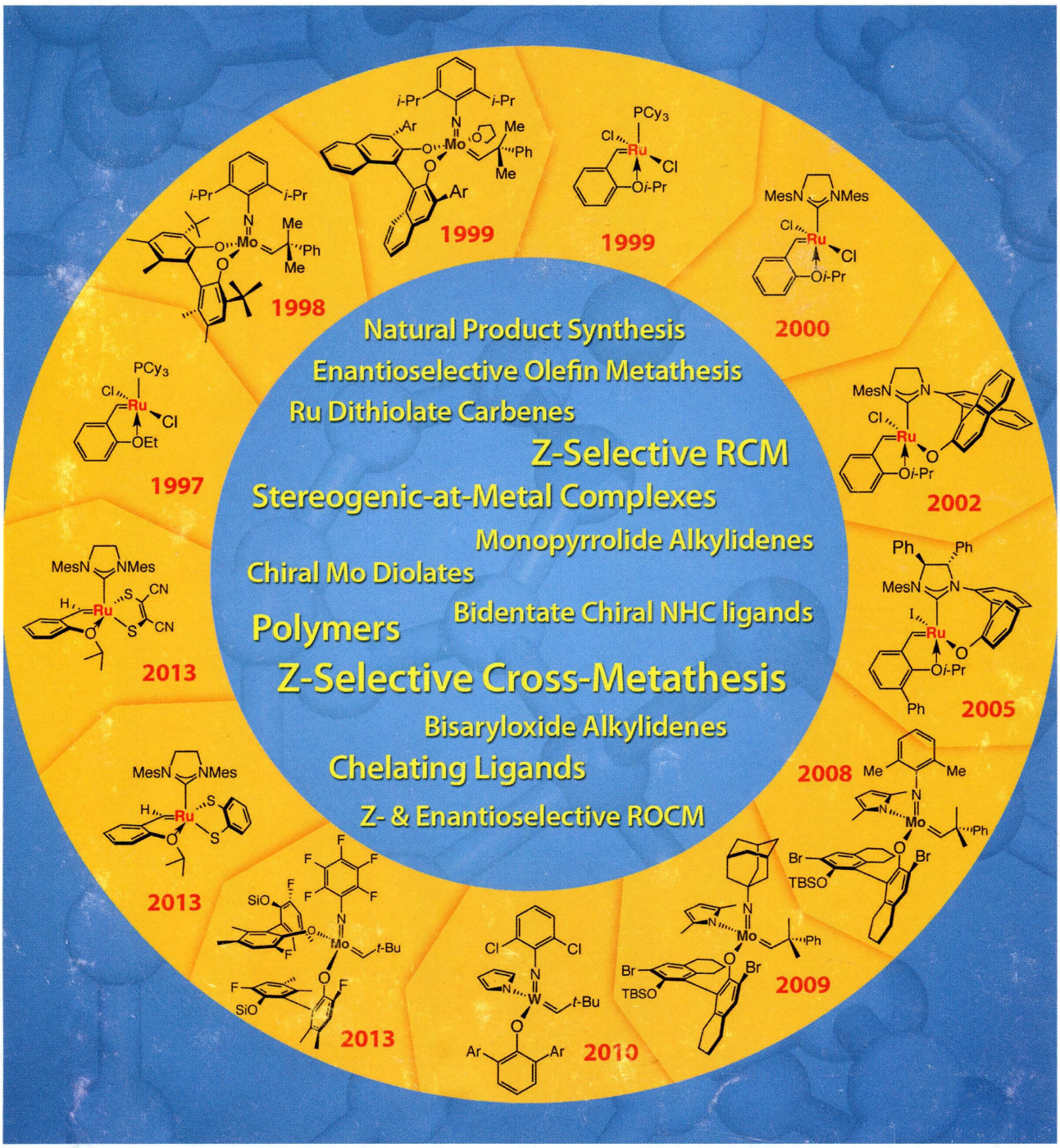
JOC

The Journal of Organic Chemistry

JUNE 6, 2014 VOLUME 79, NUMBER 11 pubs.acs.org/joc



JOC The Journal of Organic Chemistry

JUNE 6, 2014
VOLUME 79 ISSUE 11

JOCEAH 79(11) 4763–5390 (2014)
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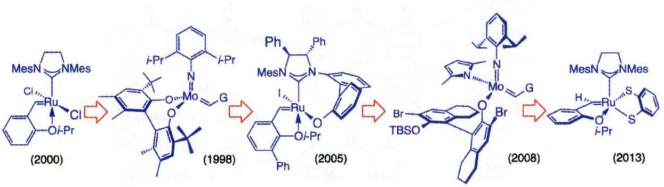
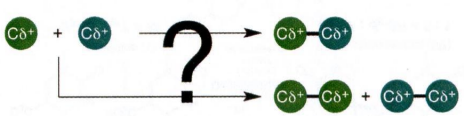
ON THE COVER: Many exciting developments in stereoselective olefin metathesis involve the cycles of catalyst discovery that encompass complexes containing Ru, Mo, or W centers. For a critical overview of related development during the last two decades, see Hoveyda, p 4763. Professor Hoveyda is the recipient of the 2014 ACS Award for Creative Work in Synthetic Organic Chemistry.

