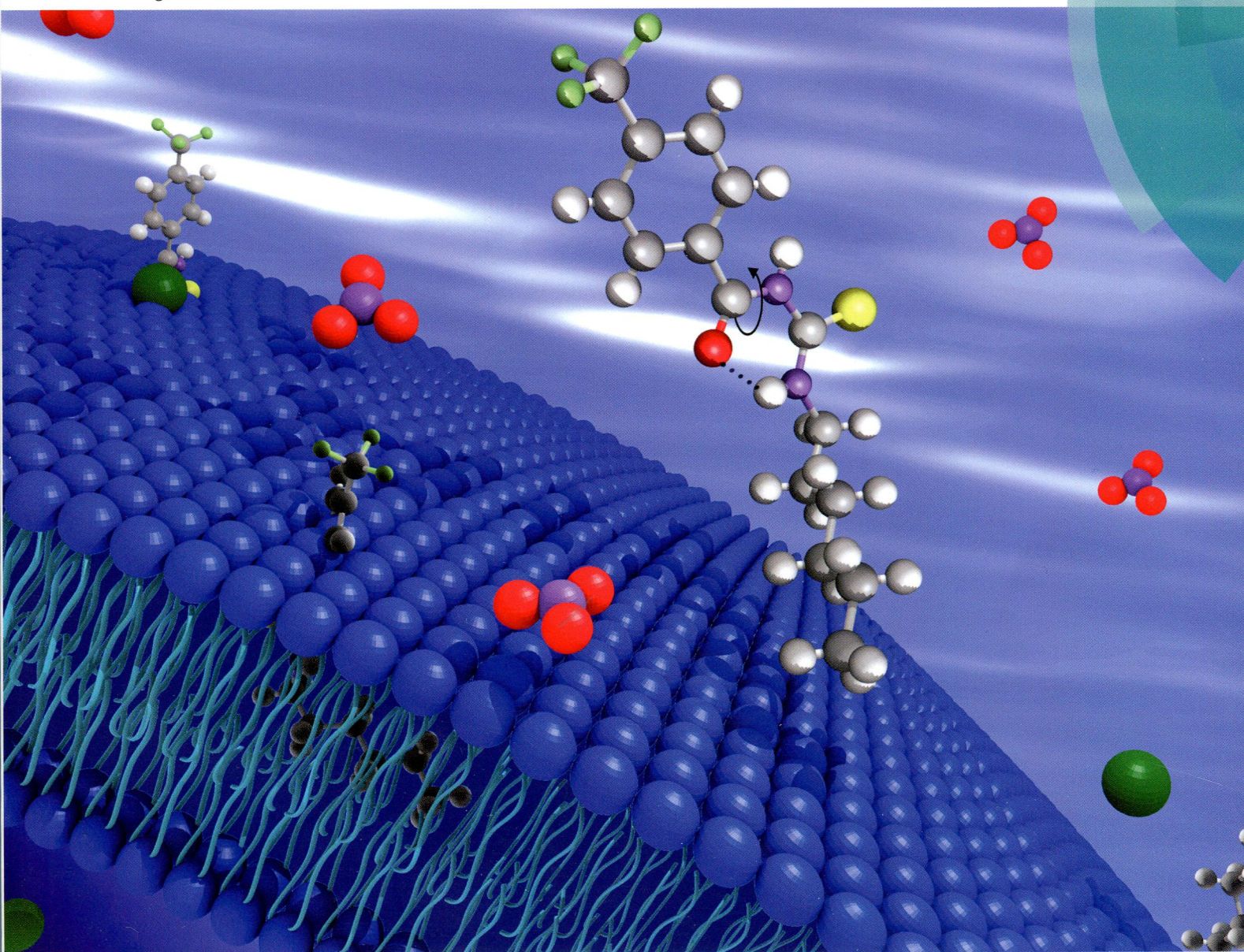


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PAPER

Philip A. Gale *et al.*
Acylthioureas as anion transporters: the effect of intramolecular hydrogen bonding

