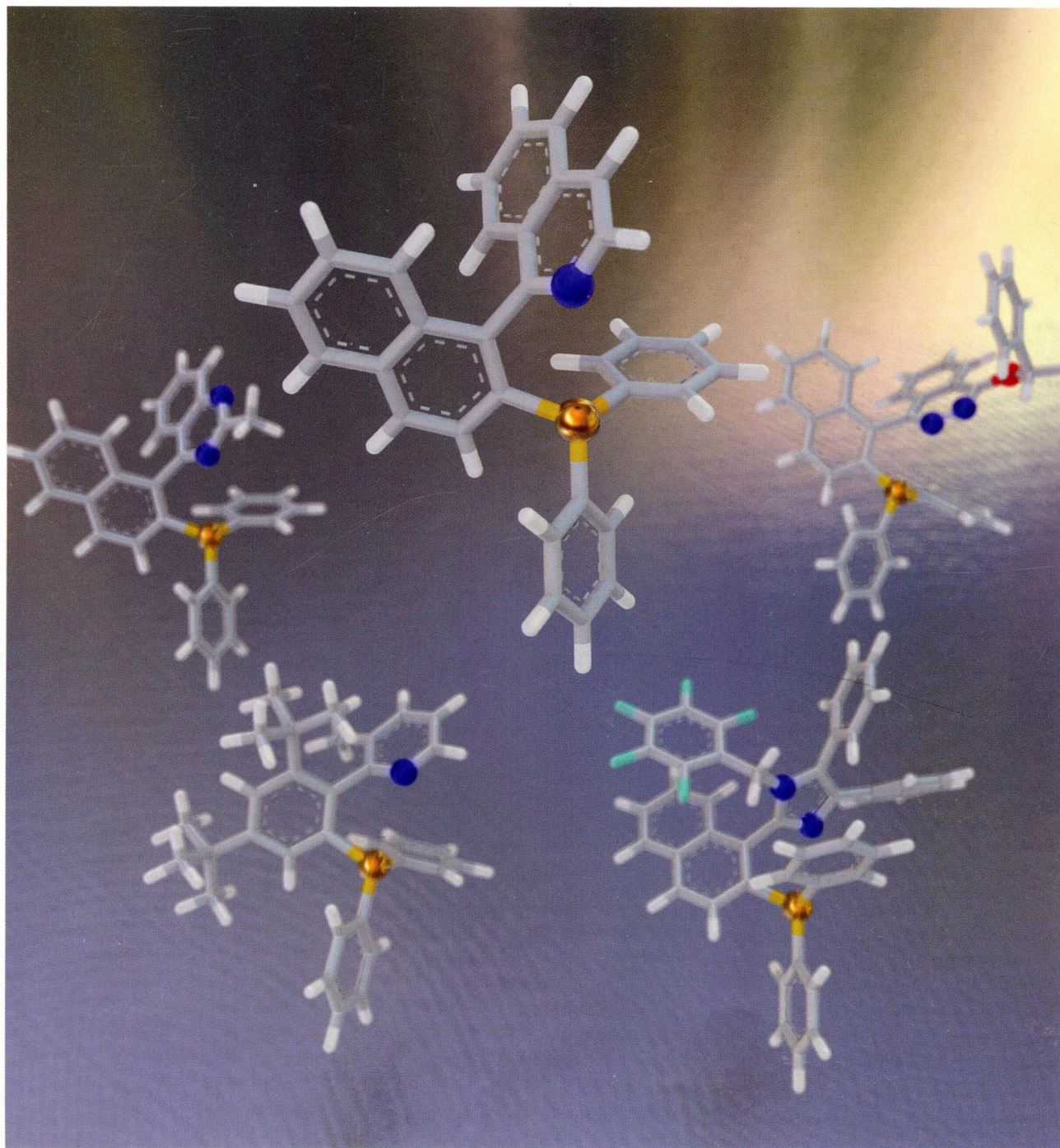


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# JOC

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**ON THE COVER:** Atropisomeric PN ligands have contributed to distinct areas of asymmetric catalysis, among them hydroboration, diboration, 1,3-dipolar cycloaddition, and alkylation. The cover paper describes developments in both ligand synthesis and application. See Brown and co-workers, p 5391. Professor Brown is the recipient of the 2013 RSC Robert Robinson Award.

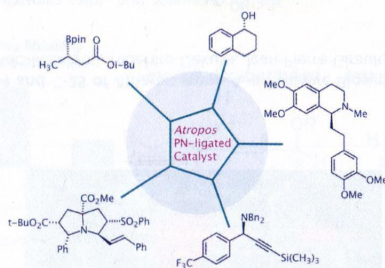
## Perspective

5391

[dx.doi.org/10.1021/jo500512s](https://doi.org/10.1021/jo500512s)

### Quinap and Congeners: Atropos PN ligands for Asymmetric Catalysis

Elena Fernández, Patrick J. Guiry, Kieran P. T. Connole, and John M. Brown\*



## Featured Articles

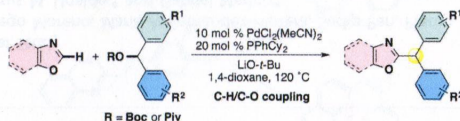
5401

5

[dx.doi.org/10.1021/jo501063e](https://doi.org/10.1021/jo501063e)