Perspective



JOCSynopsis

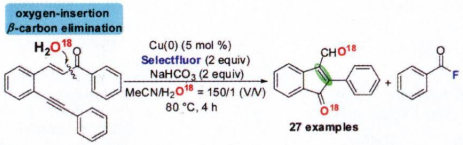


Featured Articles

4799 dx.doi.org/10.1021/jo500948b

Copper-Catalyzed Oxidative Cyclization of 1,5-Enynes with Concomitant C–C Bond Cleavage: An Unexpected Access to 3-Formyl-1-indenone Derivatives

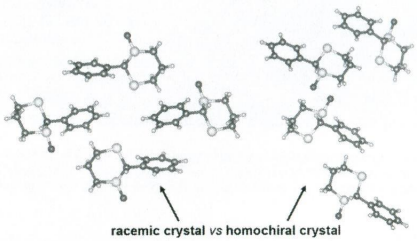
Jian Zhang, Degui Wu, Xiaoling Chen, Yunkui Liu,* and Zhenyuan Xu



4809 dx.doi.org/10.1021/jo500528k

Are Racemic Crystals Favored over Homochiral Crystals by Higher Stability or by Kinetics? Insights from Comparative Studies of Crystalline Stereoisomers

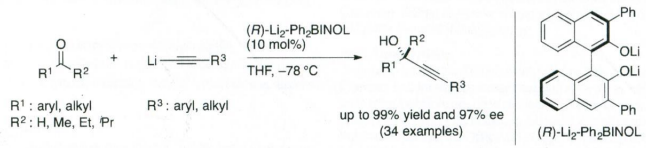
Angelo Gavezzotti and Silvia Rizzato*



4817 dx.doi.org/10.1021/jo5005394

Lithium Binaphtholate-Catalyzed Asymmetric Addition of Lithium Acetylides to Carbonyl Compounds

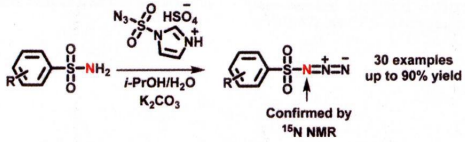
Shunsuke Kotani, Kenji Kukita, Kana Tanaka, Tomonori Ichibakase, and Makoto Nakajima*

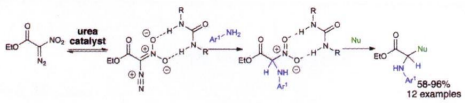


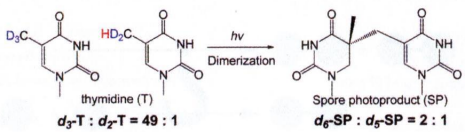
4826 dx.doi.org/10.1021/jo500553q

Synthesis of Sulfonyl Azides via Diazotransfer using an Imidazole-1-sulfonyl Azide Salt: Scope and ^{15}N NMR Labeling Experiments

Marc Y. Stevens, Rajiv T. Sawant, and Luke R. Odell*



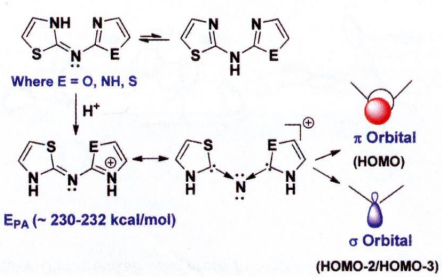




d_3-T : d_2-T = 49 : 1

d_6-SP : d_5-SP = 2 : 1

Articles

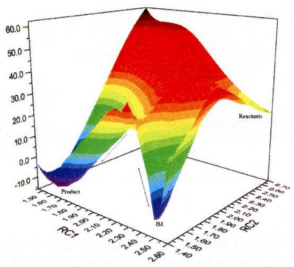


E_{PA} (~ 230-232 kcal/mol)

4863 S dx.doi.org/10.1021/jo500184f

Medium Effects on the 1,3-Dipolar Cycloaddition of Pyridazinium Dicyanomethanide with Ethyl Vinyl Ketone in Pure and Mixed Solvents from QM/MM Simulations

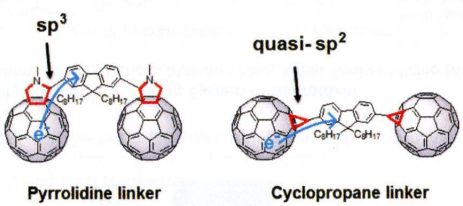
Xin Yang and Ying Xue*



4871 S dx.doi.org/10.1021/jo500342x

Does a Cyclopropane Ring Enhance the Electronic Communication in Dumbbell-Type C_{60} Dimers?

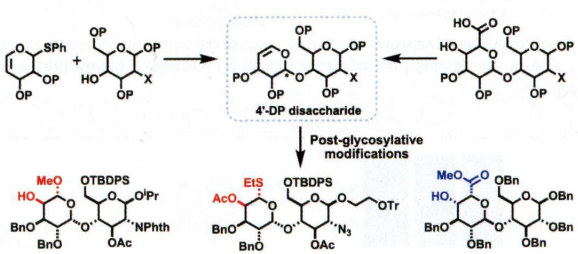
Andrea La Rosa, Katalin Gillemot, Edmund Leary,* Charalambos Evangeli, María Teresa González, Salvatore Filippone, Gabino Rubio-Bollinger, Nicolás Agraït, Colin J. Lambert, and Nazario Martín*



4878 S dx.doi.org/10.1021/jo500449h

Synthesis and Reactivity of 4′-Deoxypentenosyl Disaccharides

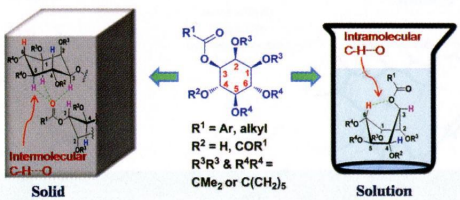
Panuwat Padungros, Ren-Hua Fan, Matthew D. Casselman, Gang Cheng, Hari R. Khatri, and Alexander Wei*



4892 S dx.doi.org/10.1021/jo5004778

Strength from Weakness: Conformational Divergence between Solid and Solution States of Substituted Cyclitols Facilitated by CH···O Hydrogen Bonding