Organic & Biomolecular Chemistry

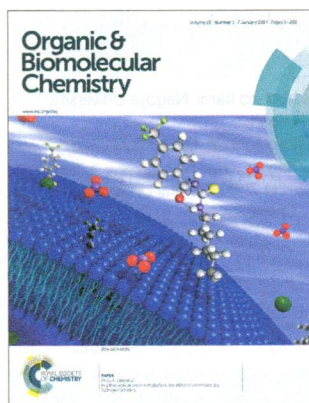
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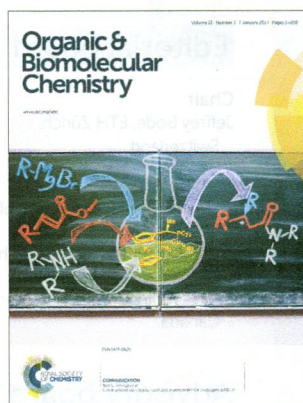
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Cover

See Philip A. Gale *et al.*,
pp. 62–72.

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Inside cover

See Ben L. Feringa *et al.*,
pp. 36–41.

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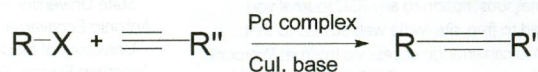
REVIEW

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To be or not to be metal-free: trends and advances in coupling chemistries

Rick Arneil D. Arancon,* Carol Sze Ki Lin,
Carolina Vargas and Rafael Luque*

Coupling reactions have been part of several extensive studies in order to develop innovative and greener protocols that can generate a wide range of compounds with applications in pharmaceuticals, agrochemicals and biologically active compounds.



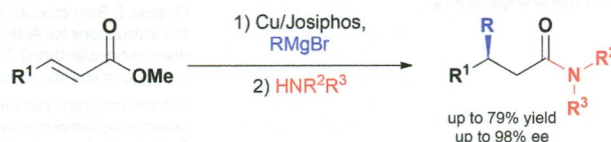
COMMUNICATIONS

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Chiral amides via copper-catalysed enantioselective conjugate addition

Anne K. Schoonen, M. Ángeles Fernández-Ibáñez,
Martín Fañanás-Mastral, Johannes F. Teichert and
Ben L. Feringa*

A highly enantioselective one pot procedure for the synthesis of β -substituted amides was developed using copper-catalysed enantioselective conjugate addition to α,β -unsaturated esters and subsequent quenching of the intermediate enolate with an amine.



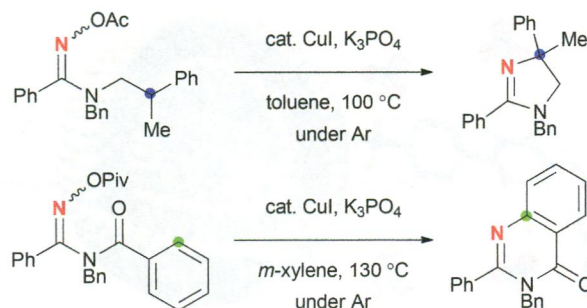
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Уральского отделения
Российской академии наук (ЦНБ УрО РАН)

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Copper-catalyzed redox-neutral C–H amination with amidoximes

Hui Chen and Shunsuke Chiba*

CuI-catalyzed reactions of *N*-alkylamidoximes afforded dihydroimidazoles *via* sp^3 C–H amination. On the other hand, the reactions of *N*-benzoylamidoximes resulted in sp^2 C–H amination to form quinazolinones. The reaction mechanisms could be characterized as a redox-neutral radical pathway including a Cu(I)–Cu(II) redox catalytic cycle.

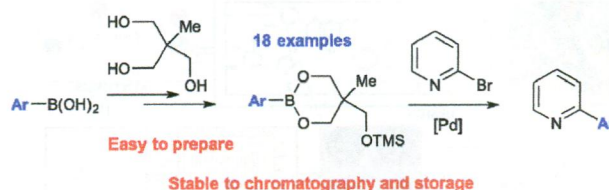


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Silyl-protected dioxaborinanes: application in the Suzuki cross-coupling reaction

Sean Goggins, Eleanor Rosevere, Clément Bellini, Joseph C. Allen, Barrie J. Marsh, Mary F. Mahon and Christopher G. Frost*

The synthesis of a range of novel silyl-protected dioxaborinanes as a column- and bench-stable boron reagent were found to be advantageous to achieving good yields of 2-arylpyridines *via* palladium-catalysed cross-coupling reactions.

