinyl Ketones via Binary Acid Strategy

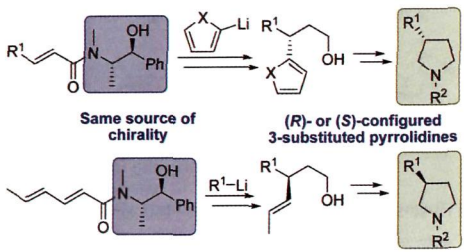
Zhi-Guo Xi, Lihui Zhu, Sanzhong Luo,* and Jin-Pei Cheng



614 S dx.doi.org/10.1021/jo302438k

Using Heteroaryl-lithium Reagents as Hydroxycarbonyl Anion Equivalents in Conjugate Addition Reactions with (*S,S*)-(+)-Pseudoephedrine as Chiral Auxiliary; Enantioselective Synthesis of 3-Substituted Pyrrolidines

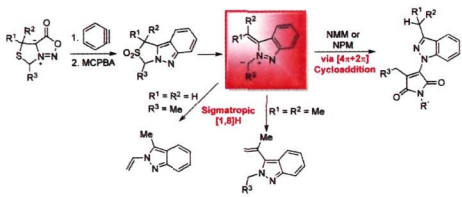
Beatriz Alonso, Marta Ocejo, Luisa Carrillo,* Jose L. Vicario,* Efraim Reyes, and Uxue Uria



628 S dx.doi.org/10.1021/jo302463q

Thiazolo[3,4-*b*]indazole-2,2-dioxides as Masked Extended Dipoles: Pericyclic Reactions of Benzodiazafulvenium Methides

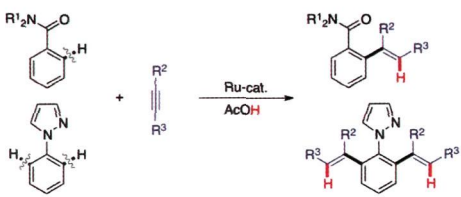
Maria I. L. Soares, Cláudio M. Nunes, Clara S. B. Gomes, and Teresa M. V. D. Pinho e Melo*



638 S dx.doi.org/10.1021/jo3025237

Regioselective C–H Bond Cleavage/Alkyne Insertion under Ruthenium Catalysis

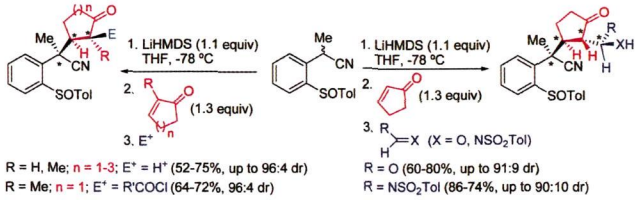
Yuto Hashimoto, Koji Hirano, Tetsuya Satoh,* Fumitoshi Kakiuchi, and Masahiro Miura*



647 S dx.doi.org/10.1021/jo3025434

Use of Lithiated Chiral *o*-Sulfinylbenzyl Carbanions for the One-Pot Building of Linear Fragments Containing up to Four Connected Stereocenters

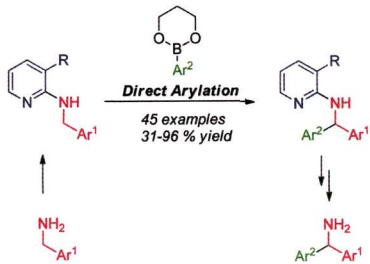
José Luis García Ruano,* Esther Torrente, and Ana M. Martín-Castro*



658 S dx.doi.org/10.1021/jo302547q

Mechanistic Investigations and Substrate Scope Evaluation of Ruthenium-Catalyzed Direct sp^3 Arylation of Benzylic Positions Directed by 3-Substituted Pyridines

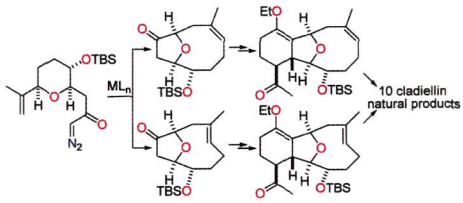
Navid Dastbaravardeh, Karl Kirchner, Michael Schnürch,* and Marko D. Mihovilovic



