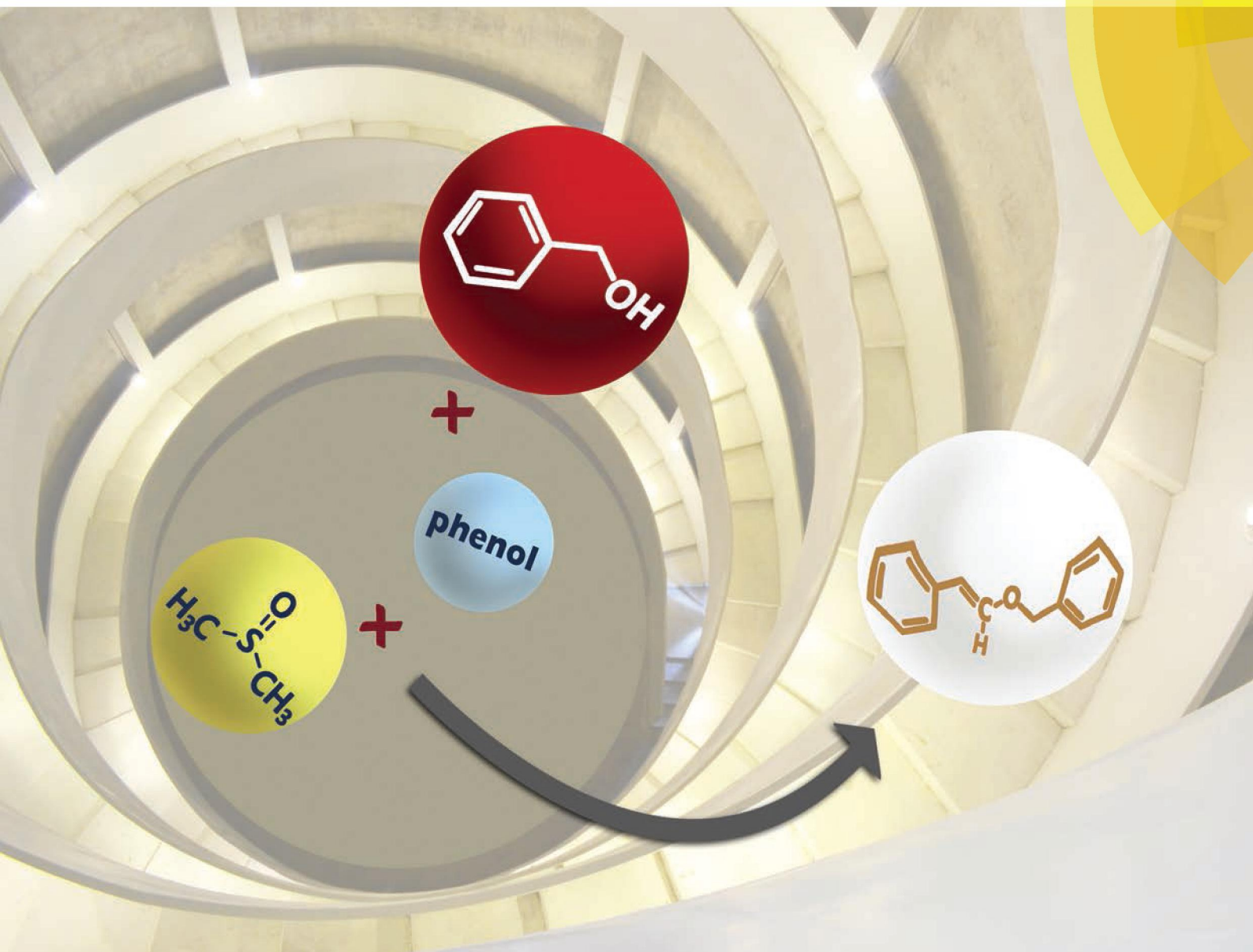


Organic & Biomolecular Chemistry

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ISSN 1477-0520



PAPER

Kai Yang and Qiuling Song
Styryl ether formation from benzyl alcohols under transition-metal-free
basic DMSO conditions

Organic & Biomolecular Chemistry

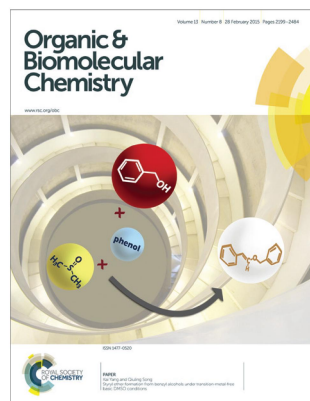
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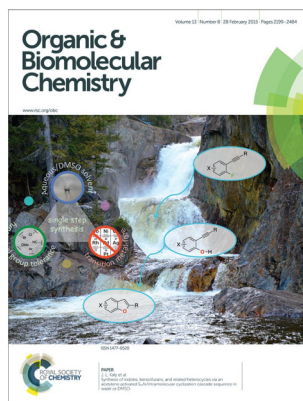
ISSN 1477-0520 CODEN OBCRAK 13(8) 2199–2484 (2015)



Cover

See Kai Yang and Qiuling Song, pp. 2267–2272.