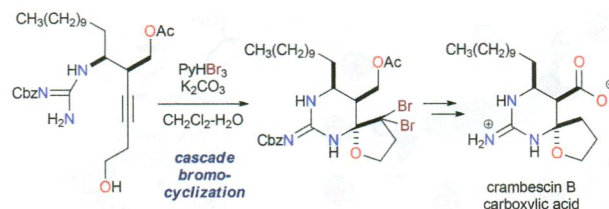


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Synthesis of crambescic acid, a potent inhibitor of voltage-gated sodium channels

Atsuo Nakazaki, Yuki Ishikawa, Yusuke Sawayama, Mari Yotsu-Yamashita and Toshio Nishikawa*

Stereocontrolled cascade cyclization of a guanidino-acetylene with bromocyclizations provided crambescic acid, which exhibited a potent inhibitory activity of voltage-gated sodium channels.

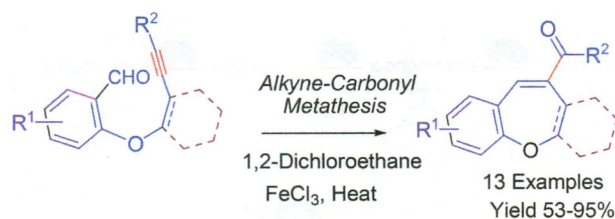


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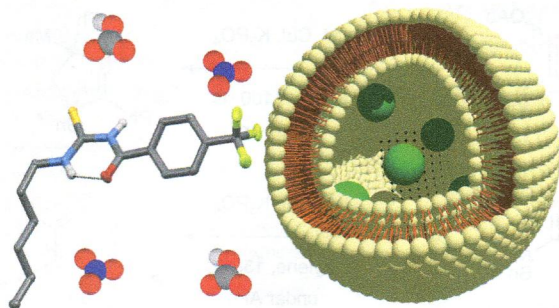
FeCl₃-catalyzed synthesis of functionally diverse dibenzo[*b,f*]oxepines and benzo[*b*]oxepines *via* alkyne–aldehyde metathesis

Krishnendu Bera, Swapnadeep Jalal, Soumen Sarkar and Umasish Jana*

An efficient synthesis of dibenzo[*b,f*]oxepines and benzo[*b*]oxepines *via* FeCl₃-catalyzed alkyne–aldehyde metathesis reaction is described.



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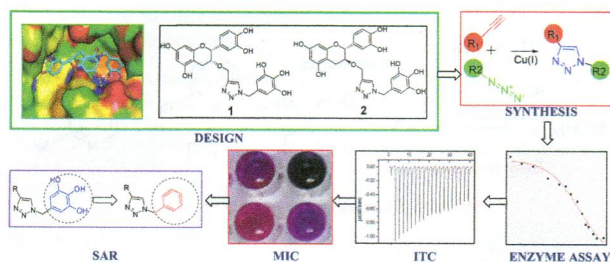


Acylthioureas as anion transporters: the effect of intramolecular hydrogen bonding

Cally J. E. Haynes, Nathalie Busschaert, Isabelle L. Kirby, Julie Herniman, Mark E. Light, Neil J. Wells, Igor Marques, Vitor Félix and Philip A. Gale*

The effects of intramolecular hydrogen bonding on the efficiency of anion transport are explored in a series of acylthioureas.