673 S dx.doi.org/10.1021/jo302542h

Total Syntheses of Multiple Cladiellin Natural Products by Use of a Completely General Strategy

J. Stephen Clark,* Raphaëlle Berger, Stewart T. Hayes, Hans Martin Senn, Louis J. Farrugia, Lynne H. Thomas, Angus J. Morrison, and Luca Gobbi

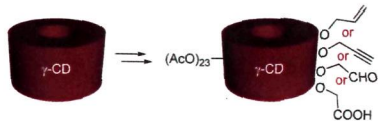


Notes

697 S dx.doi.org/10.1021/jo301656p

Complete Sets of Monosubstituted γ-Cyclodextrins as Precursors for Further Synthesis

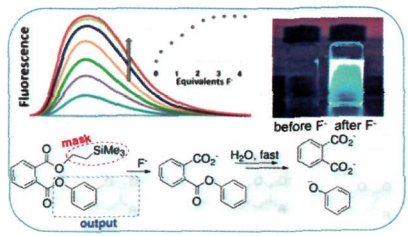
Markéta Bláhová, Eva Bednářová, Michal Řezanka, and Jindřich Jindřich*



702 S dx.doi.org/10.1021/jo301698v

Self-Immolative Aryl Phthalate Esters

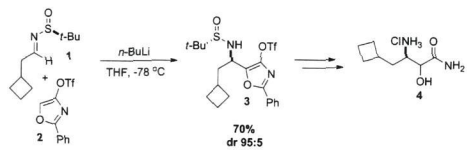
Kaitlyn M. Mahoney, Pratik P. Goswami, and Arthur H. Winter*



706 S dx.doi.org/10.1021/jo301856f

Stereoselective Addition of 2-Phenyloxazol-4-yl Trifluoromethanesulfonate to *N*-Sulfinyl Imines: Application to the Synthesis of the HCV Protease Inhibitor Boceprevir

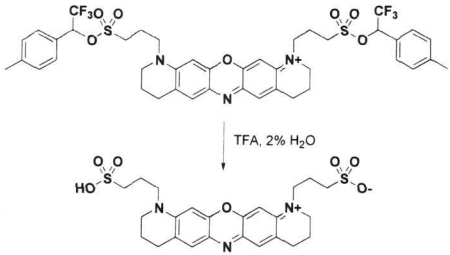
William J. Morris,* Kiran K. Muppalla,* Cameron Cowden, and Richard G. Ball



711 S dx.doi.org/10.1021/jo302065u

A Trifluoroacetic Acid-labile Sulfonate Protecting Group and Its Use in the Synthesis of a Near-IR Fluorophore

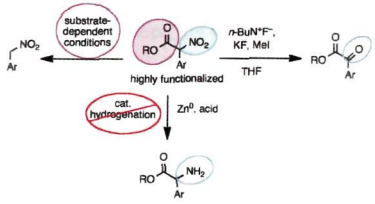
Steven M. Pauff and Stephen C. Miller*



717 S dx.doi.org/10.1021/jo302071s

2-Aryl-2-nitroacetates as Central Precursors to Aryl Nitromethanes, α-Ketoesters, and α-Amino Acids

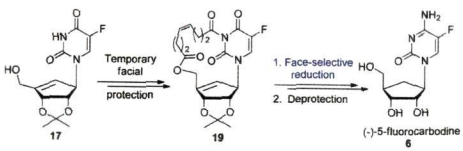
Alison E. Metz and Marisa C. Kozlowski*



723 S dx.doi.org/10.1021/jo302038d

Synthesis of Cyclopentanyl Carbocyclic 5-Fluorocytosine ((−)-5-Fluorocarbodine) Using a Facially Selective Hydrogenation Approach

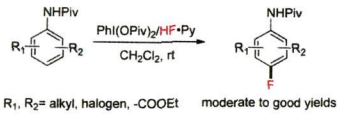
Jong Hyun Cho, Franck Amblard, Steven J. Coats, and Raymond F. Schinazi*