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Inside cover

See J. L. Katz et al., pp. 2273–2284.

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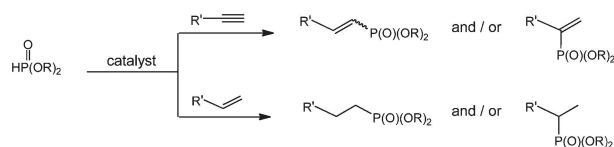
PERSPECTIVE

2212

Validating the alkene and alkyne hydrophosphonylation as an entry to organophosphonates

Alessandro Dondoni* and Alberto Marra*

The hydrophosphonylation of terminal alkenes and alkynes by *H*-phosphonates affords Markovnikov and/or anti-Markovnikov adducts depending on the catalyst (a metal or a radical initiator) and the reaction conditions.



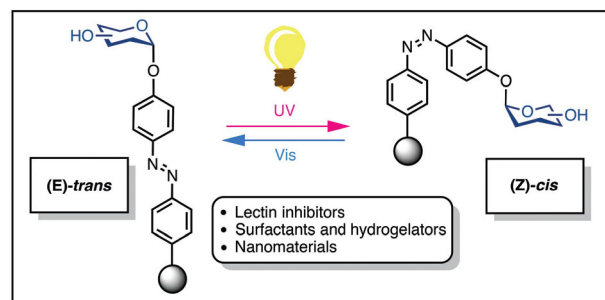
REVIEWS

2216

Sweetness and light: design and applications of photo-responsive glycoconjugates

Yingxue Hu, Rico F. Tabor and Brendan L. Wilkinson*

Photoswitchable glycoconjugates are promising tools for studying biomolecular interactions and for the development of stimuli-responsive materials.



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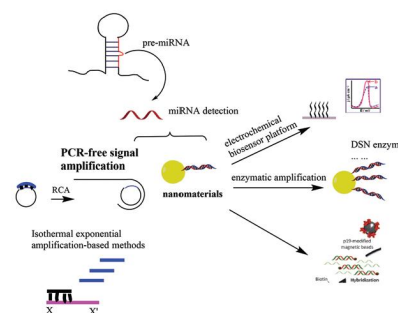
REVIEWS

2226

A review: microRNA detection methods

Tian Tian,* Jiaqi Wang and Xiang Zhou*

MicroRNA (miRNA) detection is of considerable significance in both disease diagnosis and in the study of miRNA function.



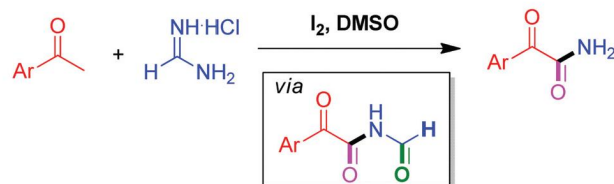
COMMUNICATIONS

2239

Formamidinium hydrochloride as an amino surrogate: I₂-catalyzed oxidative amidation of aryl methyl ketones leading to free (N–H) α-ketoamides

Shan Liu, Qinghe Gao, Xia Wu, Jingjing Zhang, Kerong Ding and Anxin Wu*

A highly efficient molecular iodine catalyzed oxidative amidation of aryl methyl ketones has been developed. This reaction represents a novel strategy for the synthesis of free (N–H) α-ketoamides.

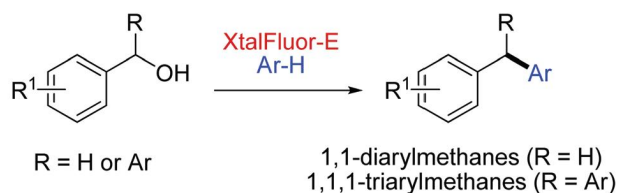


2243

In situ activation of benzyl alcohols with XtalFluor-E: formation of 1,1-diarylmethanes and 1,1,1-triarylmethanes through Friedel–Crafts benzylation

Justine Desroches, Pier Alexandre Champagne, Yasmine Benhassine and Jean-François Paquin*

The Friedel–Crafts benzylation of arenes using benzyl alcohols activated *in situ* with XtalFluor-E is described. A wide range of 1,1-diarylmethanes and 1,1,1-triarylmethanes were prepared under simple and mild conditions, without the need for a transition metal or a strong Lewis acid.