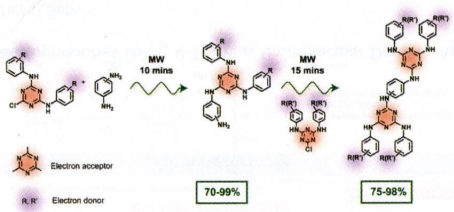
Amol M. Vibhute and Kana M. Sureshan*



4909 S dx.doi.org/10.1021/jo500480r

Microwave-Assisted Selective Synthesis of Mono- and Bistriazines with π-Conjugated Spacers and Study of the Optoelectronic Properties

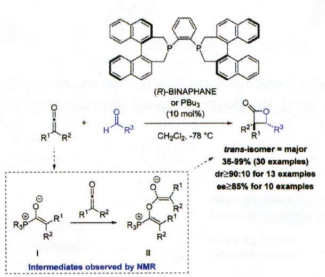
A. Ruiz-Carretero, O. Noguez, T. Herrera, J. R. Ramírez, A. Sánchez-Migallón,* and A. de la Hoz*

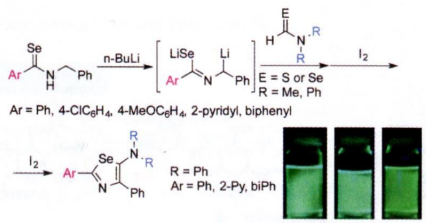


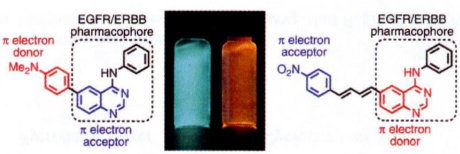
4920 S dx.doi.org/10.1021/jo500486e

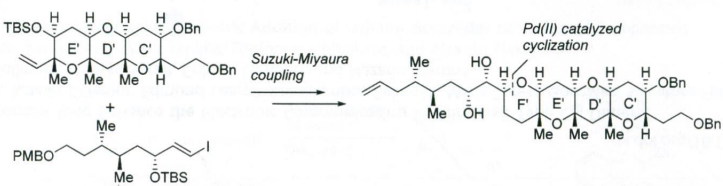
Phosphine-Catalyzed Asymmetric Synthesis of β-Lactones from Disubstituted Ketenes and Aldehydes

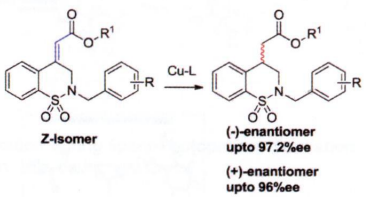
Shi Chen, Mukulesh Mondal, Ahmad A. Ibrahim, Kraig A. Wheeler, and Nessan J. Kerrigan*

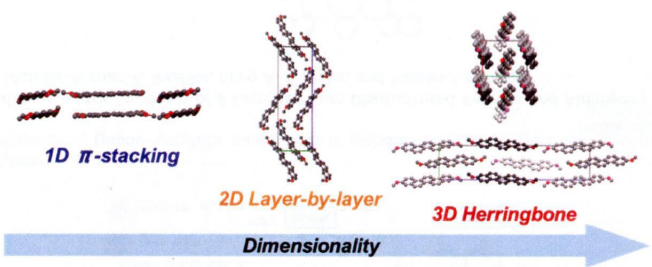


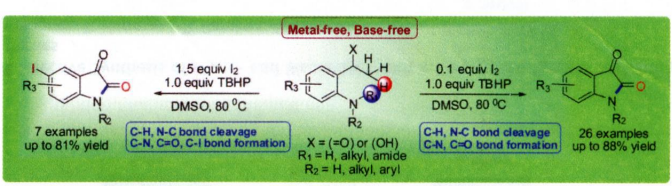








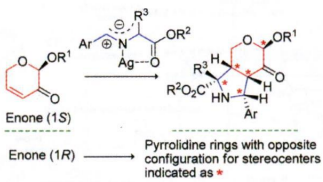




4992 S dx.doi.org/10.1021/jo500547y

Stereospecific Synthesis of Pyrrolidines with Varied Configurations via 1,3-Dipolar Cycloadditions to Sugar-Derived Enones

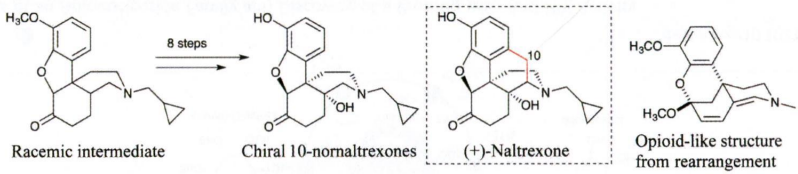
Guillermo A. Oliveira Udry, Evangelina Repetto, and Oscar Varela*



5007 S dx.doi.org/10.1021/jo500568s

Synthesis of Enantiopure 10-Nornaltrexones in the Search for Toll-like Receptor 4 Antagonists and Opioid Ligands

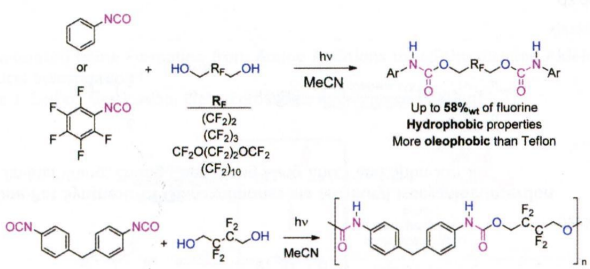
Brandon R. Selfridge, Jeffrey R. Deschamps, Arthur E. Jacobson, and Kenner C. Rice*



