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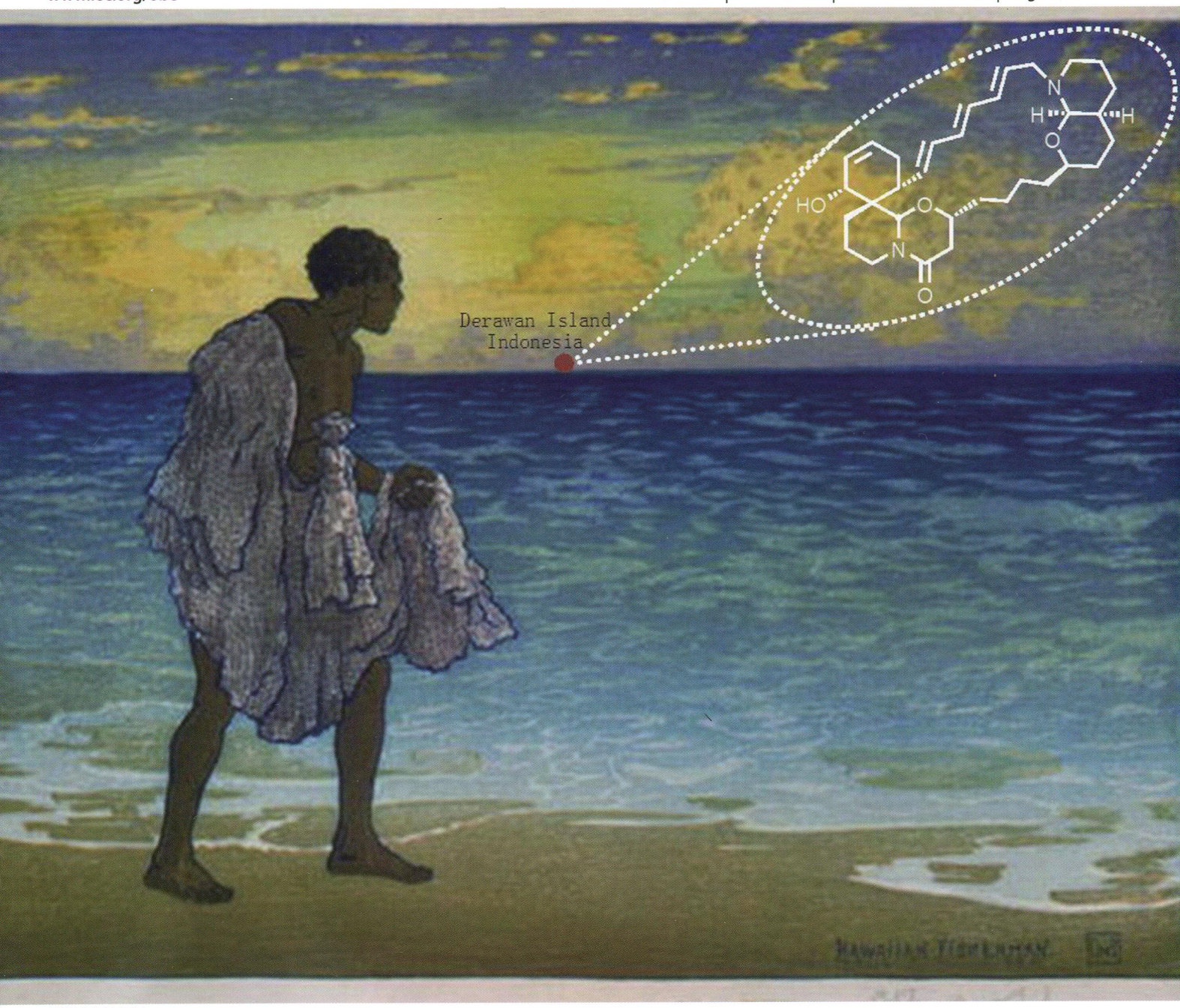

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REVIEW ARTICLE
William P. Unsworth and Richard J. K. Taylor
'Upenamide: trials and tribulations

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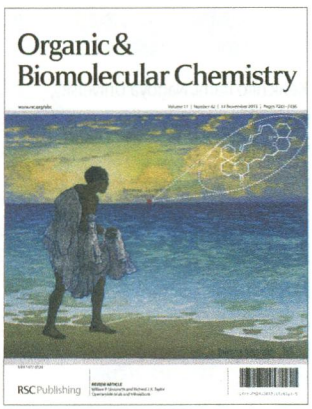

Cover
See William P. Unsworth and Richard J. K. Taylor, pp. 7250–7261.