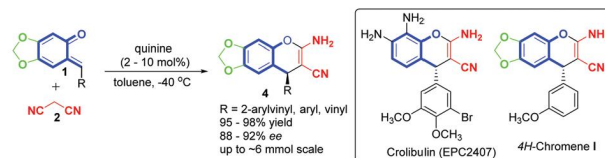


2247

Quinine-catalyzed highly enantioselective cycloannulation of *o*-quinone methides with malononitrile

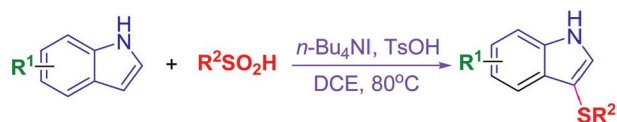
Alafate Adili, Zhong-Lin Tao, Dian-Feng Chen and Zhi-Yong Han*

2-Amino-3-cyano-4*H*-chromenes show great potential as novel anticancer agents. Here we report a quinine-catalyzed highly enantioselective formal 4 + 2 cycloaddition of *ortho*-quinone methides and malononitrile, providing a unique approach to 4-arylvinylyl, 4-aryl and 4-vinyl 2-amino-3-cyano-4*H*-chromenes with excellent yields and enantioselectivities.



COMMUNICATIONS

2251



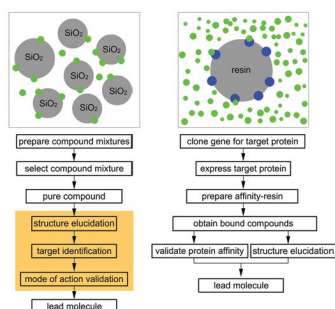
R¹: Cl, Br, NO₂, CO₂Me, Me, Ph, OMe
R²: Alkyl, Aryl, Naphthyl

Byproduct promoted regioselective sulfenylation of indoles with sulfinic acids

Cong-Rong Liu* and Liang-Hui Ding

An unprecedented method to synthesise 3-sulfenylindoles is demonstrated *via* byproduct promoted sulfenylation of indoles with sulfinic acids.

2255

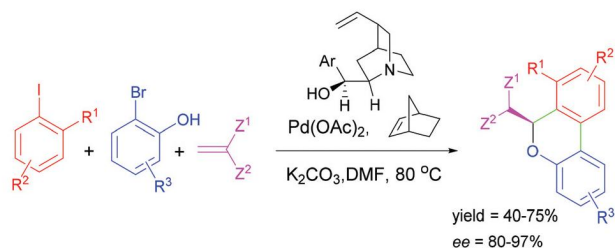


Functional chromatographic technique for natural product isolation

Eric C. Lau, Damian J. Mason, Nicole Eichhorst, Pearce Engelder, Celestina Mesa, E. M. Kithsiri Wijeratne, G. M. Kamal B. Gunaherath, A. A. Leslie Gunatilaka, James J. La Clair* and Eli Chapman*

Natural product discovery arises through a unique interplay between chromatographic purification and protein affinity.

2260



A novel enantioselective synthesis of 6H-dibenzopyran derivatives by combined palladium/norbornene and cinchona alkaloid catalysis

Di Xu, Li Dai, Marta Catellani, Elena Motti, Nicola Della Ca' and Zhiming Zhou*

Chiral dibenzopyran derivatives were obtained by cinchona alkaloid, as organocatalyst, in combination, for the first time, with palladium/norbornene catalytic system.

2264



Copper-catalyzed oxidative alkenylation of thioethers *via* Csp³-H functionalization

Hao Cao, Dong Liu, Chao Liu, Xinquan Hu* and Aiwen Lei*

The first copper-catalyzed oxidative alkenylation of thioethers *via* Csp³-H functionalization to construct allylic thioethers is demonstrated.

PAPERS

2267

Styryl ether formation from benzyl alcohols under transition-metal-free basic DMSO conditions

Kai Yang and Qiuling Song*

A phenol-catalyzed aerobic oxidative styryl ether formation method was developed with benzyl alcohol under basic DMSO.