5019 S dx.doi.org/10.1021/jo5005789

Photochemical Activation of Extremely Weak Nucleophiles: Highly Fluorinated Urethanes and Polyurethanes from Polyfluoro Alcohols

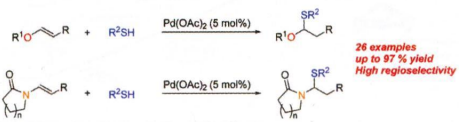
Marc Soto, Rosa María Sebastián,* and Jordi Marquet*



5028 S dx.doi.org/10.1021/jo500586a

Regioselective Hydrothiolation of Alkenes Bearing Heteroatoms with Thiols Catalyzed by Palladium Diacetate

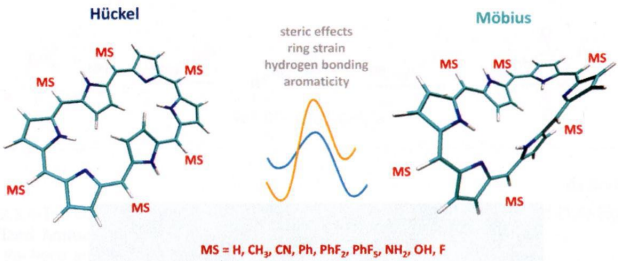
Taichi Tamai and Akiya Ogawa*



5036 S dx.doi.org/10.1021/jo500569p

Effect of the Meso-Substituent in the Hückel-to-Möbius Topological Switches

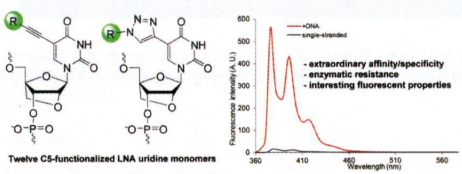
Enrique Marcos,* Josep M. Anglada, and Miquel Torrent-Sucarrat*



5047 S dx.doi.org/10.1021/jo500614a

Synthesis and Biophysical Properties of C5-Functionalized LNA (Locked Nucleic Acid)

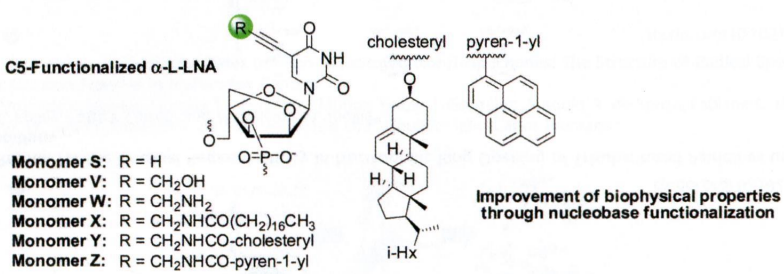
Pawan Kumar, Michael E. Østergaard, Bharat Baral, Brooke A. Anderson, Dale C. Guenther, Mamta Kaura, Daniel J. Raible, Pawan K. Sharma, and Patrick J. Hrdlicka*



5062 S dx.doi.org/10.1021/jo5006153

C5-Alkynyl-Functionalized α-L-LNA: Synthesis, Thermal Denaturation Experiments and Enzymatic Stability

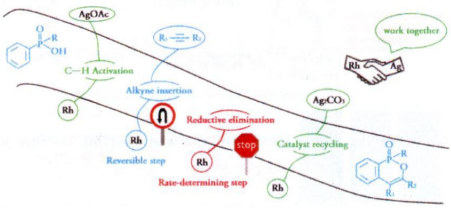
Pawan Kumar, Bharat Baral, Brooke A. Anderson, Dale C. Guenther, Michael E. Østergaard, Pawan K. Sharma, and Patrick J. Hrdlicka*



5074 dx.doi.org/10.1021/jo500616g

Mechanism, Reactivity, and Selectivity in Rh(III)-Catalyzed Phosphoryl-Directed Oxidative C−H Activation/Cyclization: A DFT Study

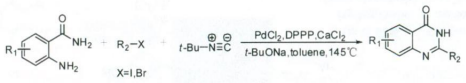
Liu Liu, Yile Wu, Tao Wang, Xiang Gao, Jun Zhu,* and Yufen Zhao*



5082 dx.doi.org/10.1021/jo500636y

Palladium-Catalyzed One-Pot Synthesis of Quinazolinones via *tert*-Butyl Isocyanide Insertion

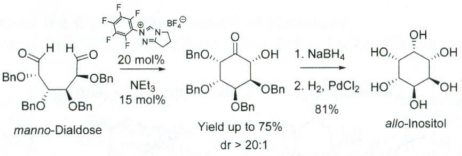
Xiao Jiang, Ting Tang, Jin-Mei Wang, Zhong Chen, Yong-Ming Zhu,* and Shun-Jun Ji



5088 dx.doi.org/10.1021/jo500645z

Synthesis of *allo*- and *epi*-Inositol via the NHC-Catalyzed Carbocyclization of Carbohydrate-Derived Dialdehydes

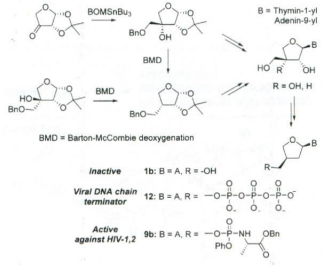
Kieran P. Stockton, Ben W. Greatrex,* and Dennis K. Taylor



5097 dx.doi.org/10.1021/jo500659e

Synthesis of an Apionucleoside Family and Discovery of a Prodrug with Anti-HIV Activity

