Volume 13 | Number 19 | 21 May 2015 | Pages 5291–5558

Organic & Biomolecular Chemistry

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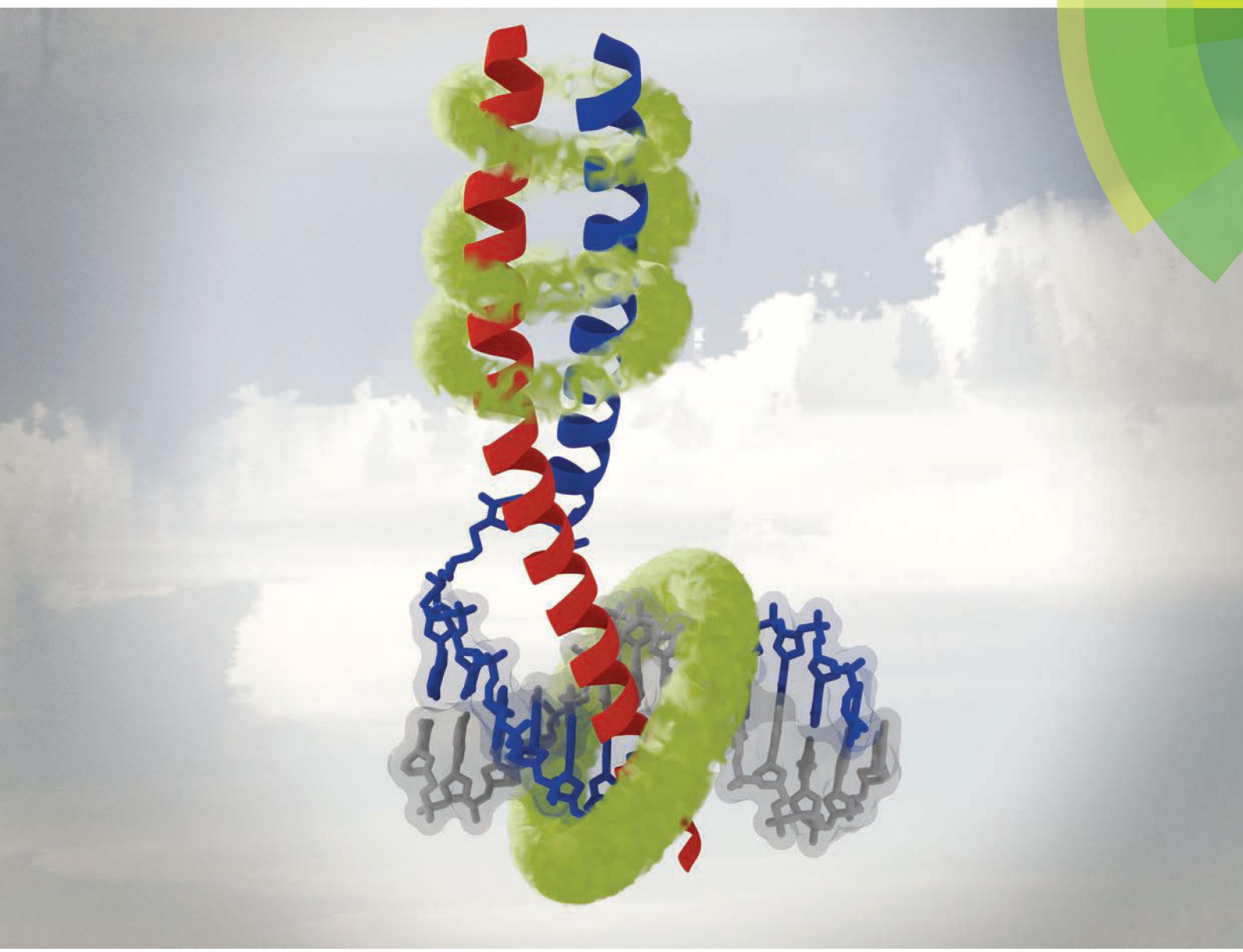

ISSN 1477-0520

ROYAL SOCIETY OF CHEMISTRY

PAPER

José L. Mascareñas *et al.*

Peptide–DNA conjugates as tailored bivalent binders of the oncoprotein c-Jun

Organic & Biomolecular Chemistry

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ISSN 1477-0520 CODEN OBCRAK 13(19) 5291–5558 (2015)

Cover
See José L. Mascareñas *et al.*, pp. 5385–5390.