### Synthesis of Triarylmethanes by Palladium-Catalyzed C–H/C–O Coupling of Oxazoles and Diarylmethanol Derivatives

Sho Tabuchi, Koji Hirano,\* Tetsuya Satoh, and Masahiro Miura\*

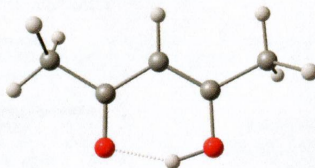


5412 **S**

dx.doi.org/10.1021/jo402814c

## Tautomeric Properties and Gas-Phase Structure of Acetylacetone

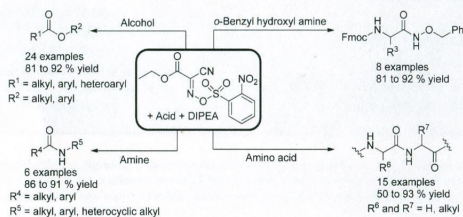
Natalya V. Belova, Heinz Oberhammer, Nguen Hoang Trang, and Georgiy V. Girichev\*

5420 **S**

dx.doi.org/10.1021/jo500292m

Ethyl 2-Cyano-2-(2-nitrobenzenesulfonyloxyimino)acetate (*o*-NosylOXY): A Recyclable Coupling Reagent for Racemization-Free Synthesis of Peptide, Amide, Hydroxamate, and Ester

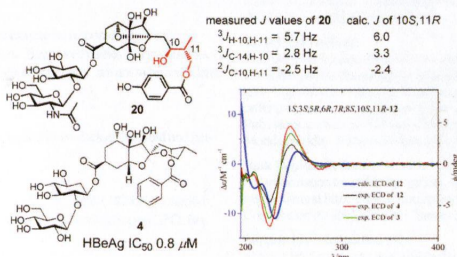
Dharm Dev, Nani Babu Palakurthy, Kishore Thalluri, Jyoti Chandra, and Bhubaneswar Mandal\*

5432 **S**

dx.doi.org/10.1021/jo5004604

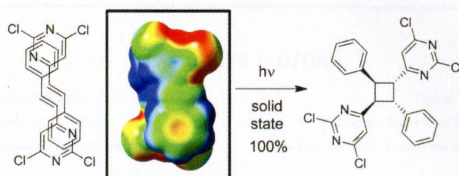
Anti-Hepatitis B Virus Norbisabolane Sesquiterpenoids from *Phyllanthus acidus* and the Establishment of Their Absolute Configurations Using Theoretical Calculations

Jun-Jiang Lv, Shan Yu, Ya-Feng Wang, Dong Wang, Hong-Tao Zhu, Rong-Rong Cheng, Chong-Ren Yang, Min Xu,\* and Ying-Jun Zhang\*



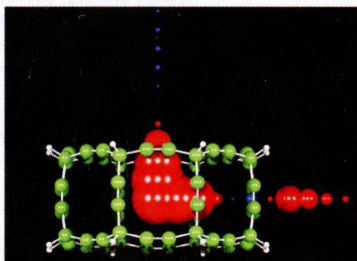
$\pi$ - $\pi$  Interaction Energies as Determinants of the Photodimerization of Mono-, Di-, and Triazastilbenes

Alexander A. Parent, Daniel H. Ess, and John A. Katzenellenbogen\*



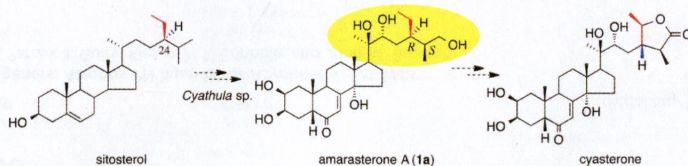
## Carbo-Cages: A Computational Study

Jon M. Azpiroz, Rafael Islas, Diego Moreno, María A. Fernández-Herrera, Sudip Pan, Pratim K. Chattaraj, Gerardo Martínez-Guajardo, Jesus M. Ugalde,\* and Gabriel Merino\*



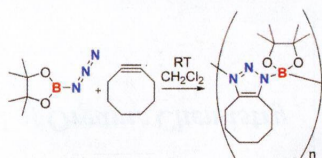
## Stereochemical Assignment of C-24 and C-25 of Amarasterone A, a Putative Biosynthetic Intermediate of Cyasterone

Yui Hirayama, Keiko Okuzumi, Hironori Masubuti, Hidehiro Uekusa, Jean-Pierre Girault, and Yoshinori Fujimoto\*



## Boryl Azides in 1,3-Dipolar Cycloadditions

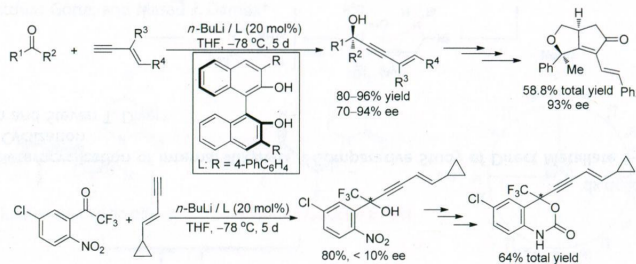
Matthias Müller, Cécilia Maichle-Mössmer, and Holger F. Bettinger\*