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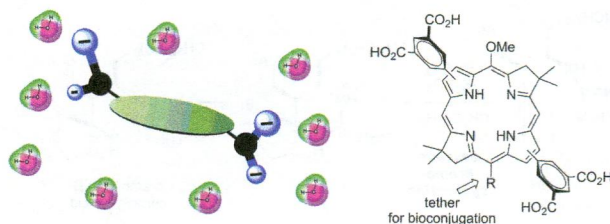


Design, synthesis and characterization of novel inhibitors against mycobacterial β -ketoacyl CoA reductase FabG4

Deb Ranjan Banerjee, Debajyoti Dutta, Baisakhee Saha, Sudipta Bhattacharyya, Kalyan Senapati, Amit K. Das* and Amit Basak*

We report the design and synthesis of triazole-polyphenol hybrid compounds **1** and **2** as inhibitors of the FabG4 (Rv0242c) enzyme of *Mycobacterium tuberculosis* for the first time.

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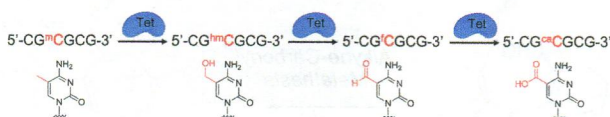


Hydrophilic tetracarboxy bacteriochlorins for photonics applications

Jianbing Jiang, Potheppan Vairaprakash, Kanumuri Ramesh Reddy, Tuba Sahin, M. Phani Pavan, Elisa Lubian and Jonathan S. Lindsey*

A new molecular design affords near-infrared absorbing fluorophores that are soluble in aqueous media and can be equipped with a bioconjugatable handle.

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CGmCGCG is a versatile substrate with which to evaluate Tet protein activity

Seiichiro Kizaki and Hiroshi Sugiyama*

Tet family proteins have the ability to convert 5-methylcytosine (mC) to 5-hydroxymethylcytosine, and further to 5-formylcytosine and 5-carboxycytosine.

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A step toward polytwistane: synthesis and characterization of C_2 -symmetric tritwistane

Martin Olbrich, Peter Mayer and Dirk Trauner*

Twistane is a classic hydrocarbon with fascinating stereochemical properties. Herein we describe a series of oligomers of twistane that converges on a chiral nanorod, which we term polytwistane. A member of this series, C_2 -symmetric tritwistane, has been synthesized for the first time.

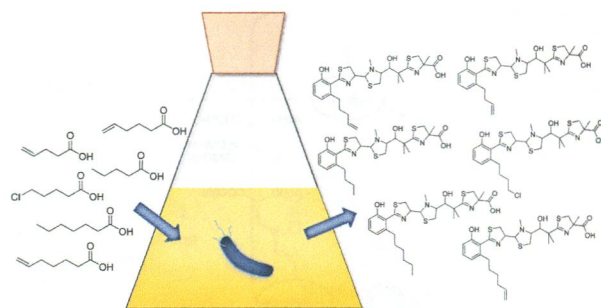


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Precursor-directed biosynthesis of micacocidin derivatives with activity against *Mycoplasma pneumoniae*

Martin F. Kreutzer, Hirokazu Kage, Jennifer Herrmann, Julia Pauly, Ron Hermenau, Rolf Müller, Dirk Hoffmeister and Markus Nett*

Supplementation of *Ralstonia solanacearum* cultures with hexanoic acid analogues yields novel derivatives of the antibiotic micacocidin.

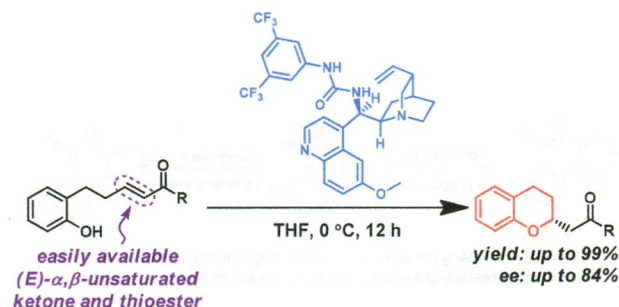


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Asymmetric chroman synthesis via an intramolecular oxy-Michael addition by bifunctional organocatalysts

Ryota Miyaji, Keisuke Asano* and Seiji Matsubara*

Cinchona-alkaloid-urea-based bifunctional organocatalysts facilitate asymmetric chroman synthesis via an intramolecular oxy-Michael addition from phenol derivatives bearing an easily available (*E*)- α,β -unsaturated ketone or thioester moiety.