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Inside cover
See Shina C. L. Kamerlin *et al.*, pp. 5391–5398.

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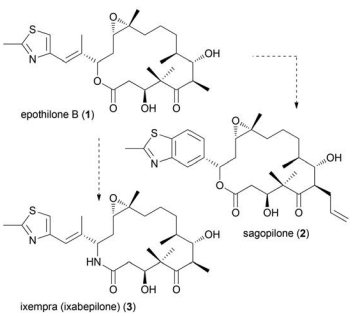
REVIEW

5302

Design and synthesis of analogues of natural products

Martin E. Maier

In this article strategies for the design and synthesis of natural product analogues are summarized and illustrated with some selected examples.



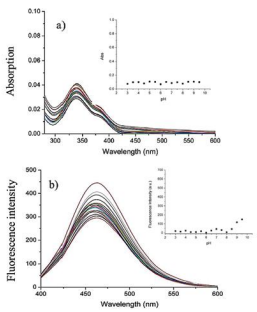
COMMUNICATIONS

5344

An ESIPT-based fluorescent probe for sensitive detection of hydrazine in aqueous solution

Ji Zhou, Ruiyan Shi, Jianxu Liu, Rui Wang, Yufang Xu* and Xuhong Qian*

A fluorescent probe for sensitive detection of hydrazine based on an ESIPT mechanism and a substitution–cyclization–elimination cascade was developed.



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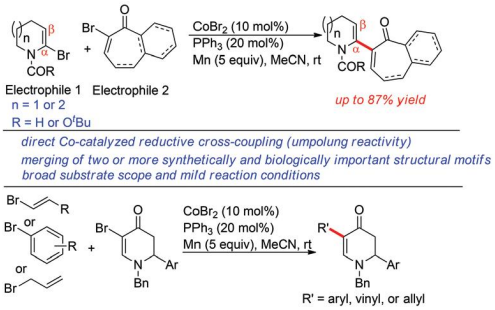
COMMUNICATIONS

5349

Direct access to functionalized benzotropones, azepanes, and piperidines by reductive cross-coupling of α-bromo enones with α-bromo enamides

T. K. Beng,* K. Sincavage, A. W. V. Silaire, A. Alwali, D. P. Bassler, L. E. Spence and O. Beale

High-yielding syntheses of functionalized azepenes and piperidines, bearing an α-benzotropone derivative, have been achieved through cobalt-catalysed reductive cross-coupling of α-bromo enamides with α-bromo enones.

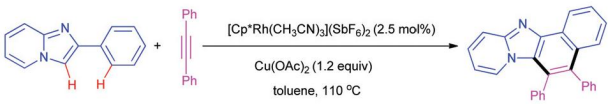


5354

Rhodium-catalyzed annulation between 2-arylimidazo[1,2-*a*]pyridines and alkynes leading to pyrido[1,2-*a*]benzimidazole derivatives

Haibo Peng, Jin-Tao Yu, Yan Jiang, Lei Wang and Jiang Cheng*

A rhodium-catalyzed annulation between 2-arylimidazo-[1,2-*a*]pyridines and alkynes was developed, leading to pyrido[1,2-*a*]benzimidazole derivatives in moderate to excellent yields.

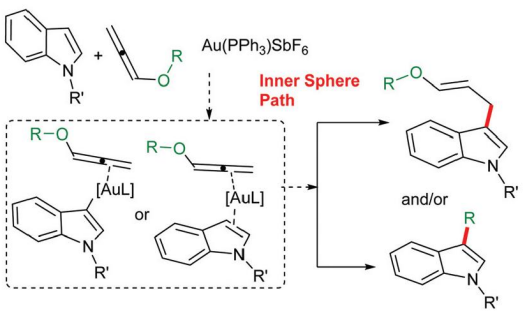


5358

Gold(I)-catalyzed hydroindolylation of allenyl ethers

Chandrababu Naidu Kona, Mahesh H. Shinde and Chepuri V. Ramana*

Nucleophilicity game: the gold(I)-catalyzed reaction/rearrangement of allenyl ethers has been investigated in the presence of indoles. The reaction outcome seems to be decided mainly by the nature of the pendant group of allenyl ether. Control experiments are indicative of an inner sphere mechanism for the hydroindolylation reaction.