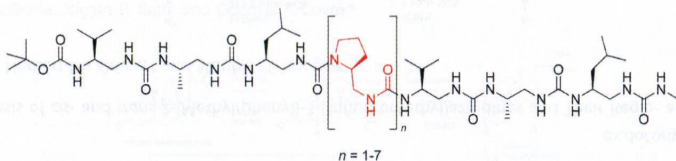
### Lithium Binaphtholate-Catalyzed Enantioselective Enyne Addition to Ketones: Access to Enynylated Tertiary Alcohols

Hua Cai, Jing Nie, Yan Zheng, and Jun-An Ma\*



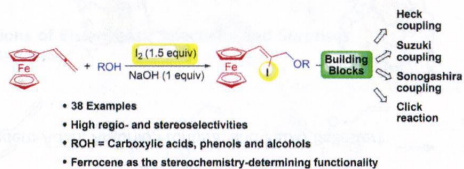
### Synthesis and Folding Propensity of Aliphatic Oligoureas Containing Repeats of Proline-Type Units

Juliette Fremaux, Brice Kauffmann, and Gilles Guichard\*

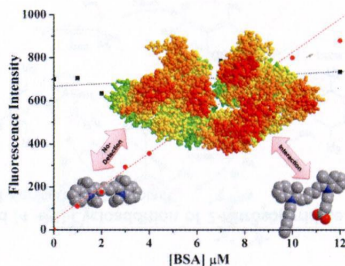


### Regio- and Stereoselective Synthesis of Ferrocene-Containing $\beta$ -Iodoallylic Esters and Ethers from the Iodofunctionalization of Ferrocenylallene with Carboxylic Acids, Phenols, and Alcohols

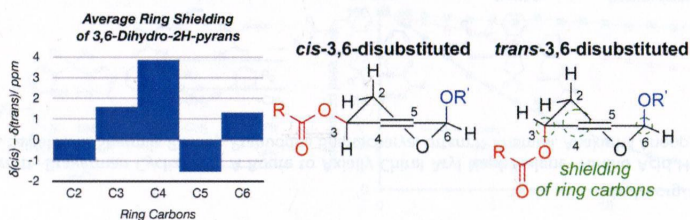
Shufeng Chen,\* Hongli Zhang, Qing Yan, Chenjun Wang, Fei Han, Kaixin Zhang, Haiying Zhao, and Baoguo Li\*



**Symmetrical and Asymmetrical Cyanine Dyes. Synthesis, Spectral Properties, and BSA Association Study**  
 Diego S. Pisoni, Leticia Todeschini, Antonio César A. Borges, Cesar L. Petzhold, Fabiano S. Rodembusch,\* and Leandra F. Campo\*

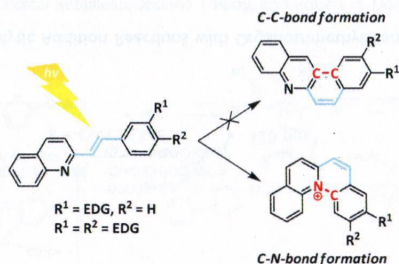


**<sup>13</sup>C NMR Analysis of 3,6-Dihydro-2H-pyrans: Assignment of Remote Stereochemistry Using Axial Shielding Effects**  
 Mark J. Bartlett, Peter T. Northcote, Matthias Lein,\* and Joanne E. Harvey\*



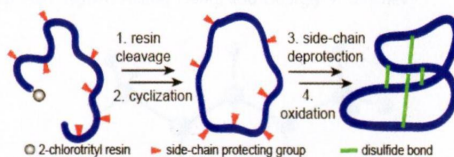
**Regiospecific C–N Photocyclization of 2-Styrylquinolines**

Elena N. Gulakova, Daria V. Berdnikova,\* Tseimur M. Aliyev, Yuri V. Fedorov, Ivan A. Godovikov, and Olga A. Fedorova

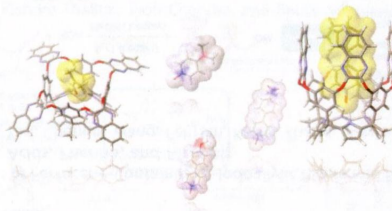


**Fmoc-Based Synthesis of Disulfide-Rich Cyclic Peptides**

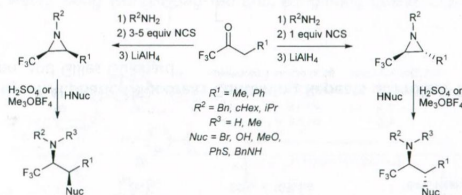
Olivier Cheneval, Christina I. Schroeder, Thomas Durek, Phillip Walsh, Yen-Hua Huang, Spiros Liras, David A. Price, and David J. Craik\*