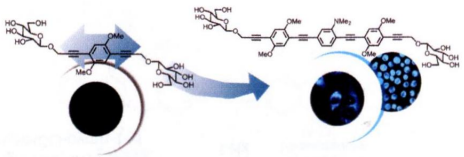
Kiran S. Toti, Marco Derudas, Fabrizio Pertusati, Davy Sinnaeve, Freya Van den Broeck, Lia Margamuljana, José C. Martins, Piet Herdewijn, Jan Balzarini, Christopher McGuigan, and Serge Van Calenbergh*



5113 Ⓢ dx.doi.org/10.1021/jo500661u

Oligo(phenylene ethynylene) Glucosides: Modulation of Cellular Uptake Capacity Preserving Light ON

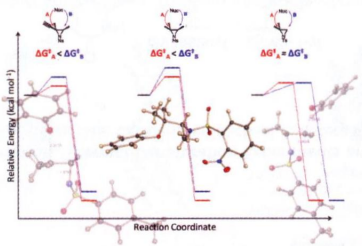
Anna Barattucci,* Elisa Deni, Paola Bonaccorsi, Maria Grazia Ceraolo, Teresa Papalia, Antonio Santoro, Maria Teresa Sciortino,* and Fausto Puntoriero*



5121 Ⓢ dx.doi.org/10.1021/jo5006685

Possible Reason for the Unusual Regioselectivity in Nucleophilic Ring Opening of Trisubstituted Aziridines under Mildly Basic Conditions

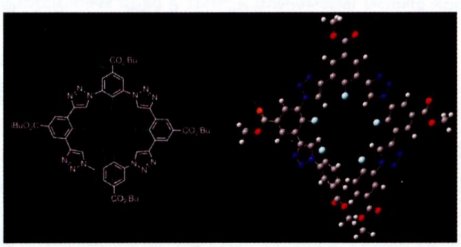
Brandon T. Kelley, Patrick Carroll, and Madeleine M. Joullié*



5134 Ⓢ dx.doi.org/10.1021/jo500582c

Aromatic Triazole Foldamers Induced by C–H···X (X = F, Cl) Intramolecular Hydrogen Bonding

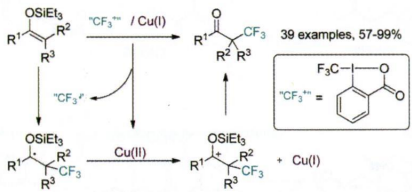
Jie Shang, Nolan M. Gallagher, Fusheng Bie, Qiaolian Li, Yanke Che, Ying Wang,* and Hua Jiang*



5145 dx.doi.org/10.1021/jo500713f

Synthesis of α-Trifluoromethyl Ketones via the Cu-Catalyzed Trifluoromethylation of Silyl Enol Ethers Using an Electrophilic Trifluoromethylating Agent

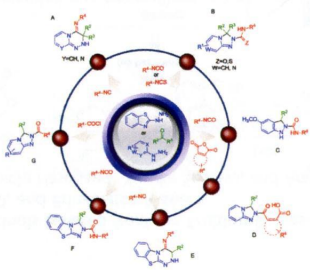
Lun Li, Qing-Yun Chen,* and Yong Guo*



5153 dx.doi.org/10.1021/jo500723d

Synthesis of Diverse Nitrogen-Enriched Heterocyclic Scaffolds Using a Suite of Tunable One-Pot Multicomponent Reactions

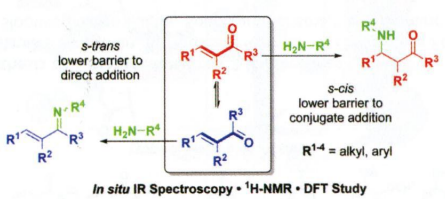
Guillermo Martinez-Ariza, Muhammad Ayaz, Federico Medda, and Christopher Hulme*



5163 dx.doi.org/10.1021/jo5007366

Understanding α,β-Unsaturated Imine Formation from Amine Additions to α,β-Unsaturated Aldehydes and Ketones: An Analytical and Theoretical Investigation

Adam D. J. Calow, Jorge J. Carbó,* Jessica Cid, Elena Fernández, and Andrew Whiting*



5173 dx.doi.org/10.1021/jo500745u

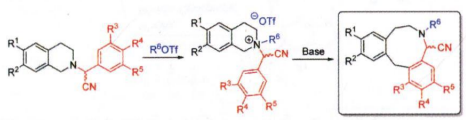
Fluoroalkylated α,β-Unsaturated Imines as Synthons for the Preparation of Fluorinated Triazinane-2,4-diones and Dihydropyrimidin-2(1*H*)-ones

Guillermo Fernández de Trocóniz, Ana M. Ochoa de Retana, Gloria Rubiales, and Francisco Palacios*

5182 dx.doi.org/10.1021/jo500749x

Ring Expansion of 1,2,3,4-Tetrahydroisoquinolines to Dibenzo[*c*,*f*]azonines. An Unexpected [1,4]-Sigmatropic Rearrangement of Nitrile-Stabilized Ammonium Ylides

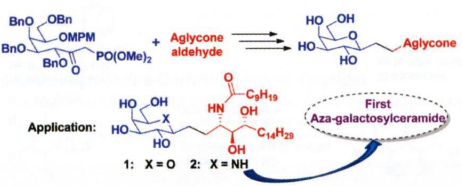
Julio Cesar Orejarena Pacheco and Till Opatz*



5193 dx.doi.org/10.1021/jo500769f

Synthesis of β-*C*-Galactosyl Ceramide and Its New Aza Variant via the Horner–Wadsworth–Emmons Reaction

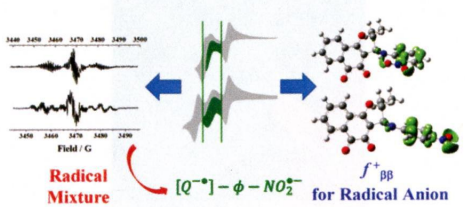
Jaggaiah N. Gorantla and Ravi S. Lankalapalli*