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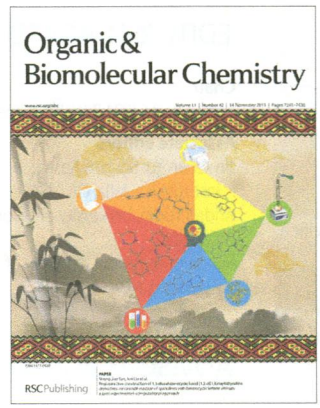

Inside cover
See Sheng-Jiao Yan, Jun Lin *et al.*, pp. 7276–7288.

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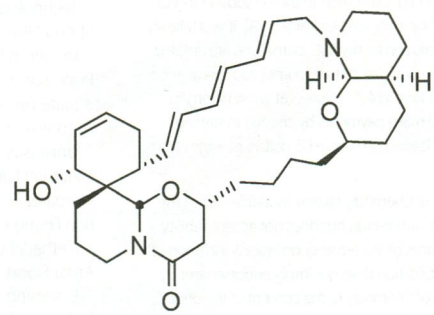
REVIEW

7250

'Upenamide: trials and tribulations

William P. Unsworth* and Richard J. K. Taylor*

The work of several research groups towards the total synthesis of the macrocyclic marine natural product 'upenamide is described.



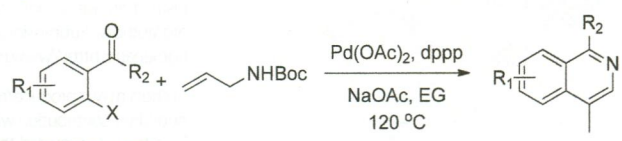
COMMUNICATIONS

7262

One-pot synthesis of 4-methylisoquinolines *via* a sequential Pd-catalyzed Heck reaction and intramolecular cyclization

Yulin Tian, Jianguo Qi, Chenbin Sun, Dali Yin, Xiaojian Wang* and Qiong Xiao

An efficient, one-pot synthesis of 4-methylisoquinolines *via* a sequential Pd-catalyzed Heck reaction and intramolecular cyclization has been developed with a wide substrate scope.



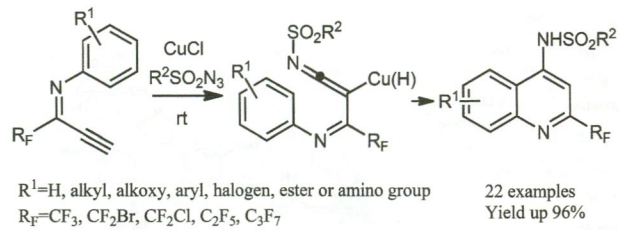
X= I, Br, OTf

7267

Cu-catalyzed tandem reactions of fluorinated alkynes with sulfonyl azides en route to 2-trifluoromethylquinolines

Yajun Li, Lisi Zhang, Li Zhang, Yongming Wu* and Yuefa Gong*

A novel method for the synthesis of 2-trifluoromethylquinolines *via* Cu-catalyzed tandem reactions was reported.

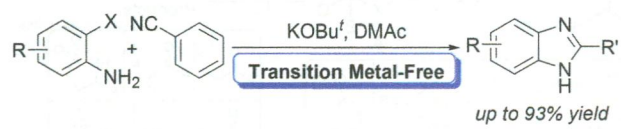


7271

Synthesis of benzimidazoles by potassium *tert*-butoxide-promoted intermolecular cyclization reaction of 2-iodoanilines with nitriles

Shi-Kai Xiang,* Wen Tan, Dong-Xue Zhang, Xian-Li Tian, Chun Feng, Bi-Qin Wang,* Ke-Qing Zhao, Ping Hu and Hua Yang

The synthesis of benzimidazoles by intermolecular cyclization reaction of 2-iodoanilines with nitriles has been developed. These reactions could proceed just using potassium *tert*-butoxide as the base.