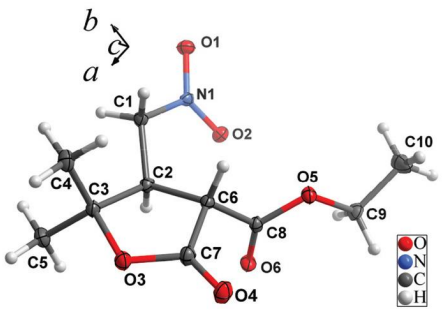


5363

Asymmetric Michael addition reactions of nitroalkanes to 2-furanones catalyzed by bifunctional thiourea catalysts

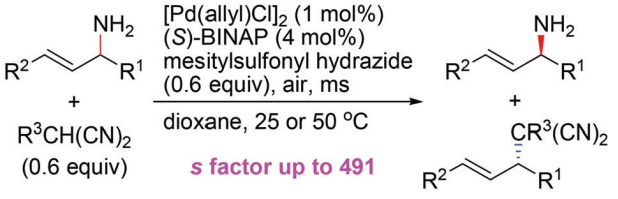
Zhushuang Bai, Ling Ji, Zemei Ge, Xin Wang* and Runtao Li*

The first bifunctional thiourea catalyzed asymmetric Michael addition reactions of nitroalkanes to 2-furanones are described.



COMMUNICATIONS

5367

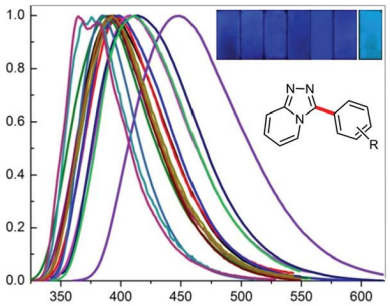


Kinetic resolution of primary allylic amines *via* palladium-catalyzed asymmetric allylic alkylation of malononitriles

Yong Wang, Ya-Nan Xu, Guo-Sheng Fang, Hong-Jian Kang, Yonghong Gu* and Shi-Kai Tian*

A new strategy has been developed for the catalytic kinetic resolution of primary allylic amines *via* enantioselective C–N bond cleavage.

5372

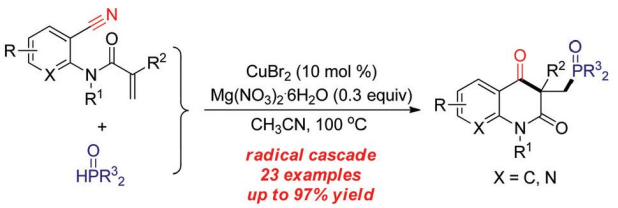


Cu-catalysed direct C–H (hetero)arylation of [1,2,4]triazolo[4,3-*a*]pyridine to construct deep-blue-emitting luminophores

Jie Wu, Qiulin You, Jingbo Lan,* Qiang Guo, Xiaoyu Li, Ying Xue and Jingsong You*

An efficient protocol for the synthesis of 3-aryl-[1,2,4]-triazolo[4,3-*a*]pyridines has been developed *via* Cu-catalysed direct C–H (hetero)arylation. The resulting compounds exhibit deep-blue emission with high quantum yields, photostability, and thermal stability.

5376

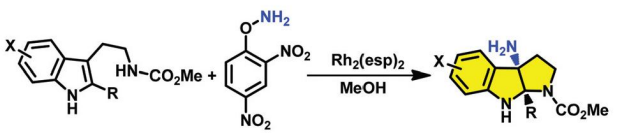


Copper-catalyzed cascade addition/cyclization: highly efficient access to phosphonylated quinoline-2,4(1*H*,3*H*)-diones

Ya-Min Li,* Shi-Sheng Wang, Fuchao Yu, Yuehai Shen and Kwen-Jen Chang

A novel Cu-catalyzed addition/cyclization cascade of *o*-cyanoarylacrylamide has been developed for the synthesis of various phosphonylated quinoline-2,4(1*H*,3*H*)-diones.