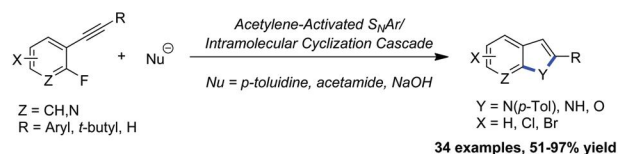


2273

Synthesis of indoles, benzofurans, and related heterocycles via an acetylene-activated S_NAr /intramolecular cyclization cascade sequence in water or DMSO

R. Hudson, N. P. Bizier, K. N. Esdale and J. L. Katz*

The synthesis of 2-substituted indoles and benzofurans was achieved by nucleophilic aromatic substitution, followed by subsequent 5-endo-dig cyclization between the nucleophile and an *ortho* acetylene.

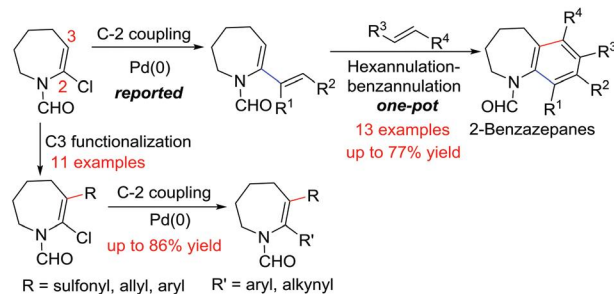


2285

Expedient access to α,β -difunctionalized azepenes using α -halo eneformamides: application to the one-pot synthesis of 2-benzazepanes

Daniel P. Bassler, Laura Spence, Amir Alwali, Oliver Beale and Timothy K. Beng*

The regioselective synthesis of α,β -difunctionalized (alkenyl, aryl, sulfonyl, allyl, or alkynyl) azepenes has been accomplished through α -halo eneformamides.

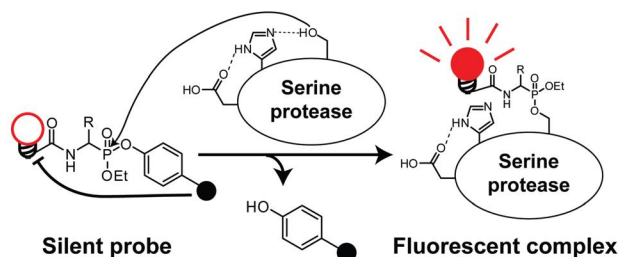


2293

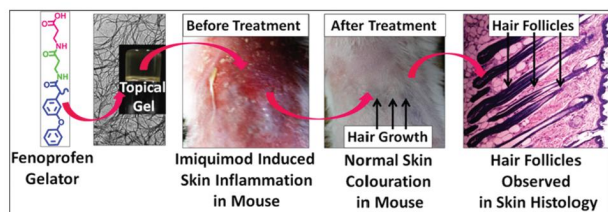
Mixed alkyl aryl phosphonate esters as quenched fluorescent activity-based probes for serine proteases

Sevnur Serim, Philipp Baer and Steven H. L. Verhelst*

The synthesis of quenched fluorescent activity-based probes for serine proteases based on a phosphonate reactive group is reported.



2300

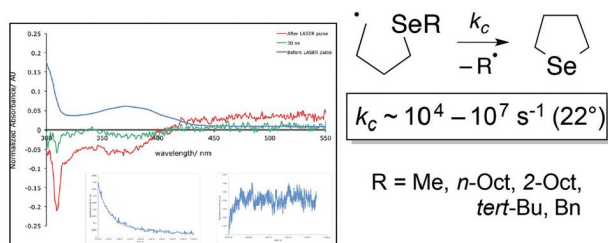


A supramolecular topical gel derived from a non-steroidal anti-inflammatory drug, fenopropfen, is capable of treating skin inflammation in mice

Joydeb Majumder, Pavani Yedoti and Parthasarathi Dastidar*

A small β -di-peptide functionalized fenopropfen bioconjugate forms supramolecular gel with menthol containing methylsalicylate solvent. The resulting gel shows topical self-delivery application in treating imiquimod induced skin inflammation in mice.