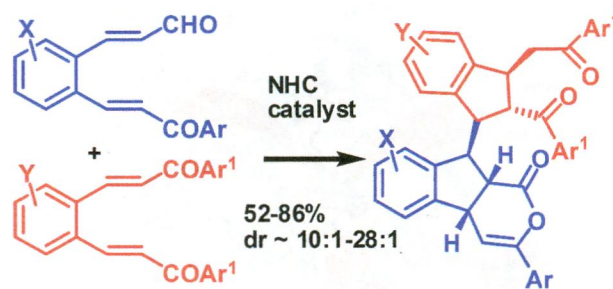


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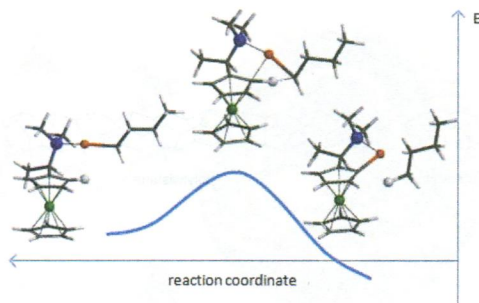
N-Heterocyclic carbene-catalyzed cascade reaction of 2-arylvinylcinnamaldehydes with 2-arylvinylchalcones: rapid assembly of six contiguous stereogenic centers with high diastereoselectivity

Xing-Wen Fan and Ying Cheng*

NHC-catalyzed reaction of 2-arylvinylcinnamaldehydes with 2-arylvinylchalcones produced good yields of novel 9-(2-aryl-3-arylmethyl-1-indanyl)-3-arylindeno[2,1-*c*]-pyran-1-ones with high diastereoselectivity.



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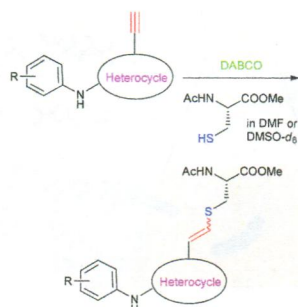


Computational study of diastereoselective *ortho*-lithiations of chiral ferrocenes

Andrea Škvorcová and Radovan Šebesta*

DFT calculations provide an explanation of the governing effects of diastereoselective *ortho*-lithiations of chiral ferrocenes.

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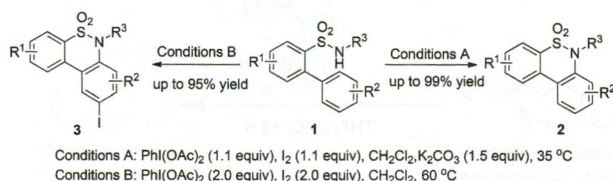


Model system for irreversible inhibition of Nek2: thiol addition to ethynylpurines and related substituted heterocycles

H. Lebraud, C. R. Coxon, V. S. Archard, C. M. Bawn, B. Carbain, C. J. Matheson, D. M. Turner, C. Cano, R. J. Griffin, I. R. Hardcastle, U. Baisch, R. W. Harrington and B. T. Golding*

Model studies reveal a 50-fold rate variation for the capture of the ethynyl group in a series of ethynyl-heterocycles by *N*-acetylcysteine methyl ester catalysed by 1,4-diazabicyclo[2.2.2]octane in dimethyl sulfoxide.

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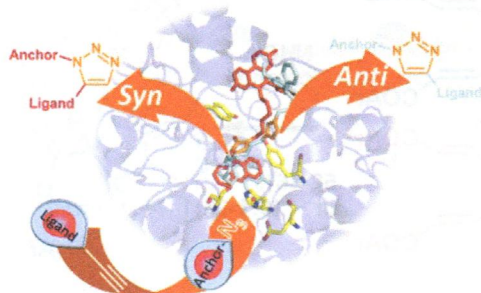


Synthesis of benzosultams via an intramolecular sp^2 C–H bond amination reaction of *o*-arylbenzenesulfonamides under metal-free conditions

Yuewen Li, Qiuping Ding,* Guanyinsheng Qiu and Jie Wu*

A practical synthetic method for the generation of benzosultams via an intramolecular sp^2 C–H bond amination reaction of *o*-arylbenzenesulfonamides with $\text{PhI}(\text{OAc})_2$ – I_2 under metal-free conditions is developed.