5381



Synthesis of naked amino-pyrroloindoline *via* direct aminocyclization of tryptamine

Zhigao Shen, Zilei Xia, Huijun Zhao, Jiadong Hu, Xiaolong Wan, Yisheng Lai,* Chen Zhu* and Weiqing Xie*

Direct access to unprotected amino-pyrroloindoline *via* aminocyclization of tryptamine and tryptophan catalyzed by $Rh_2(esp)_2$ has been described using *O*-(2,4-dinitrophenyl)hydroxylamine (DPH) as the nitrogen source.

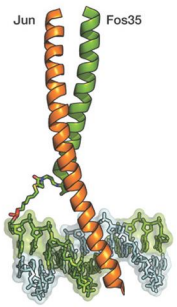
PAPERS

5385

Peptide–DNA conjugates as tailored bivalent binders of the oncoprotein c-Jun

Elena Pazos, Cecilia Portela, Cristina Penas, M. Eugenio Vázquez and José L. Mascareñas*

A designed disrupter of the DNA complexes of oncoproteins Fos and Jun is reported.

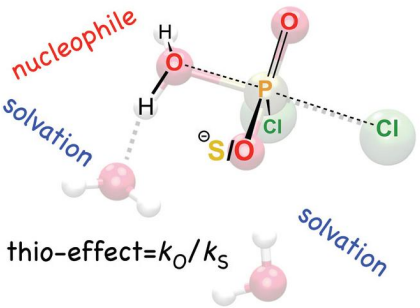


5391

Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge

Alexandra T. P. Carvalho, AnnMarie C. O'Donoghue, David R. W. Hodgson and Shina C. L. Kamerlin*

Detailed quantum chemical calculations provide insight on the origin of large differences in experimental thio-effects for the hydrolysis of (thio)phosphodichloridates by water and hydroxide nucleophiles.

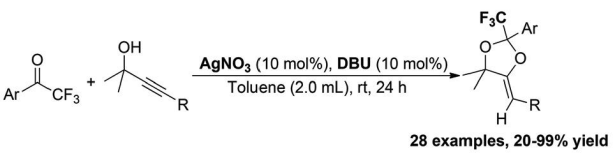


5399

Silver salts and DBU cooperatively catalyzed nucleophilic addition/cyclization of propargylic alcohols with trifluoromethyl ketones

Jingjing Wang,* Wei-Guang Kong, Feng Li, Jie Liu, Qin Shen, Lantao Liu and Wen-Xian Zhao*

A general and efficient synthesis of trifluoromethyl substituted 5-alkylidene-1,3-dioxolane using a silver salt and DBU cooperatively catalyzed nucleophilic addition/cyclization of propargylic alcohols and trifluoromethyl ketones is described.

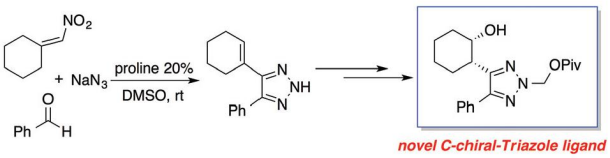


5407

Facile synthesis and stereo-resolution of chiral 1,2,3-triazoles

Ye Shi, Xiaohan Ye, Qiang Gu, Xiaodong Shi* and Zhiguang Song*

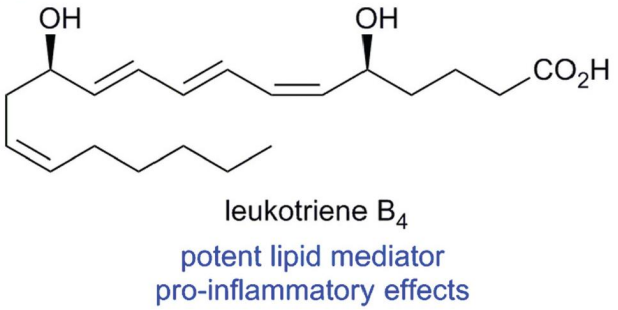
We describe herein the first facile synthesis of chiral triazoles through side chain functionalization.



- High efficient CalB resolution, S>200
- Gram scale synthesis
- Successfully asymmetric diethylzinc addition to aldehyde

PAPERS

5412

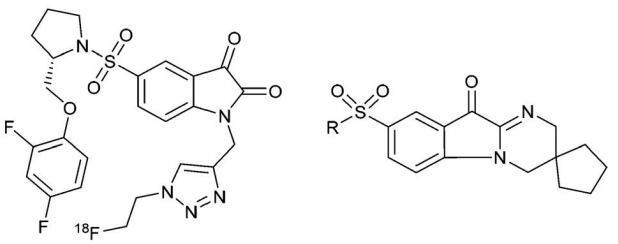


An efficient total synthesis of leukotriene B_4

Karoline Gangestad Primdahl, Jørn Eivind Tungen, Marius Aursnes, Trond Vidar Hansen and Anders Vik*

A convergent and stereoselective synthesis of leukotriene B_4 has been achived in 5% yield over 10 steps in the longest linear sequence.