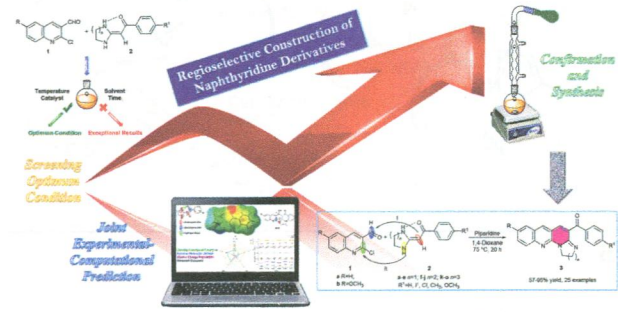


7276

Regioselective construction of 1,3-diazaheterocycle fused [1,2-*a*][1,8]naphthyridine derivatives *via* cascade reaction of quinolines with heterocyclic ketene aminals: a joint experimental–computational approach

Yi-Chuan Zhang, Zhi-Cheng Liu, Rui Yang, Ji-Hong Zhang, Sheng-Jiao Yan* and Jun Lin*

A joint experimental–computational approach for regioselective construction of 1,8-naphthyridines *via* cascade reaction of HKAs has been reported.

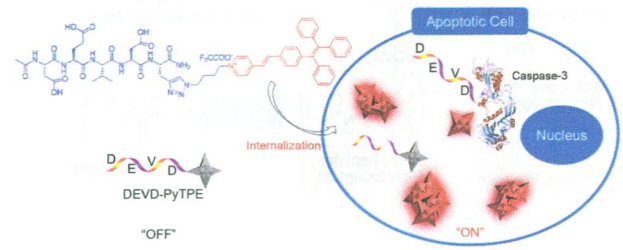


7289

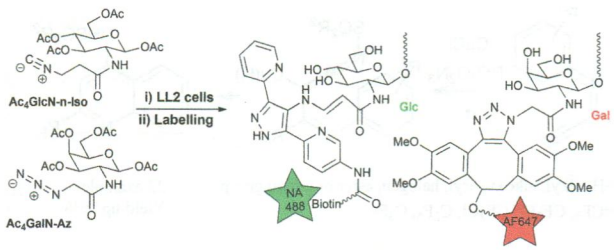
Fluorescent light-up probe with aggregation-induced emission characteristics for *in vivo* imaging of cell apoptosis

Haibin Shi, Na Zhao, Dan Ding, Jing Liang, Ben Zhong Tang* and Bin Liu*

A live-cell permeable, fluorescent light-up AIE probe has been developed for real-time *in vivo* cell apoptosis imaging and drug screening.



7297

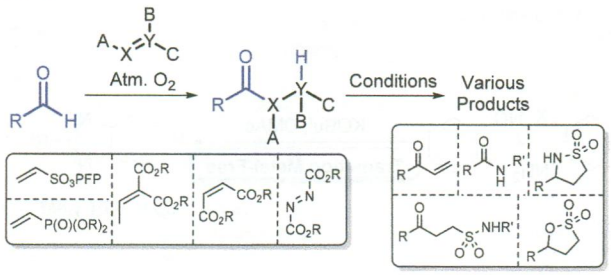


Dual-sugar imaging using isonitrile and azido-based click chemistries

Yéléna A. Wainman, André A. Neves, Shaun Stairs, Henning Stöckmann, Heather Ireland-Zecchini, Kevin M. Brindle and Finian J. Leeper*

We report the first account of metabolically labelling *N*-acetylglucosamine, in conjunction with either *N*-acetylgalactosamine or *N*-acetylmannosamine using a combination of isonitrile- and azide-based chemistries.