**Synthesis, Structure, and Binding Properties of Lipophilic Cavitands Based on a Calix[4]pyrrole-Resorcinarene Hybrid Scaffold**

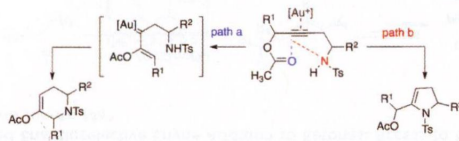
Albano Galán, Eduardo C. Escudero-Adán, Antonio Frontera, and Pablo Ballester\*

**Selective Synthesis of *cis*- and *trans*-2-(Methyl/phenyl)-3-(trifluoromethyl)aziridines and Their Regio- and Stereospecific Ring Opening**

Matthias Moens, Norbert De Kimpe,\* and Matthias D'hooghe\*

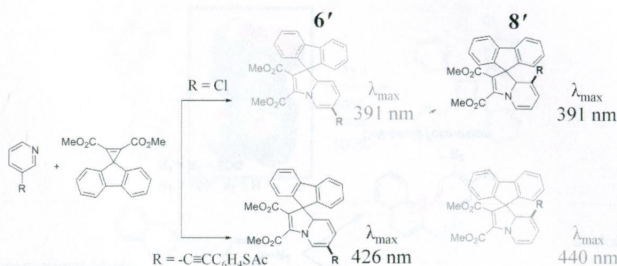
**Gold(I)-Promoted Heterocyclization of Internal Alkynes: A Comparative Study of Direct Metallate *5-endo-dig* Cyclization versus a Stepwise Cyclization**

Jonathan M. French and Steven T. Diver\*



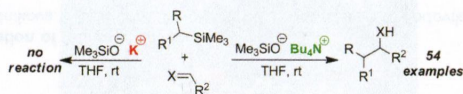
### Substituent Parameters Impacting Isomer Composition and Optical Properties of Dihydroindolizine Molecular Switches

Matthew A. Bartucci and Jacob W. Ciszek\*



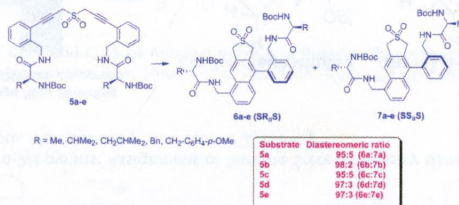
### $Bu_4N^+$ Alkoxide-Initiated/Autocatalytic Addition Reactions with Organotrimethylsilanes

Manas Das and Donal F. O'Shea\*



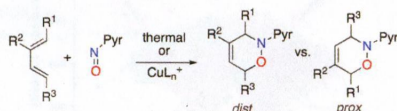
### Asymmetric Garratt–Braverman Cyclization: A Route to Axially Chiral Aryl Naphthalene–Amino Acid Hybrids

Tapobrata Mitra, Saibal Jana, Sharmila Pandey, Prabuddha Bhattacharya, Uttam K. Khamrai, Anakuthil Anoop,\* and Amit Basak\*



### Regioselectivity in the Cu(I)-Catalyzed [4 + 2]-Cycloaddition of 2-Nitrosopyridine with Unsymmetrical Dienes

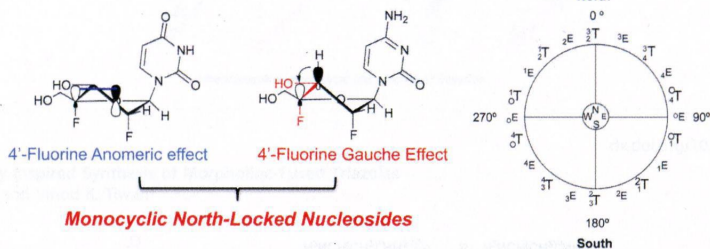
Anh T. Tran, Peng Liu, K. N. Houk, and Kenneth M. Nicholas\*





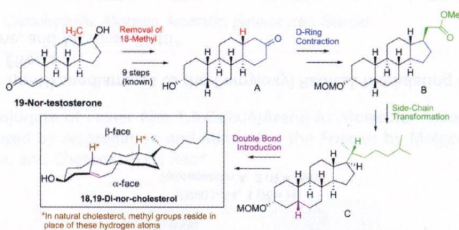
### Rigid 2',4'-Difluororibonucleosides: Synthesis, Conformational Analysis, and Incorporation into Nascent RNA by HCV Polymerase

Saúl Martínez-Montero, Glen F. Deleavey, Anupriya Kulkarni, Nerea Martín-Pintado, Petra Lindovska, Michael Thomson, Carlos González, Matthias Götte, and Masad J. Damha\*



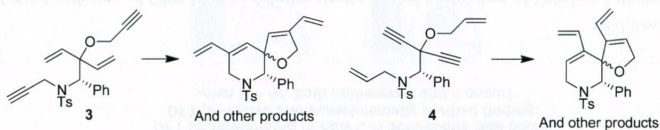
### Synthesis of a Smoothened Cholesterol: 18,19-Di-nor-cholesterol