5418

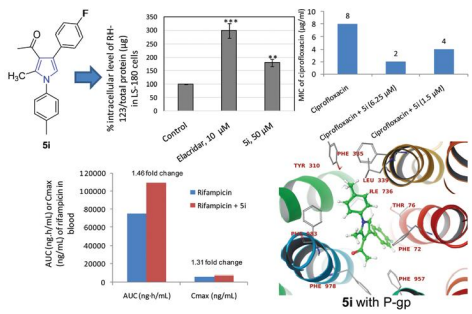


Design, synthesis and initial characterisation of a radiolabelled [^{18}F]pyrimidoindolone probe for detecting activated caspase-3/7

A. Udemba, G. Smith, Q.-D. Nguyen, M. Kaliszczak, L. Carroll, R. Fortt, M. J. Fuchter and E. O. Aboagye*

Evasion of apoptosis is one of the six initially proposed hallmarks of cancer, and as such, a method to detect apoptosis in a tumour would be of considerable interest in both clinical trials of new cancer therapeutics, as well as for routine patient management.

5424

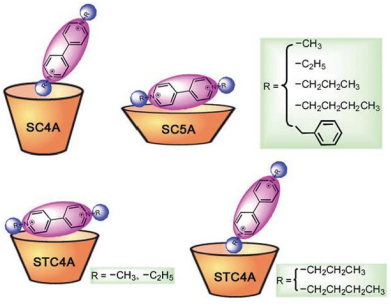


Discovery of 4-acetyl-3-(4-fluorophenyl)-1-(*p*-tolyl)-5-methylpyrrole as a dual inhibitor of human P-glycoprotein and *Staphylococcus aureus* Nor A efflux pump

Jaideep B. Bharate, Samsher Singh, Abubakar Wani, Sadhana Sharma, Prashant Joshi, Inshad A. Khan, Ajay Kumar,* Ram A. Vishwakarma* and Sandip B. Bharate*

Pyrroles showed dual inhibition of human P-gp and *S. aureus* Nor A efflux pump.

5432



The effect of terminal groups of viologens on their binding behaviors and thermodynamics upon complexation with sulfonated calixarenes

Kui Wang,* Si-Yang Xing,* Xiu-Guang Wang and Hong-Xi Dou

The effect of terminal groups of viologens on their binding behaviors with sulfonated calixarenes was systematically studied in this study.

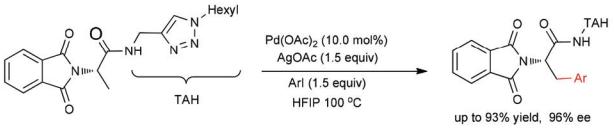
PAPERS

5444

Pd(II)-catalyzed C(sp^3)–H arylation of amino acid derivatives with click-triazoles as removable directing groups

Guofu Zhang, Xiaoqiang Xie, Jianfei Zhu, Shasha Li, Chengrong Ding* and Ping Ding

An effective Pd(II)-catalyzed C(sp^3)–H arylation of amino acid derivatives using 1,2,3-triazoles as removable directing groups has been developed.

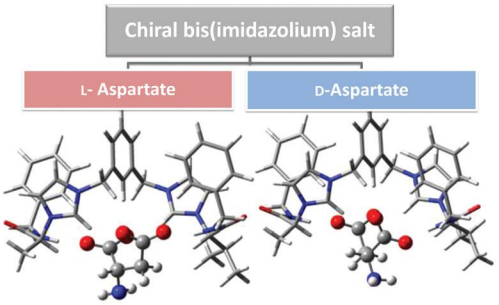


5450

Application of optically active chiral bis(imidazolium) salts as potential receptors of chiral dicarboxylate salts of biological relevance

Laura González-Mendoza, Jorge Escorihuela, Belén Altava,* M. Isabel Burguete and Santiago V. Luis*

New chiral ionic liquids as receptors for dicarboxylic acid derivatives.