7301

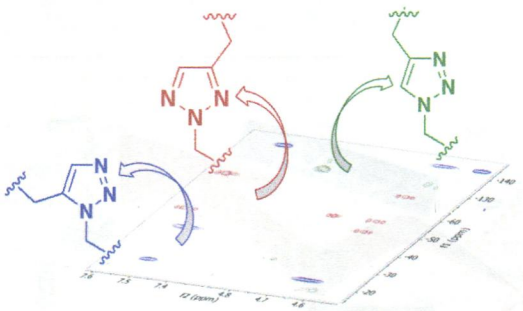


Metal-free, hydroacylation of C=C and N=N bonds *via* aerobic C–H activation of aldehydes, and reaction of the products thereof

Vijay Chudasama, Ahmed R. Akhbar, Karim A. Bahou, Richard J. Fitzmaurice and Stephen Caddick*

A clean, efficient and wide-ranging method for hydroacylation using *only* atmospheric oxygen for initiation, and reaction of the products thereof.

7318

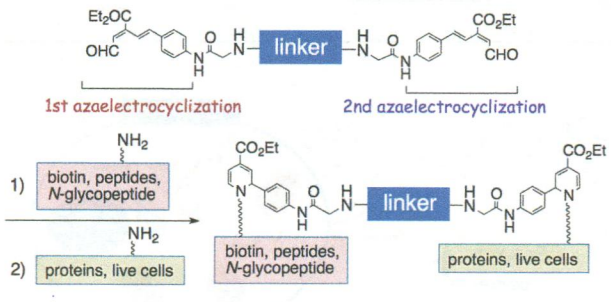


^{15}N NMR spectroscopic and theoretical GIAO-DFT studies for the unambiguous characterization of disubstituted 1,2,3-triazoles

Miriam Corredor, Jordi Bujons, Àngel Messeguer and Ignacio Alfonso*

The three possible isomers of disubstituted 1,2,3-triazoles have been unambiguously assigned by a combination of the ^{1}H/^{15}N gHMBC experiments and theoretical calculations of the corresponding chemical shifts.

7326



Development of bis-unsaturated ester aldehydes as amino-glue probes: sequential double azaelectrocyclization as a promising strategy for bioconjugation

Katsunori Tanaka,* Yuka Nakamoto, Eric R. O. Siwu, Ambara R. Pradipta, Koji Morimoto, Takeshi Fujiwara, Suguru Yoshida, Takamitsu Hosoya, Yuki Tamura, Go Hirai, Mikiko Sodeoka and Koichi Fukase*

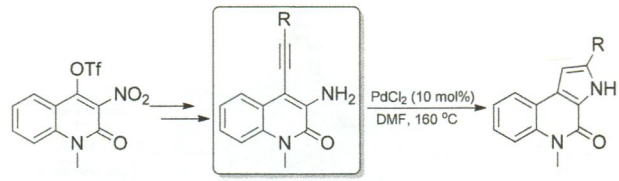
The unsaturated ester aldehyde, (*E*)-3-alkoxycarbonyl-5-phenyl-2,4-dienal, was developed to achieve highly efficient bioconjugation between the biological amines.

7334

Synthesis of 3*H*-pyrrolo[2,3-*c*]quinolin-4(5*H*)-ones *via Pd-catalyzed cross*-coupling reaction and cyclization

Zhiyong Wang,* Xiaoxiao Xing, Lijun Xue, Fang Gao and Ling Fang*

An efficient and concise manner for the synthesis of biologically active 3*H*-pyrrolo[2,3-*c*]quinolin-4(5*H*)-ones through the palladium catalyzed sequential cross-coupling reaction and cyclization process was described.

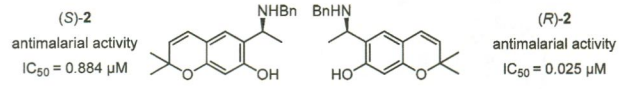


7342

Enantioselective synthesis of encecaline-derived potent antimalarial agents

Dipak Harel, Dirk Schepmann, Reto Brun, Thomas J. Schmidt and Bernhard Wünsch*

The high antiplasmodial activity of racemic benzylamines *rac*-**1** and *rac*-**2** stimulated the synthesis of pure enantiomers. (*R*)-**2** is 34-fold more potent than (*S*)-**2**.