Laurel Mydock-McGrane, Nigam P. Rath, and Douglas F. Covey\*



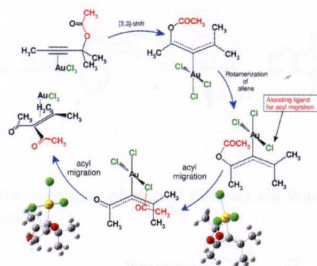
### Ring-Closing Metathesis Reactions of Bis(enynes): Selectivity and Surprises

Debra J. Wallace\* and Robert A. Reamer

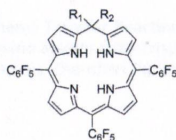


**Ligand-Assisted Acyl Migration in Au-Catalyzed Isomerization of Propargylic Ester to Diketone: A DFT Study**

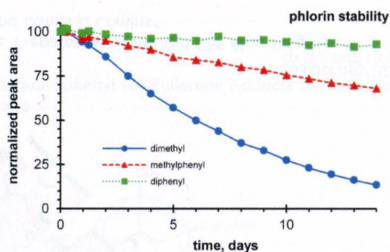
Animesh Ghosh, Atanu Basak, Kuheli Chakrabarty, Boyli Ghosh, and Gourab Kanti Das\*

**Phlorins Bearing Different Substituents at the  $sp^3$ -Hybridized Meso-Position**

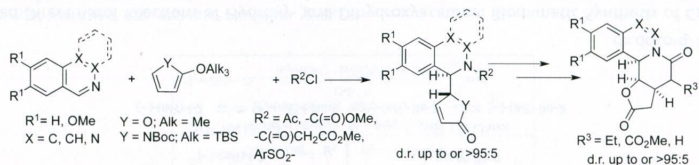
Alexandra M. Bruce, Emily S. Weyburne, James T. Engle, Christopher J. Ziegler,\* and G. Richard Geier III\*



R <sub>1</sub>	R <sub>2</sub>
-CH <sub>3</sub>	-CH <sub>3</sub>
-CH <sub>3</sub>	-Ph
-Ph	-Ph

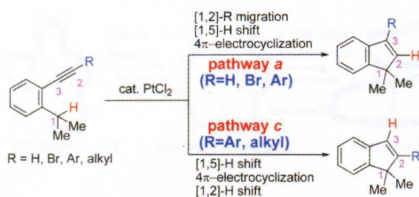
**Diastereoselective Three-Component Vinyllogous Mannich Reaction of Nitrogen Heterocycles, Acyl/Sulfonyl Chlorides, and Silyloxyfurans/pyrroles**

Simon Janody, Philippe Hermange, Pascal Retailleau, Josiane Thierry, and Robert H. Dodd\*



### Mechanisms of the PtCl<sub>2</sub>-Catalyzed Intramolecular Cyclization of *o*-Isopropyl-Substituted Aryl Alkynes for the Synthesis of Indenes and Comparison of Three sp<sup>3</sup> C–H Bond Activation Modes

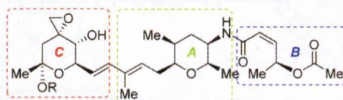
Yi Wang, Wei Liao, Genping Huang, Yuanzhi Xia, and Zhi-Xiang Yu\*



DFT understanding of how C-H activations take place;  
DFT predicted and experimentally verified finding:  
when R = Ar, both pathways a and c occur!

### Enantioselective Total Syntheses of FR901464 and Spliceostatin A and Evaluation of Splicing Activity of Key Derivatives

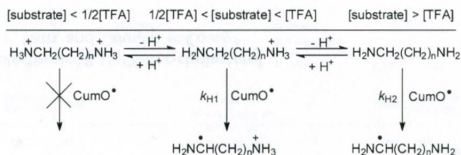
Arun K. Ghosh,\* Zhi-Hua Chen, Kerstin A. Effenberger, and Melissa S. Jurica



FR901464, **1** (R = H)  
Spliceostatin A, **2** (R = Me)

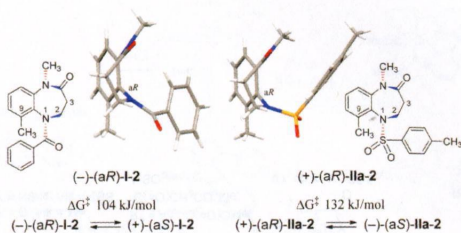
### Hydrogen Atom Transfer from 1,*n*-Alkanediamines to the Cumyloxy Radical. Modulating C–H Deactivation Through Acid–Base Interactions and Solvent Effects

Michela Milan, Michela Salamone, and Massimo Bietti\*

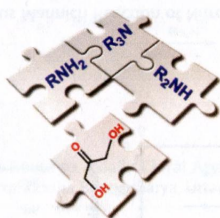




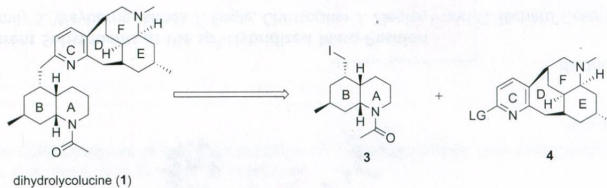
***N*-Benzoyl- and *N*-Sulfonyl-1,5-benzodiazepines: Comparison of Their Atropisomeric and Conformational Properties**  
Tetsuya Yoneda, Hidetsugu Tabata, Jun Nakagomi, Tomohiko Tasaka, Tetsuta Oshitari, Hideyo Takahashi, and Hideaki Natsugari\*