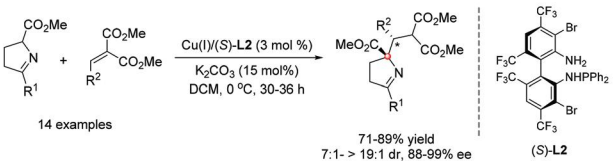


5460

Cu(I)/TF-BiphamPhos-catalyzed asymmetric Michael addition of cyclic ketimino esters to alkylidene malonates

Zhi-Yong Xue, Zhi-Min Song and Chun-Jiang Wang*

Cu(I)-catalyzed asymmetric Michael addition of cyclic ketimino esters with alkylidene malonates has been developed for efficient construction of β-branched α-amino acids containing adjacent quaternary and tertiary stereogenic centers in good yields with excellent diastereo-/enantioselectivities.

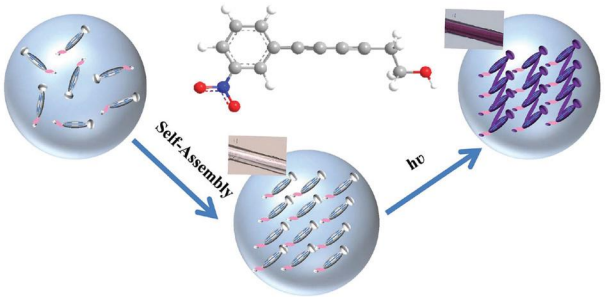


5467

Topochemical polymerization of unsymmetrical aryldiacetylene supramolecules with nitrophenyl substituents utilizing C–H···π interactions

Shichao Wang, Yong Li, Hui Liu, Jinpeng Li, Tiesheng Li, * Yangjie Wu,* Shuji Okada and Hachiro Nakanishi

The synthesis and solid-state polymerization of unsymmetrical aryldiacetylene supramolecules with nitrophenyl substituents.



PAPERS

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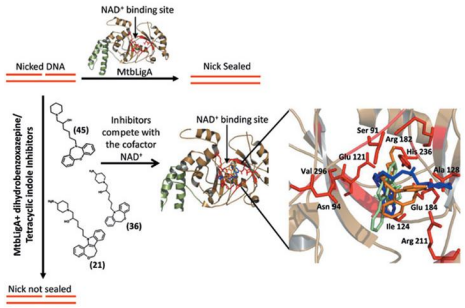
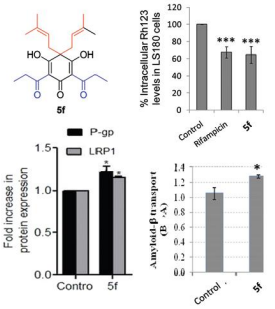


Tricyclic dihydrobenzoxazepine and tetracyclic indole derivatives can specifically target bacterial DNA ligases and can distinguish them from human DNA ligase I

Nisha Yadav, Taran Khanam, Ankita Shukla, Niyati Rai, Kanchan Hajela* and Ravishankar Ramachandran*

DNA ligases are critical components for DNA metabolism in all organisms.

5488

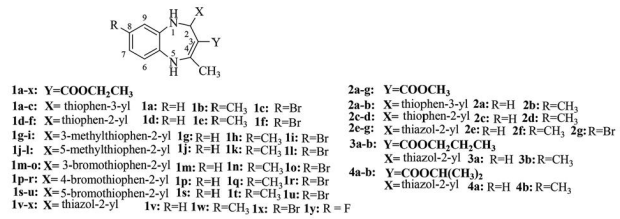


Synthesis and P-glycoprotein induction activity of colupulone analogs

Jaideep B. Bharate, Yazan S. Batarseh, Abubakar Wani, Sadhana Sharma, Ram A. Vishwakarma, Amal Kaddoumi,* Ajay Kumar* and Sandip B. Bharate*

A diprenylated acylphloroglucinol was identified as a potent P-gp inducer and showing ability to increase amyloid-beta transport across BBB, thus it is a potential anti-Alzheimer lead compound.