2310



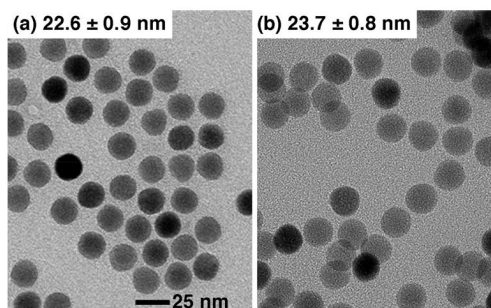
The effect of leaving radical on the formation of tetrahydroselephenone by S_{Hi} ring closure: an experimental and computational study

Amber N. Hancock, Sofia Lobachevsky, Naomi L. Haworth, Michelle L. Coote and Carl H. Schiesser*

Competition kinetic studies augmented with laser-flash photolysis and high-level computational techniques [G3(MP2)-RAD], with [COSMO-RS, SMD] and without solvent correction, provide kinetic parameters for the ring closures of a series of 4-(alkylseleno)butyl radicals.

laser-flash, competition kinetics and G3(MP2)-RAD

2317

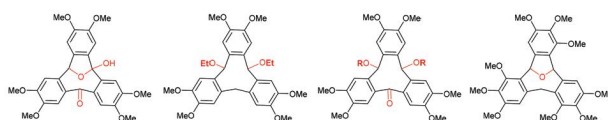


Energy transfer between amphiphilic porphyrin polymer shells and upconverting nanoparticle cores in water-dispersible nano-assemblies

T. Wu, S. Kaur and N. R. Branda*

The synthesis and optical properties of water-dispersible nano-assemblies containing upconverting nanoparticles (UCNPs) and porphyrin molecules using a one-pot method is described.

2323



Pd-catalyzed benzylic C–H oxidation of cyclotriveratrylene – product diversity

B. Senthilkumar, R. G. Gonnade and C. V. Ramana*

The inner-rim oxidation of CTV has been explored with palladium and an interesting array of CTV derivatives has been obtained by simple changes in the solvent/conditions employed.

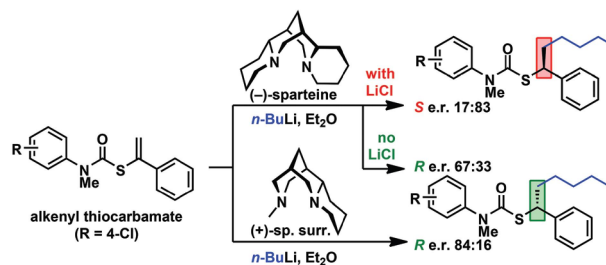
PAPERS

2330

Enantioselective carbolithiation of *S*-alkenyl-*N*-aryl thiocarbamates: kinetic and thermodynamic control

Daniele Castagnolo, Leonardo Degennaro, Renzo Luisi and Jonathan Clayden*

Carbolithiation of vinyl thiocarbamates may proceed with the same sense of enantioselectivity with either (–)-sparteine and (+)-sparteine surrogate ligands.

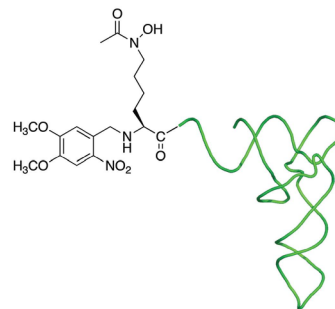


2341

Tetrahydrofuranyl and tetrahydropyranyl protection of amino acid side-chains enables synthesis of a hydroxamate-containing aminoacylated tRNA

Lester J. Lambert, Marvin J. Miller and Paul W. Huber*

O-protection using tetrahydrofuranyl or tetrahydropyranyl enabled addition of a hydroxamate-containing unnatural amino acid to a suppressor tRNA, allowing subsequent site-specific incorporation of the amino acid into the transcription factor, TFIIIA.

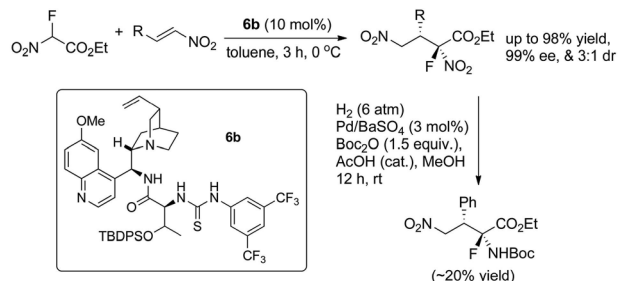


2350

Asymmetric Michael addition of α -fluoro- α -nitro esters to nitroolefins: towards synthesis of α -fluoro- α -substituted amino acids

Jacek Kwiatkowski and Yixin Lu*

α -Fluoro- α -nitro esters were used as reaction partners in Michael addition to nitroalkenes, and the products were obtained in excellent chemical yields and with high enantioselectivities.