5201 dx.doi.org/10.1021/jo500787q

Nature of Electrogenerated Intermediates in Nitro-Substituted Nor-β-lapachones: The Structure of Radical Species during Successive Electron Transfer in Multiredox Centers

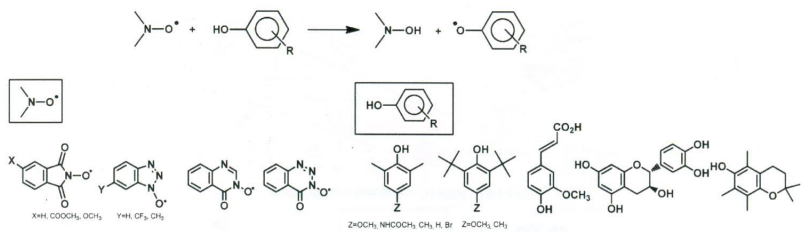
Georgina Armendáriz-Vidales, Lindsay S. Hernández-Muñoz, Felipe J. González, Antonio A. de Souza, Fabiane C. de Abreu, Guilherme A. M. Jardim, Eufrânio N. da Silva Jr., Marilia O. F. Goulart,* and Carlos Frontana*



5209 dx.doi.org/10.1021/jo500789v

Importance of π-Stacking Interactions in the Hydrogen Atom Transfer Reactions from Activated Phenols to Short-Lived *N*-Oxyl Radicals

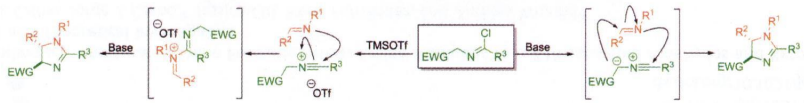
Marco Mazzonna, Massimo Bietti, Gino A. DiLabio,* Osvaldo Lanzalunga,* and Michela Salamone



5219 dx.doi.org/10.1021/jo500790n

Diastereoselective One-Pot Synthesis of Tetrafunctionalized 2-Imidazolines

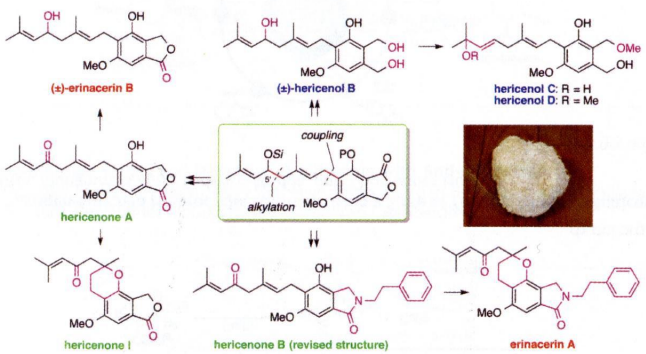
Guido V. Janssen, Paul Slobbe, Maurice Mooijman, Art Kruithof, Andreas W. Ehlers, Célia Fonseca Guerra, F. Matthias Bickelhaupt, J. Chris Slootweg, Eelco Ruijter, Koop Lammertsma,* and Romano V. A. Orru*



5227 dx.doi.org/10.1021/jo500795z

Divergent Synthesis of Bioactive Resorcinols Isolated from the Fruiting Bodies of *Hericium erinaceum*: Total Syntheses of Hericenones A, B, and I, Hericenols B–D, and Erinacerins A and B

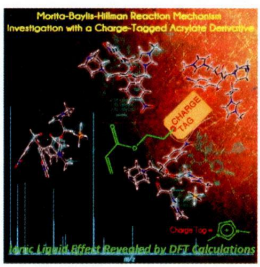
Shoji Kobayashi,* Hidetsugu Tamanoi, Yuichi Hasegawa, Yusuke Segawa, and Araki Masuyama



5239 (S) dx.doi.org/10.1021/jo500799j

Morita–Baylis–Hillman Reaction: ESI-MS(/MS) Investigation with Charge Tags and Ionic Liquid Effect Origin Revealed by DFT Calculations

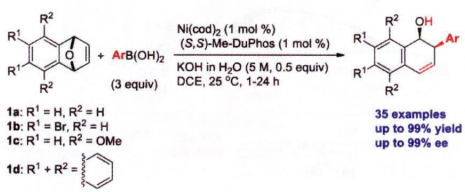
Thyago S. Rodrigues, Valter H. C. Silva, Priscila M. Lalli, Heibbe C. B. de Oliveira, Wender A. da Silva, Fernando Coelho, Marcos N. Eberlin, and Brenno A. D. Neto*



5249 (S) dx.doi.org/10.1021/jo500821m

Nickel-Catalyzed Asymmetric Ring Opening of Oxabenzonorbornadienes with Arylboronic Acids

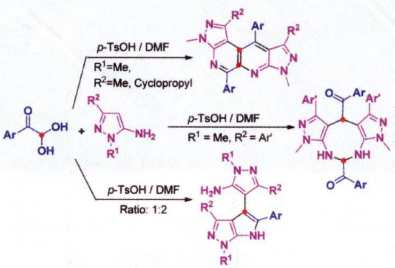
Zhongyi Zeng, Dingqiao Yang,* Yuhua Long,* Xuejing Pan, Guobao Huang, Xiongjun Zuo, and Wen Zhou



5258 (S) dx.doi.org/10.1021/jo500823z

Domino Reaction of Arylglyoxals with Pyrazol-5-amines: Selective Access to Pyrazolo-Fused 1,7-Naphthyridines, 1,3-Diazocanes, and Pyrroles