5497

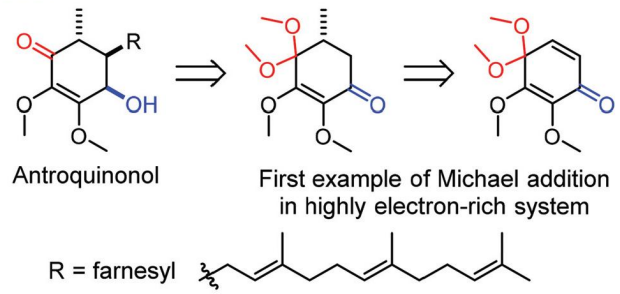


1,5-Benzodiazepine derivatives as potential antimicrobial agents: design, synthesis, biological evaluation, and structure–activity relationships

Lan-Zhi Wang,* Xiao-Qing Li and Ying-Shuang An

36 novel 1,5-benzodiazepine derivatives were synthesized and evaluated for their *in vitro* antimicrobial activity. The results revealed that most of the 1,5-benzodiazepine derivatives exhibited considerable potency against all of the tested strains.

5510



A short synthesis of (±)-antroquinonol in an unusual scaffold of 4-hydroxy-2-cyclohexenone

Che-Sheng Hsu, Ho-Hsuan Chou and Jim-Min Fang*

A short synthesis of the anticancer agent antroquinonol having an unusual core structure of 2,3-dimethoxy-4-hydroxycyclohex-2-enone with substituents at three contiguous stereocenters.

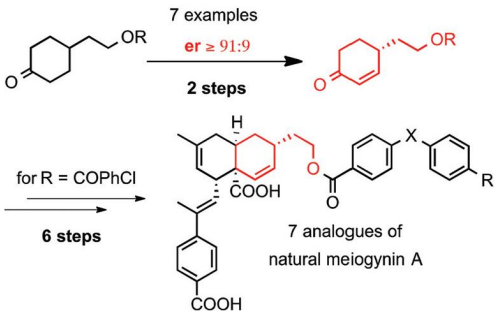
PAPERS

5520

Development of an efficient route toward meiogynin A-inspired dual inhibitors of Bcl-xL and Mcl-1 anti-apoptotic proteins

Sandy Desrat, Camille Remeur and Fanny Roussi*

The synthesis, on a large scale, with very good yield and er *via* an efficient strategy, of a chiral 4-substituted 2-cyclohexenone intermediate, was a milestone in the synthesis of seven analogues of meiogynin A, a natural sesquiterpenoid dimer.

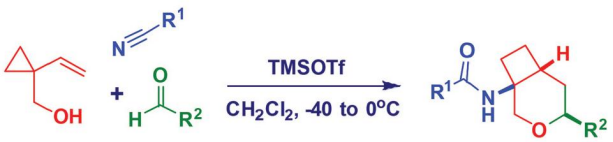


5532

Tandem Prins/Wagner/Ritter process for the stereoselective synthesis of (3-oxabicyclo[4.2.0]-octanyl)amide and (1-(5-aryltetrahydrofuran-3-yl)-cyclobutyl)amide derivatives

B. V. Subba Reddy,* K. Muralikrishna, J. S. Yadav, N. Jagdeesh Babu, K. Sirisha and A. V. S. Sarma

A novel synthesis of 4-aryl-(3-oxabicyclo[4.2.0]octan-1-yl)-amide and (1-(5-aryltetrahydrofuran-3-yl)cyclobutyl)amide derivatives was achieved through a sequential Prins/Wagner/Ritter process.

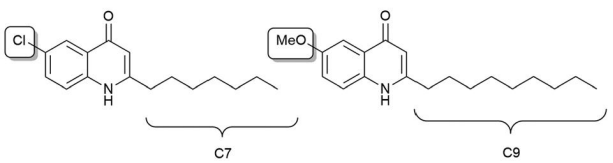


5537

A structure activity-relationship study of the bacterial signal molecule HHQ reveals swarming motility inhibition in *Bacillus atrophaeus*

F. Jerry Reen, Rachel Shanahan, Rafael Cano, Fergal O'Gara* and Gerard P. McGlacken*

Swarming motility inhibition in *Bacillus atrophaeus*.



5542

Alkynylation of steroids *via* Pd-free Sonogashira coupling

Yury N. Kotovshchikov, Gennadij V. Latyshev, Nikolay V. Lukashev* and Irina P. Beletskaya

A new biligand catalytic system was applied for the Pd-free Sonogashira syntheses of valuable steroidal enynes.