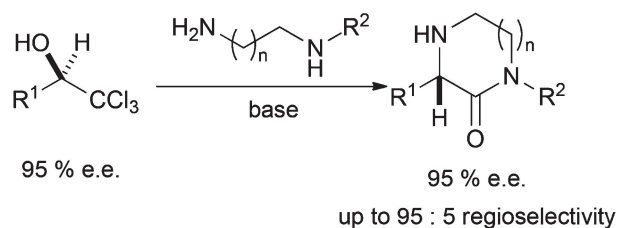


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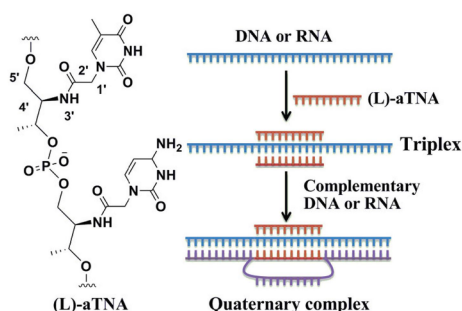
Synthesis of 1- and 4-substituted piperazin-2-ones via Jocic-type reactions with *N*-substituted diamines

Michael S. Perryman, Matthew W. M. Earl, Sam Greatorex, Guy J. Clarkson and David J. Fox*

Enantiomerically-enriched trichloromethyl-containing alcohols are transformed regioselectively into enantiomerically-enriched 1-substituted piperazinones by modified Jocic reactions.



2366

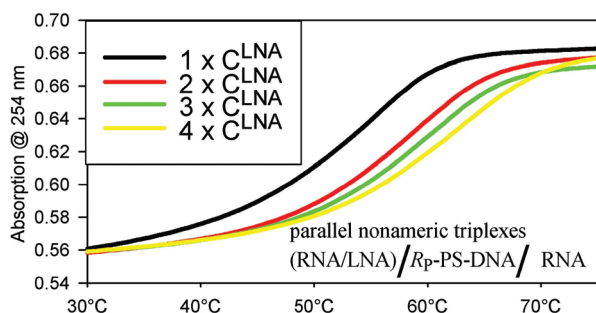


Highly stable triple helix formation by homopyrimidine (L)-acyclic threoninol nucleic acids with single stranded DNA and RNA

Vipin Kumar, Venkitasamy Kesavan* and Kurt V. Gothelf*

Homopyrimidine acyclic (L)-threoninol nucleic acid (aTNA) was synthesized and found to form highly stable (L)-aTNA–DNA–(L)-aTNA and (L)-aTNA–RNA–(L)-aTNA triple helical structures.

2375

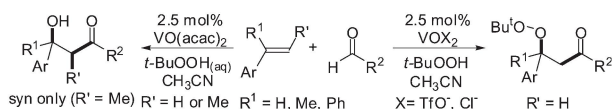


LNA units present in the (2'-OMe)-RNA strand stabilize parallel duplexes (2'-OMe)-RNA/[All-R_P-PS]-DNA and parallel triplexes (2'-OMe)-RNA/[All-R_P-PS]-DNA/RNA. An improved tool for the inhibition of reverse transcription

Anna Maciaszek, Agnieszka Krakowiak, Magdalena Janicka, Agnieszka Tomaszewska-Antczak, Milena Sobczak, Barbara Mikołajczyk and Piotr Guga*

LNA units stabilize (RNA/LNA)/R_P-PS-DNA/RNA triplexes and efficiently inhibit reverse transcription of target RNA.

2385

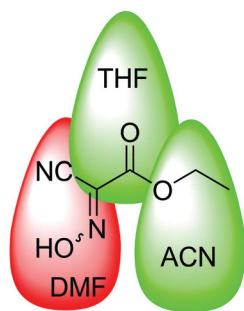


Vanadyl species-catalyzed complementary β-oxidative carbonylation of styrene derivatives with aldehydes

Wen-Chieh Yang, Shiue-Shien Weng,* Anandhan Ramasamy, Gobi Rajeshwaren, Yi-Ya Liao and Chien-Tien Chen*

By judicious choice of the counter anions in the vanadyl catalysts, we can achieve β-hydroxylated and *t*-butyl peroxy carbonylation of styrenes by aromatic 1° and 2° alkyl aldehydes in a complementary manner.