**Amine-Catalyzed Direct Aldol Reactions of Hydroxy- and Dihydroxyacetone: Biomimetic Synthesis of Carbohydrates**  
Oskar Popik, Monika Pasternak-Suder, Katarzyna Leśniak, Magdalena Jawiczuk, Marcin Górecki, Jadwiga Frelek, and Jacek Mlynarski\*

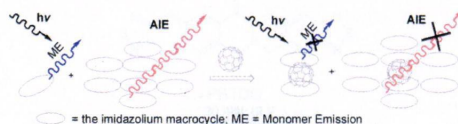


**Studies toward the Total Synthesis of Dihydrolycolucine. Preparation of AB and CEF Ring Fragments**  
Brandon M. Cash, Natacha Prevost, Florence F. Wagner, and Daniel L. Comins\*



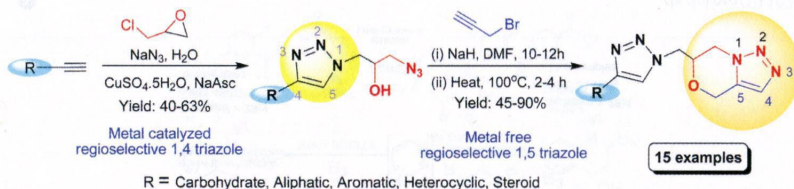
### Monomer Emission and Aggregate Emission of an Imidazolium Macrocycle Based on Bridged Tetraphenylethylene and Their Quenching by C<sub>60</sub>

Jin-Hua Wang, Hai-Tao Feng, Jun Luo, and Yan-Song Zheng\*



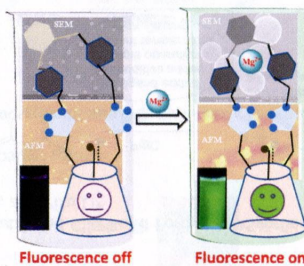
### Click Chemistry Inspired Synthesis of Morpholine-Fused Triazoles

Kunj B. Mishra and Vinod K. Tiwari\*



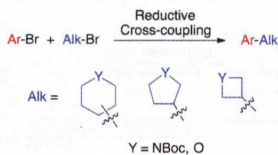
### Phenylene-Diimine-Capped Conjugate of Lower Rim 1,3-Calix[4]Arene As Molecular Receptor for Mg<sup>2+</sup> via Ar Conformational Changes Followed by Aggregation and Mimicking the Species by Molecular Mechanics

Anita Nehra, Vijaya Kumar Hinge, and Chebrolu Pulla Rao\*



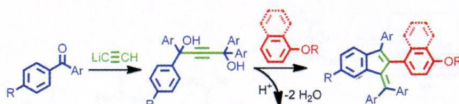
### Reductive Cross-Coupling of Nonaromatic, Heterocyclic Bromides with Aryl and Heteroaryl Bromides

Gary A. Molander,\* Kaitlin M. Traister, and Brian T. O'Neill



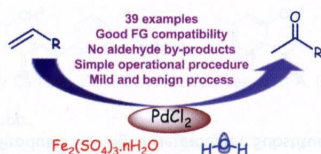
### Acid-Catalyzed Domino Reactions of Tetraarylbut-2-yne-1,4-diols. Synthesis of Conjugated Indenes and Inden-2-ones

Céu M. Sousa, Jerome Berthet, Stephanie Delbaere, and Paulo J. Coelho\*



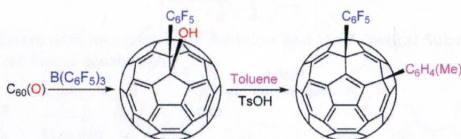
### Iron(III) Sulfate as Terminal Oxidant in the Synthesis of Methyl Ketones via Wacker Oxidation

Rodney A. Fernandes\* and Dipali A. Chaudhari



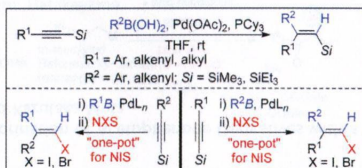
### Pentafluorophenyl Transfer Reaction: Preparation of Pentafluorophenyl [60]Fullerene Adducts through Opening of Fullerene Epoxide Moiety with Trispentafluorophenylborane

Sisi Liang, Liang Xu, Zhenshan Jia, and Liangbing Gan\*



### Pd-Catalyzed Regio- and Stereoselective Addition of Boronic Acids to Silylacetylenes: A Stereodivergent Assembly of $\beta,\beta$ -Disubstituted Alkenylsilanes and Alkenyl Halides

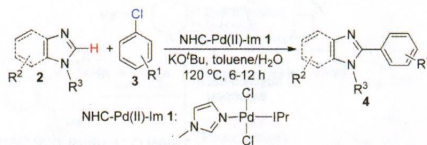
Wei Kong, Chao Che, Jialin Wu, Lai Ma, and Gangguo Zhu\*