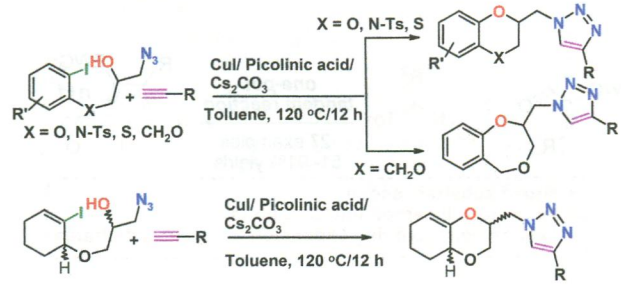


7350

Dual catalysis by Cu(I): facile single step click and intramolecular C–O bond formation leading to triazole tethered dihydrobenzodioxines/ benzoxazines/benzoxathiines/benzodioxepines

M. Nagarjuna Reddy and K. C. Kumara Swamy*

Dual copper catalysis, involving two different reactions, click (alkyne–azide) and carbon–oxygen bond formation (aryl iodide–secondary alcohol) in a single step, is reported.

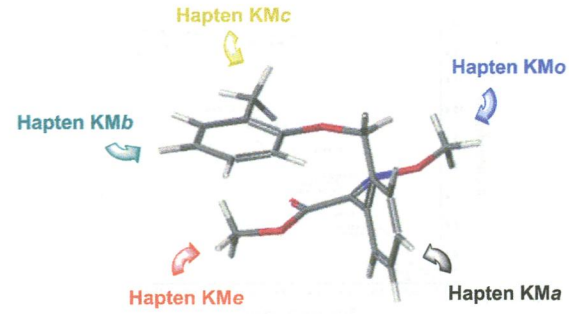


7361

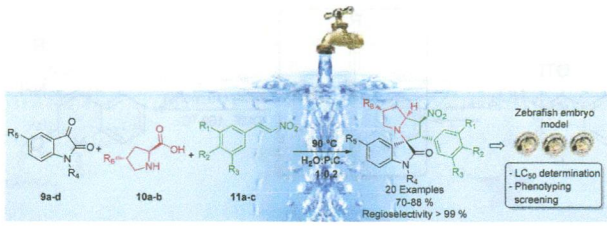
Structure–immunogenicity relationship of kresoxim-methyl regioisomeric haptens

Rosario López-Moreno, Josep V. Mercader, Consuelo Agulló, Antonio Abad-Somovilla* and Antonio Abad-Fuentes*

The antibody-eliciting capability of five kresoxim-methyl haptens with identical linkers tethered at selected sites of the molecular framework was evaluated in rabbits and mice.



7372

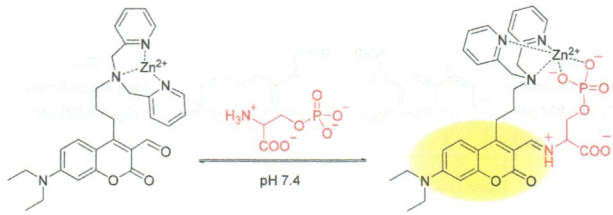


Regio- and stereoselective synthesis of spirooxindole 1′-nitro pyrrolizidines with five concurrent stereocenters under aqueous medium and their bioprospection using the zebrafish (*Danio rerio*) embryo model

Carlos E. Puerto Galvis and Vladimir V. Kouznetsov*

The synthesis of spirooxindolo 1′-nitro pyrrolizidines with five concurrent stereocenters under aqueous medium is described as well as their bioprospection using the. zebrafish embryo model.