2393



Peptide synthesis beyond DMF: THF and ACN as excellent and friendlier alternatives

Yahya E. Jad, Gerardo A. Acosta, Sherine N. Khattab, Beatriz G. de la Torre, Thavendran Govender, Hendrik G. Kruger, Ayman El-Faham* and Fernando Albericio*

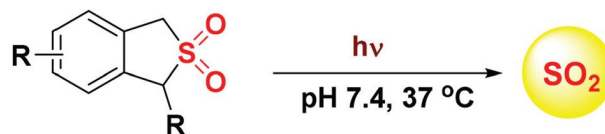
To date, DMF has been considered as the only solvent suitable for peptide synthesis.

2399

Benzosulfones as photochemically activated sulfur dioxide (SO₂) donors

Satish R. Malwal and Harinath Chakrapani*

A series of benzosulfones were synthesized and found to undergo photolysis to generate sulfur dioxide in aqueous buffer.

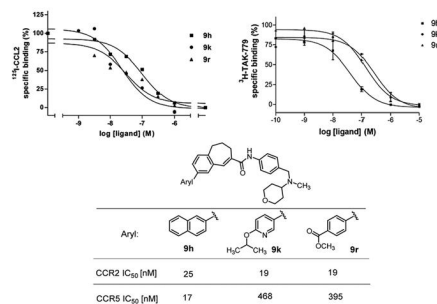


2407

Synthesis, binding affinity and structure–activity relationships of novel, selective and dual targeting CCR2 and CCR5 receptor antagonists

A. Junker, A. K. Kokornaczyk, A. J. M. Zweemer, B. Frehland, D. Schepmann, J. Yamaguchi, K. Itami, A. Faust, S. Hermann, S. Wagner, M. Schäfers, M. Koch, C. Weiss, L. H. Heitman, K. Kopka and B. Wünsch*

Late-stage diversification led to selective chemokine CCR2 receptor antagonists and dual-targeting CCR2/CCR5 receptor antagonists.

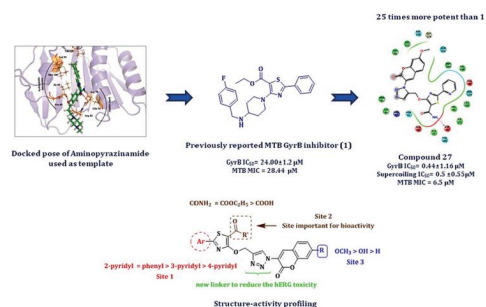


2423

Enabling the (3 + 2) cycloaddition reaction in assembling newer anti-tubercular lead acting through the inhibition of the gyrase ATPase domain: lead optimization and structure activity profiling

Variam Ullas Jeankumar, Rudraraju Srilakshmi Reshma, Renuka Janupally, Shalini Saxena, Jonnalagadda Padma Sridevi, Brahmam Medapi, Pushkar Kulkarni, Perumal Yogeewari and Dharmarajan Sriram*

Exploring the Gyrase ATPase platform to tailor novel anti-tubercular leads.

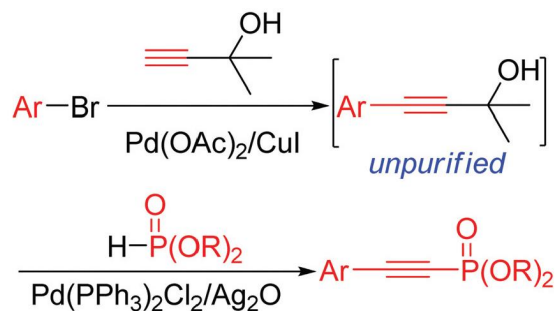


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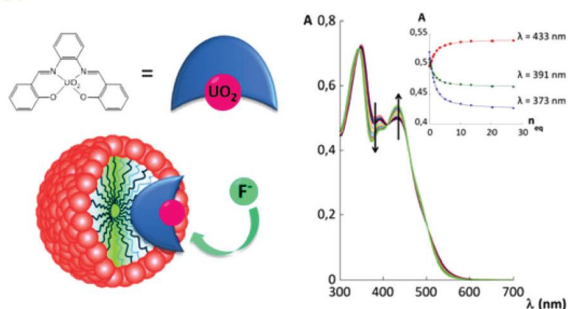
Palladium-catalyzed oxidative deacetonative coupling of 4-aryl-2-methyl-3-butyn-2-ols with H-phosphonates

Xiang Li, Suyan Sun, Fan Yang,* Jianxun Kang, Yusheng Wu* and Yangjie Wu*

A new and generally practical synthesis of alkynylphosphonates through a palladium-catalyzed consecutive Sonogashira/deacetonative process using aryl bromides, 2-methyl-3-butyn-2-ol and H-phosphonates is developed.