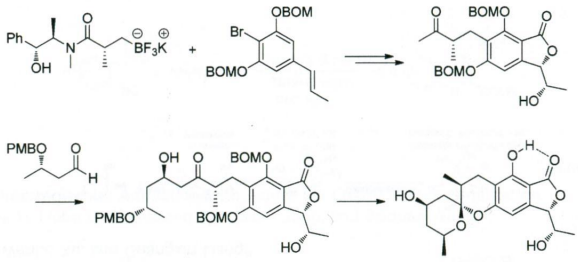
Bo Jiang,* Wei Fan, Mu-Yan Sun, Qin Ye, Shu-Liang Wang, Shu-Jiang Tu,* and Guigen Li



5269 dx.doi.org/10.1021/jo5008527

Total Synthesis of Virgatolide B via Exploitation of Intramolecular Hydrogen Bonding

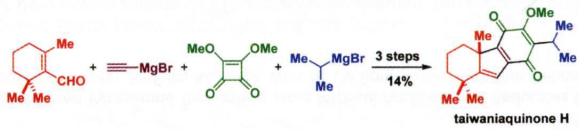
Paul A. Hume, Daniel. P. Furkert, and Margaret A. Brimble*



5282 dx.doi.org/10.1021/jo5008652

Protecting-Group-Free Synthesis of Taiwaniaquinone H Using a One-Pot Thermal Ring Expansion/4π-Electrocyclization Strategy

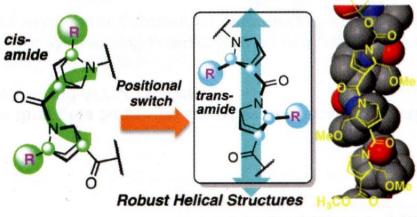
Xiuxiang Yan and Xiangdong Hu*



5287 dx.doi.org/10.1021/jo500916j

Robust *trans*-Amide Helical Structure of Oligomers of Bicyclic Mimics of β-Proline: Impact of Positional Switching of Bridgehead Substituent on Amide *cis*–*trans* Equilibrium

Siyuan Wang, Yuko Otani,* Xin Liu, Masatoshi Kawahata, Kentaro Yamaguchi, and Tomohiko Ohwada*

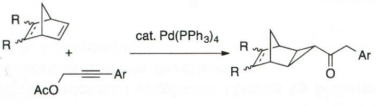


Notes

5301 dx.doi.org/10.1021/jo500357f

Palladium-Catalyzed α-Ketocyclopropanation of Norbornenes with Propargyl Acetates

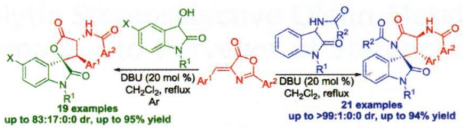
Yuta Tanioka and Naofumi Tsukada*



5305 S dx.doi.org/10.1021/jo500432c

Tandem Michael Addition–Ring Transformation Reactions of 3-Hydroxyoxindoles/3-Aminooxindoles with Olefinic Azlactones: Direct Access to Structurally Diverse Spirocyclic Oxindoles

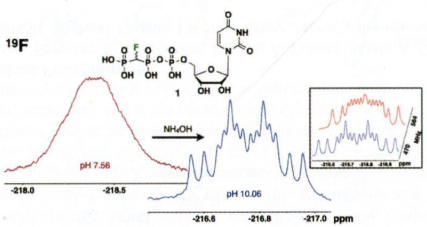
Bao-Dong Cui, Jian Zuo, Jian-Qiang Zhao, Ming-Qiang Zhou, Zhi-Jun Wu, Xiao-Mei Zhang, and Wei-Cheng Yuan*



5315 S dx.doi.org/10.1021/jo500452b

On the Observation of Discrete Fluorine NMR Spectra for Uridine 5′-β,γ-Fluoromethylenetriphosphate Diastereomers at Basic pH

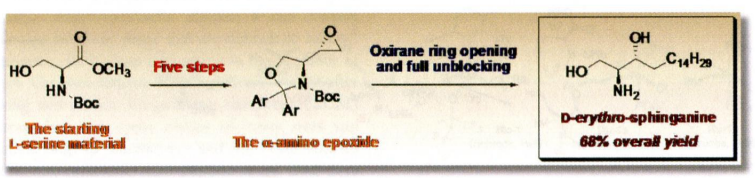
Candy S. Hwang, Boris A. Kashemirov, and Charles E. McKenna*



5320 S dx.doi.org/10.1021/jo500493c

Synthesis of D-*erythro*-Sphinganine through Serine-Derived α-Amino Epoxides

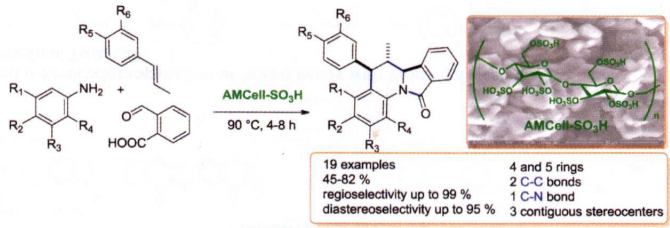
Carlo Siciliano,* Anna Barattucci, Paola Bonaccorsi, Maria Luisa Di Gioia, Antonella Leggio, Lucio Minuti, Emanuela Romio, and Andrea Temperini



5327 (S) dx.doi.org/10.1021/jo500516c

Diastereoselective Synthesis of Dihydroisoindolo[2,1-*a*]quinolin-11-ones by Solvent-Free AMCell-SO_3H-Catalyzed Imino Diels–Alder/Intramolecular Amide Cyclization Cascade Reactions