### N-Heterocyclic Carbene-Palladium(II)-1-Methylimidazole Complex-Catalyzed Direct C–H Bond Arylation of (Benz)imidazoles with Aryl Chlorides

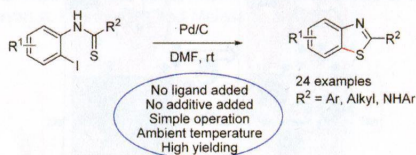
Zheng-Song Gu, Wen-Xin Chen, and Li-Xiong Shao\*



## Notes

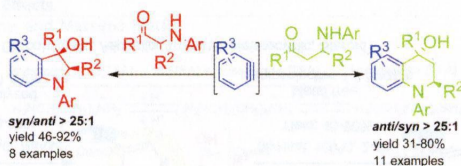
### Room-Temperature Ligand-Free Pd/C-Catalyzed C–S Bond Formation: Synthesis of 2-Substituted Benzothiazoles

Yannan Cheng, Qian Peng, Weigang Fan, and Pixu Li\*



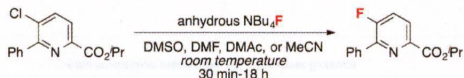
### Diastereoselective Synthesis of *N*-Aryl Tetrahydroquinolines and *N*-Aryl Indolines by the Tandem Reaction of Arynes

Ji-Xin Pian, Lin He,\* Guang-Fen Du, Hao Guo, and Bin Dai\*



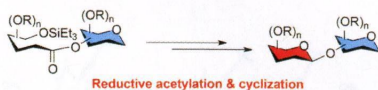
### Mild Fluorination of Chloropyridines with In Situ Generated Anhydrous Tetrabutylammonium Fluoride

Laura J. Allen, Joseck M. Muhuhi, Douglas C. Bland, Rachel Merzel, and Melanie S. Sanford\*

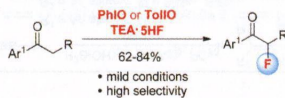


## A Stereoselective Ring-Closing Glycosylation via Nonglycosylating Pathway

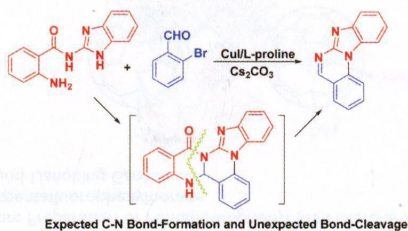
Han Liu and Xuechen Li\*

Hypervalent Iodine-Promoted  $\alpha$ -Fluorination of Acetophenone Derivatives with a Triethylamine-HF Complex

Tsugio Kitamura,\* Kensuke Muta, and Kazutaka Muta

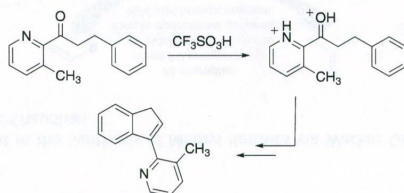
CuI-Catalyzed C–N Bond Formation and Cleavage for the Synthesis of Benzimidazo[1,2-*a*]quinazoline Derivatives

Chao Li, Wen-Ting Zhang, and Xiang-Shan Wang\*



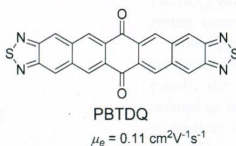
## Cyclodehydrations Leading to Indene Products Having N-Heterocyclic Substituents

Kenneth N. Boblak and Douglas A. Klumpp\*



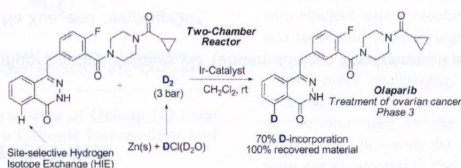
### Pentacenobis(thiadiazole)dione, an n-Type Semiconductor for Field-Effect Transistors

Zi-Fa Shi, Hayden T. Black, Afshin Davdand, and Dmitrii F. Perepichka\*



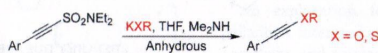
### Two-Chamber Hydrogen Generation and Application: Access to Pressurized Deuterium Gas

Amalie Modvig, Thomas L. Andersen, Rolf H. Taaning, Anders T. Lindhardt,\* and Troels Skrydstrup\*



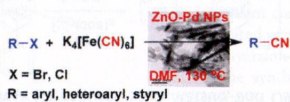
### Transition-Metal-Free Synthesis of Ynol Ethers and Thioynol Ethers via Displacement at sp Centers: A Revised Mechanistic Pathway

Vincent James Gray, James Cuthbertson, and Jonathan D. Wilden\*



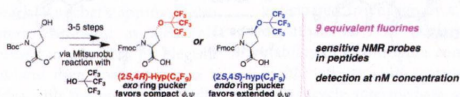
### ZnO-Supported Pd Nanoparticle-Catalyzed Ligand- and Additive-Free Cyanation of Unactivated Aryl Halides Using $\text{K}_4[\text{Fe}(\text{CN})_6]$