2437

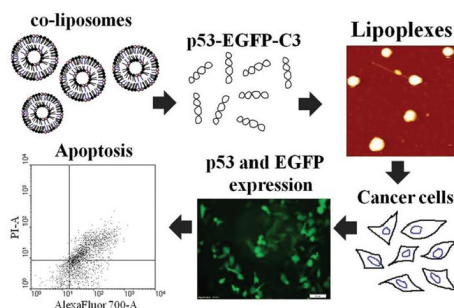


Fluoride binding in water with the use of micellar nanodevices based on salophen complexes

Flore Keymeulen, Paolo De Bernardin, Ilaria Giannicchi, Luciano Galantini, Kristin Bartik* and Antonella Dalla Cort*

Uranyl-salophen complexes incorporated into micelles are evaluated as supramolecular nanosystems for the binding of fluoride in water.

2444

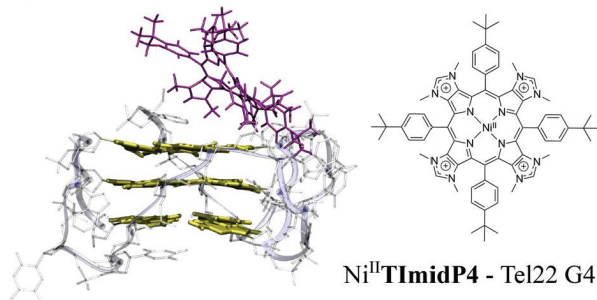


α -Tocopherol derived lipid dimers as efficient gene transfection agents. Mechanistic insights into lipoplex internalization and therapeutic induction of apoptotic activity

Krishan Kumar, Bappa Maiti, Paturu Kondaiah and Santanu Bhattacharya*

Dimeric cationic tocopheryl lipids for efficacious therapeutic pDNA delivery in cancer cell lines.

2453

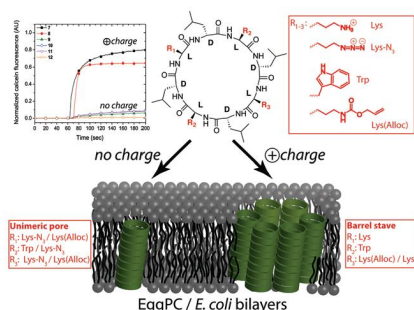


Binding modes of a core-extended metalloporphyrin to human telomeric DNA G-quadruplexes

Jenifer Rubio-Magnieto, Florent Di Meo, Mamadou Lo, Cécile Delcourt, Sébastien Clément, Patrick Norman, Sébastien Richeter,* Mathieu Linares* and Mathieu Surin*

A novel π -extended Ni^{II}-porphyrin shows a high selectivity towards human telomeric G-quadruplexes.

2464



Effect of the amino acid composition of cyclic peptides on their self-assembly in lipid bilayers

Maarten Danial, Sébastien Perrier* and Katrina A. Jolliffe*

The effect of amino acid composition on the formation of transmembrane channels in lipid bilayers upon self-assembly of alt-(L,D)- α -cyclic octapeptides has been investigated.

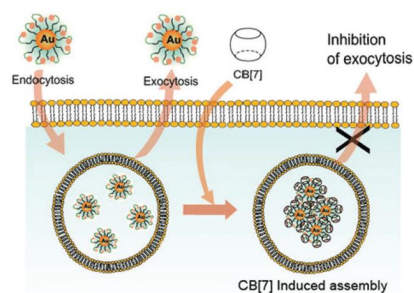
PAPERS

2474

Regulating exocytosis of nanoparticles via host–guest chemistry

Chaekyu Kim, Gulen Yesilbag Tonga, Bo Yan, Chang Soo Kim, Sung Tae Kim, Myoung-Hwan Park, Zhengjiang Zhu, Bradley Duncan, Brian Creran and Vincent M. Rotello*

Regulating exocytosis of AuNPs by using host–guest interactions between AuNPs and CB[7] molecules.



CORRECTIONS

2480

Correction: Using Hansen solubility parameters to study the encapsulation of caffeine in MOFs

Lorena Paseta, Grégory Potier, Steven Abbott and Joaquín Coronas*

2481

Correction: A novel enantioselective synthesis of 6*H*-dibenzopyran derivatives by combined palladium/norbornene and cinchona alkaloid catalysis

Di Xu, Li Dai, Marta Catellani, Elena Motti, Nicola Della Ca' and Zhiming Zhou*