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Reaction site-driven regioselective synthesis of AChE inhibitors

Emilia Oueis, Gianluca Santoni, Cyril Ronco, Olga Syzgantseva, Vincent Tognetti, Laurent Joubert, Anthony Romieu, Martin Weik, Ludovic Jean,* Cyrille Sabot,* Florian Nachon and Pierre-Yves Renard*

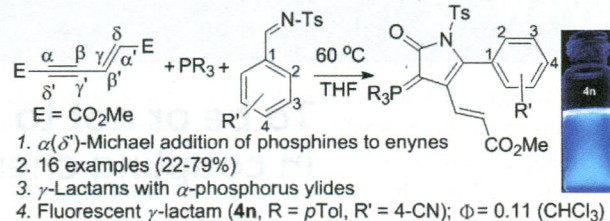
The use of the human acetylcholinesterase as a target enzyme is reported for the first time for the regioselective synthesis of potent heterodimeric huprine-based inhibitors.

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One-pot formation of fluorescent γ -lactams having an α -phosphorus ylide moiety through three-component $\alpha(\delta')$ -Michael reactions of phosphines with an enyne and *N*-tosyl aldimines

Yu-Wei Lin, Jie-Cheng Deng, You-Zung Hsieh and Shih-Ching Chuang*

Three-component reactions of phosphines, *N*-tosyl aldimines and enynes, through an initial $\alpha(\delta')$ -attack of phosphines to enynes, provided fluorescent γ -lactams.

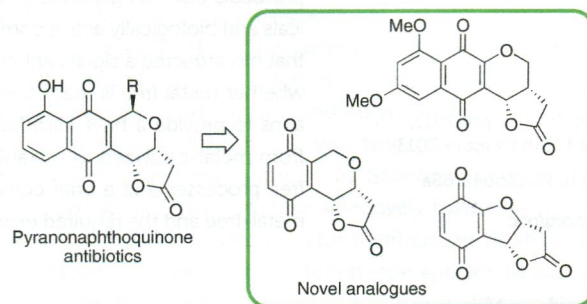


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Exploring *O*-stannyl ketyl and acyl radical cyclizations for the synthesis of γ -lactone-fused benzopyrans and benzofurans

Helen Santoso, Myriam I. Casana and Christopher D. Donner*

A series of heterocycle-fused quinones, analogues of the pyranonaphthoquinone antibiotics, are prepared in 3-4 steps by *O*-stannyl ketyl or acyl radical cyclization of benzaldehyde substrates.

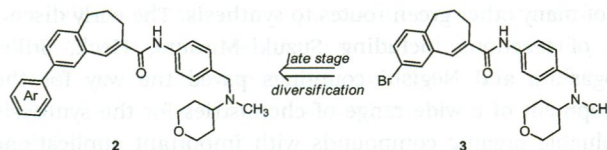


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Diverse modifications of the 4-methylphenyl moiety of TAK-779 by late-stage Suzuki–Miyaura cross-coupling

Anna Junker, Dirk Schepmann, Junichiro Yamaguchi, Kenichiro Itami, Andreas Faust, Klaus Kopka, Stefan Wagner and Bernhard Wünsch*

A new synthetic strategy for the development of TAK-779 analogs with promising CCR5 binding affinity by late stage diversification is reported.



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Unraveling polar Diels–Alder reactions with conceptual DFT analysis and the distortion/interaction model

Ariel M. Sarotti

The reaction energetics of 280 polar Diels–Alder (DA) reactions between 70 dienophiles and 4 dienes have been studied in detail using the B3LYP/6-31G* level of theory, combining conceptual density functional theory (DFT) analysis and the distortion/interaction model.