Tanmay Chatterjee, Raju Dey, and Brindaban C. Ranu\*



### (2*S*,4*R*)- and (2*S*,4*S*)-Perfluoro-*tert*-butyl 4-Hydroxyproline: Two Conformationally Distinct Proline Amino Acids for Sensitive Application in $^{19}\text{F}$ NMR

Caitlin M. Tressler and Neal J. Zondlo\*



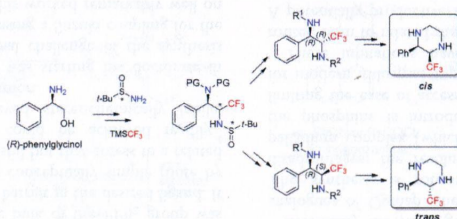


5887 **5**

dx.doi.org/10.1021/jo500832j

**Diastereoselective Synthesis of 2-Phenyl-3-(trifluoromethyl)piperazines as Building Blocks for Drug Discovery**

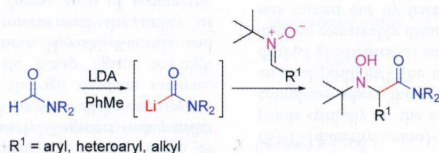
María Sánchez-Roselló,\* Oscar Delgado,\* Natalia Mateu, Andrés A. Trabanco, Michiel Van Gool, and Santos Fustero\*

5895 **5**

dx.doi.org/10.1021/jo500848a

**Carbamoyl Anion Addition to Nitrones**

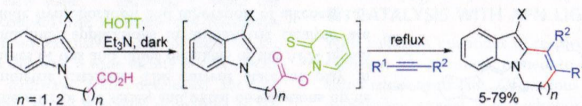
Jonathan T. Reeves,\* Chris Lorenc, Kaddy Camara, Zhibin Li, Heewon Lee, Carl A. Busacca, and Chris H. Senanayake

5903 **5**

dx.doi.org/10.1021/jo5008543

**Tandem Reactions via Barton Esters with Intermolecular Addition and Vinyl Radical Substitution onto Indole**

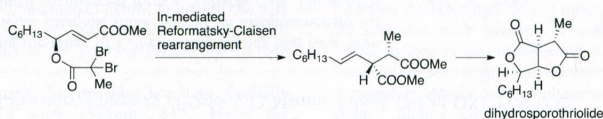
Robert Coyle, Patrick McArdle, and Fawaz Aldabbagh\*

5908 **5**

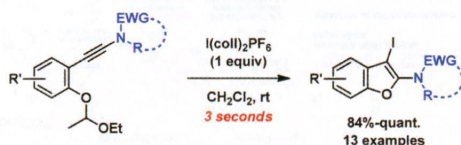
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**Total Synthesis of (–)-Dihydrospirothriolide Utilizing an Indium-Mediated Reformatsky–Claisen Rearrangement**

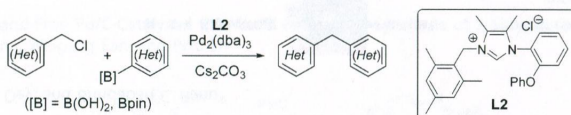
Jun Ishihara,\* Hiroaki Tsuru, and Susumi Hatakeyama



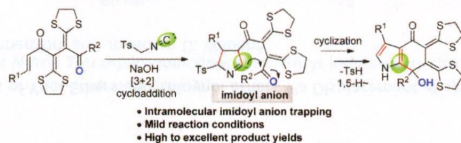
**Indocyclization of Ethoxyethyl Ethers to Ynamides: An Immediate Construction to Benzo[b]furans**  
 Takashi Okitsu,\* Kohei Nakata, Kenji Nishigaki, Naoyuki Michioka, Mitsuaki Karatani, and Akimori Wada



**Palladium-Catalyzed Synthesis of Heterocycle-Containing Diarylmethanes through Suzuki–Miyaura Cross-Coupling**  
 Masami Kuriyama,\* Mina Shinozawa, Norihisa Hamaguchi, Seira Matsuo, and Osamu Onomura\*



**Bicyclization of Isocyanides with Alkenoyl Bis(ketene dithioacetals): Access to 6,7-Dihydro-1*H*-indol-4(5*H*)-ones**  
 Yifei Li, Xianxiu Xu,\* Hui Shi, Ling Pan, and Qun Liu\*



## Additions and Corrections

**Correction to “Synthesis of Trifluoromethyl Ketones via Tandem Claisen Condensation and Retro-Claisen C–C Bond Cleavage Reaction”**

Dongmei Yang, Yuhan Zhou,\* Na Xue, and Jingping Qu\*

**Correction to Ring Expansion of Cyclic  $\beta$ -Amino Alcohols Induced by Diethylaminosulfur Trifluoride: Synthesis of Cyclic Amines with a Tertiary Fluoride at C3**

Bruno Anxionnat, Benoit Robert, Pascal George, Gino Ricci, Marc-Antoine Perrin, Domingo Gomez Pardo,\* and Janine Cossy\*