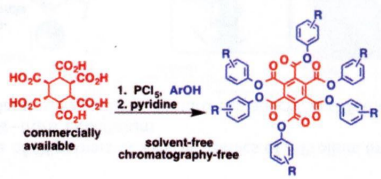
Diego R. Merchán Arenas and Vladimir V. Kouznetsov*



5334 (S) dx.doi.org/10.1021/jo5005185

Access to Aryl Mellitic Acid Esters through a Surprising Oxidative Esterification Reaction

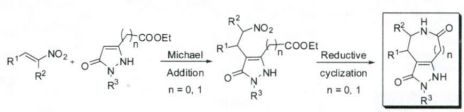
Margarita R. Geraskina, Mark J. Juetten, and Arthur H. Winter*



5338 (S) dx.doi.org/10.1021/jo5005795

Synthetic Protocol toward Fused Pyrazolone Derivatives via a Michael Addition and Reductive Ring Closing Strategy

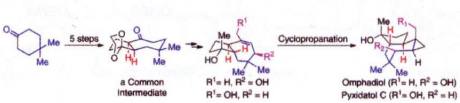
Nikita Parekh, Joice Thomas, Jubi John, Radhika Kusurkar, Wim M. De Borggraeve, and Wim Dehaen*



5345 (S) dx.doi.org/10.1021/jo5006125

Total Syntheses of (±)-Omphadiol and (±)-Pyxidatol C through a *Cis*-Fused 5,7-Carbocyclic Common Intermediate

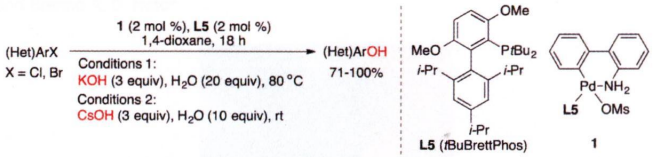
Lili Zhou, Yanmin Yao, Wenbo Xu, and Guangxin Liang*



5351 S dx.doi.org/10.1021/jo500662s

Palladium-Catalyzed Hydroxylation of Aryl and Heteroaryl Halides Enabled by the Use of a Palladacycle Precatalyst

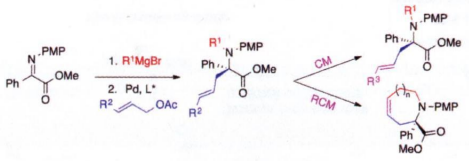
Chi Wai Cheung and Stephen L. Buchwald*



5359 S dx.doi.org/10.1021/jo500707t

α-Allyl-α-aryl α-Amino Esters in the Asymmetric Synthesis of Acyclic and Cyclic Amino Acid Derivatives by Alkene Metathesis

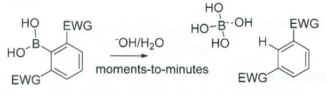
John M. Curto and Marisa C. Kozlowski*



5365 S dx.doi.org/10.1021/jo500734z

Base-Promoted Protodeboronation of 2,6-Disubstituted Arylboronic Acids

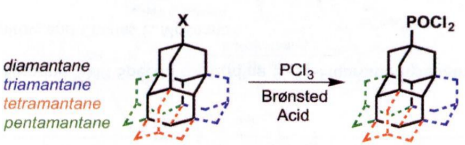
Jerome Lozada, Zhibo Liu, and David M. Perrin*



5369 S dx.doi.org/10.1021/jo500793m

Selective Preparation of Diamondoid Phosphonates

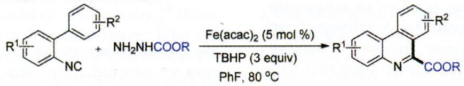
Andrey A. Fokin,* Raisa I. Yurchenko, Boryslav A. Tkachenko, Natalie A. Fokina, Maria A. Gunawan, Didier Poinsot, Jeremy E. P. Dahl, Robert M. K. Carlson, Michael Serafin, Hélène Cattey, Jean-Cyrille Hierso,* and Peter R. Schreiner*



5374 Ⓢ dx.doi.org/10.1021/jo500842e

Radical Arylalkoxycarbonylation of 2-Isocyanobiphenyl with Carbazates: Dual C–C Bond Formation toward Phenanthridine-6-carboxylates

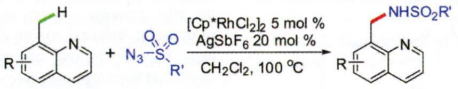
Changduo Pan, Jie Han, Honglin Zhang, and Chengjian Zhu*



5379 Ⓢ dx.doi.org/10.1021/jo5008515

Rhodium(III)-Catalyzed Intermolecular Amidation with Azides via C(sp^3)–H Functionalization

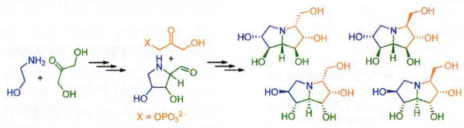
Nuancheng Wang, Renhe Li, Liubo Li, Shansheng Xu, Haibin Song, and Baiquan Wang*



5386 Ⓢ dx.doi.org/10.1021/jo500991p

Casuarine Stereoisomers from Achiral Substrates: Chemoenzymatic Synthesis and Inhibitory Properties

Alda Lisa Concia, Livia Gómez, Teodor Parella, Jesús Joglar, and Pere Clapés*



Additions and Corrections

5390 dx.doi.org/10.1021/jo5009977

Correction to $(DHQ)_2AQN$-Catalyzed Asymmetric Substitution of Isatin-Derived Hydrazones with O-Boc-Protected Morita–Baylis–Hillman Adducts: A Strategy for Synthesizing Enantioenriched Azo Compounds Incorporating an Oxindole Scaffold

Hai-Bin Yang, Yun-Zhou Zhao, Rui Sang, and Min Shi*

Ⓢ Supporting Information available via online article