728 S dx.doi.org/10.1021/jo302099d

Hypervalent Iodine Mediated *para*-Selective Fluorination of Anilides

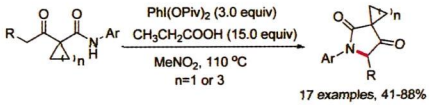
Tian Tian, Wen-He Zhong, Shuai Meng, Xiang-Bao Meng,* and Zhong-Jun Li*



733 dx.doi.org/10.1021/jo302144w

Synthesis of Tetramic Acid Derivatives via Intramolecular sp^3 C–H Amination Mediated by Hypervalent Iodine(III) Reagents/Brønsted Acids

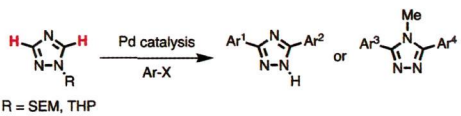
Lujia Mao, Yan Li,* Tao Xiong, Kai Sun, and Qian Zhang*



738 dx.doi.org/10.1021/jo3021677

C–H Bonds as Ubiquitous Functionality: Preparation of Multiple Regioisomers of Arylated 1,2,4-Triazoles via C–H Arylation

Jung Min Joo, Pengfei Guo, and Dalibor Sames*



744 dx.doi.org/10.1021/jo302173a

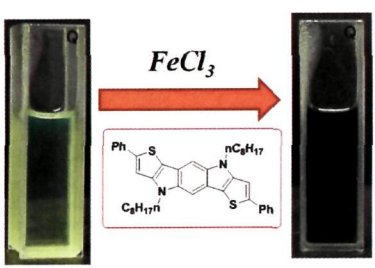
Per-6-amino-β-cyclodextrin as a Chiral Base Catalyst Promoting One-Pot Asymmetric Synthesis of 2-Aryl-2,3-dihydro-4-quinolones

Kuppusamy Kanagaraj and Kasi Pitchumani*

752 dx.doi.org/10.1021/jo3022154

Electron-Rich Pyrroloindacenodithiophenes: Synthesis, Characterization, and Spectroscopic Studies

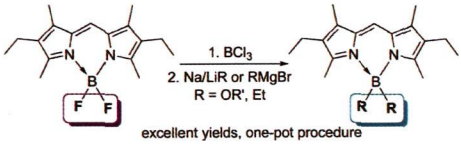
Yu Xiong, Qinghe Wu, Jie Li, Shitao Wang, Xike Gao, and Hongxiang Li*



757 dx.doi.org/10.1021/jo302277d

Conversion of *F*-BODIPYs to *Cl*-BODIPYs: Enhancing the Reactivity of *F*-BODIPYs

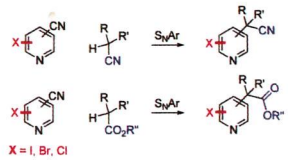
Travis Lundrigan and Alison Thompson*



762 dx.doi.org/10.1021/jo302307y

Cyanide Anion as a Leaving Group in Nucleophilic Aromatic Substitution: Synthesis of Quaternary Centers at Azine Heterocycles

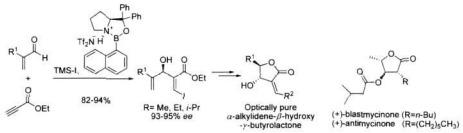
Alexander D. Thompson and Malcolm P. Huestis*



770 dx.doi.org/10.1021/jo302369q

Asymmetric Synthesis of α-Alkylidene-β-hydroxy-γ-butyrolactones via Enantioselective Tandem Michael–Aldol Reaction

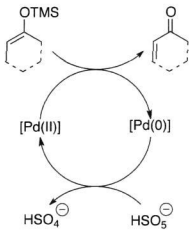
Sung Il Lee, Jin Hee Jang, Geum-Sook Hwang,* and Do Hyun Ryu*



776 dx.doi.org/10.1021/jo302465v

Palladium-Catalyzed Saegusa–Ito Oxidation: Synthesis of α,β-Unsaturated Carbonyl Compounds from Trimethylsilyl Enol Ethers

Yingdong Lu, Pierre Long Nguyen, Nicolas Lévaray, and Hélène Lebel*



Additions and Corrections

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