7387

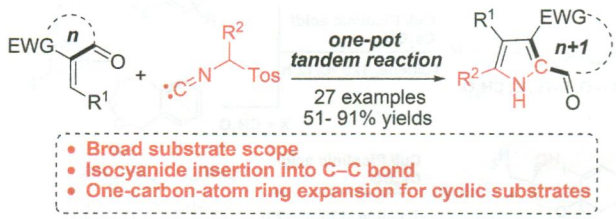


A selective fluorescent chemosensor for phosphoserine

Chad M. Cooley, Kenneth S. Hettie, Jessica L. Klockow, Shana Garrison and Timothy E. Glass*

A Zn^{2+}–DPA-substituted coumarin aldehyde chemosensor demonstrates a 30-fold fluorescence enhancement to phosphoserine in buffered aqueous conditions.

7393

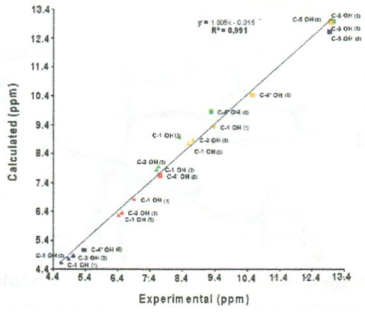


Tandem Michael addition/isocyanide insertion into the C–C bond: a novel access to 2-acylpyrroles and medium-ring fused pyrroles

Lingjuan Zhang, Xianxiu Xu,* Qiu-rong Shao, Ling Pan and Qun Liu*

The first example of tandem Michael addition/isocyanide insertion into the C–C bond is described, which enables a facile one-pot synthesis of polyfunctionalized 2-acylpyrroles and seven-/eight-membered-ring fused pyrroles in good to excellent yields under mild conditions.

7400



Investigation of solute–solvent interactions in phenol compounds: accurate *ab initio* calculations of solvent effects on ^{1}H NMR chemical shifts

Michael G. Siskos,* Vassiliki G. Kontogianni, Constantinos G. Tsiafoulis, Andreas G. Tzakos and Ioannis P. Gerothanassis*

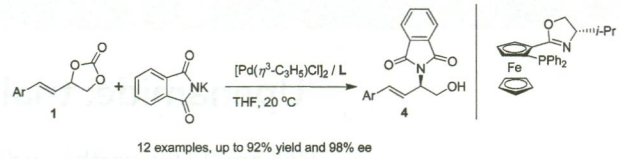
Molecular level solvent effects: Accurate *ab initio* calculations of solvent effects on ^{1}H NMR chemical shifts of the –OH groups of phenol compounds and excellent correlation with experimental data are demonstrated.

7412

The synthesis of chiral β-aryl-α,β-unsaturated amino alcohols *via* a Pd-catalyzed asymmetric allylic amination

Mao Quan, Nicholas Butt, Jiefeng Shen, Kaiji Shen, Delong Liu* and Wanbin Zhang*

A series of chiral β-aryl-α,β-unsaturated aminoalcohols were synthesized *via* a Pd-catalyzed asymmetric allylic amination with up to 92% yield and 98% ee.

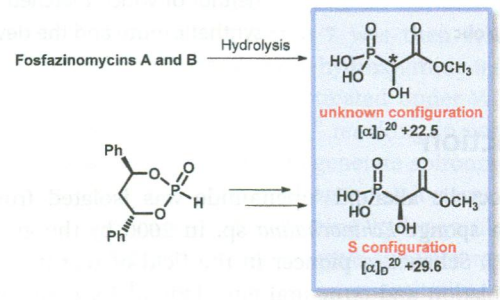


7420

Determination of absolute configuration of the phosphonic acid moiety of fosfazinomycins

Katharina Schiessl, Alexander Roller and Friedrich Hammerschmidt*

The absolute configuration of the phosphonic acid moiety of fosfazinomycins could be deduced by comparison with both synthetically obtained enantiomers.



7427

Synthesis and C2-functionalization of indoles with allylic acetates under rhodium catalysis

Mirim Kim, Jihye Park, Satyasheel Sharma, Sangil Han, Sang Hoon Han, Jong Hwan Kwak, Young Hoon Jung and In Su Kim*

Tandem rhodium-catalyzed oxidative allylation and annulation of acetanilides with allyl acetate to afford the corresponding indoles are described. In addition, the site-selective C2-allylation, crotylation and prenylation of indoles using allylic acetates under rhodium catalysis are reported.