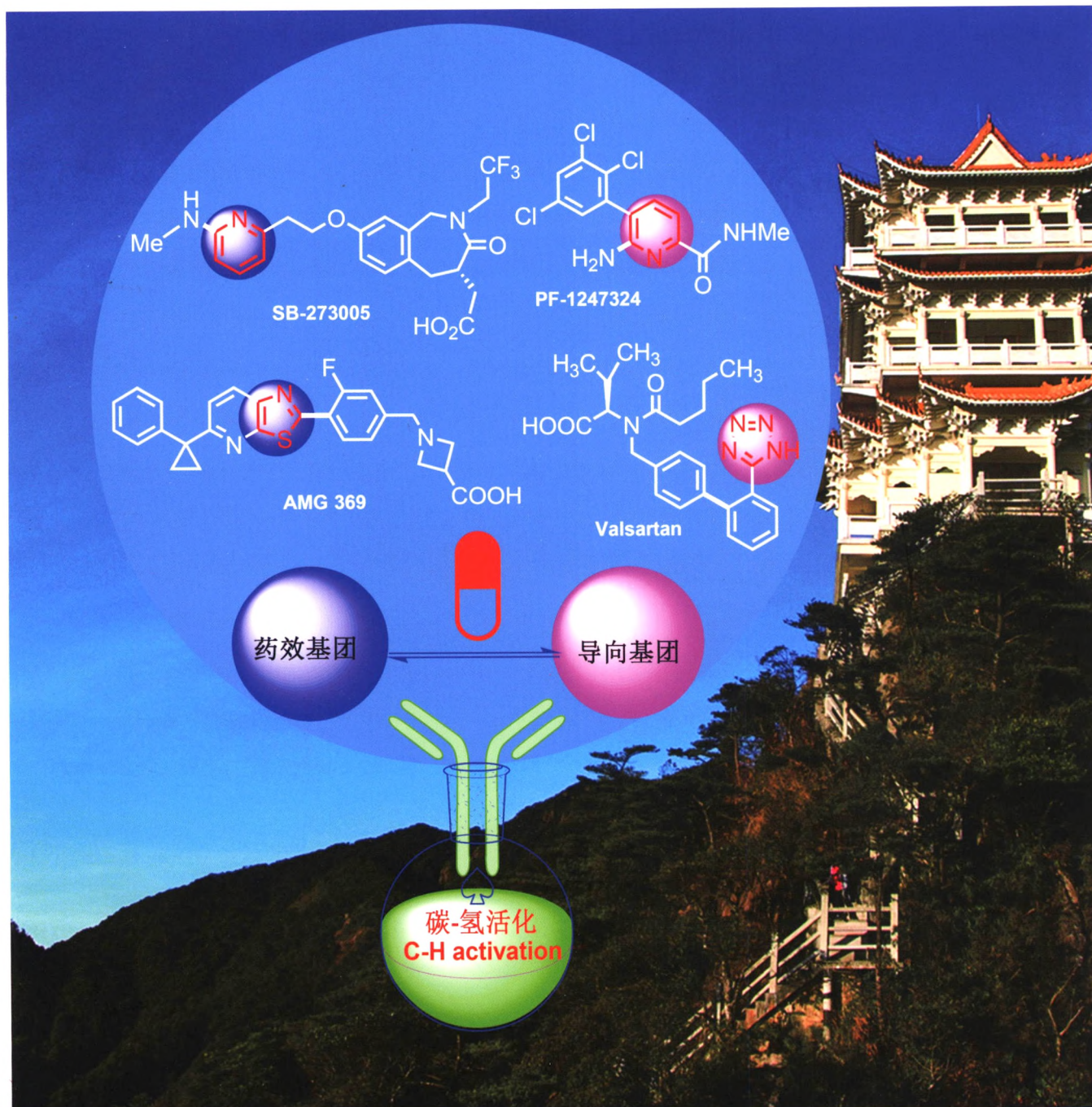


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中国科学院上海有机化学研究所

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(YOUJI HUAXUE)

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* 通讯联系人.

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研究简报

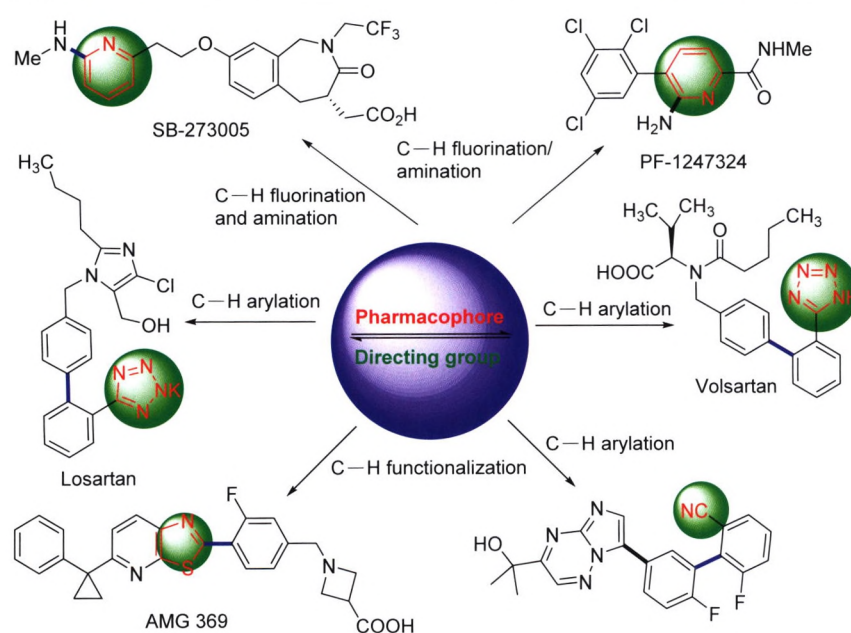
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On the Cover

Many pharmacophores are ideal directing groups for C—H activation enabling the subsequent stages of drug synthesis, and showing that there is a correlation between directing group and pharmacophore. The latest breakthroughs of C—H activation via functional switch between pharmacophore and directing group, and their application in the drug discovery and process development are reviewed in detail by Ren, Nie and Zhang on page 2465.

REVIEWS

Functional Switch between Pharmacophore and Directing Group and Their Application in Drug Discovery and Development via C—H Activation and Functionalization

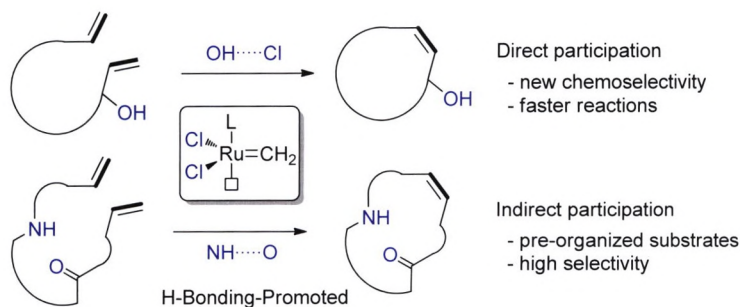


The functional switch of a C—H activation directing group to a pharmacophore is introduced and analyzed, and the value of pharmacophore and application of C—H activation are exemplified. The latest breakthroughs of C—H activation and application in the drug discovery process are reviewed as case studies, providing several industrial examples of using a pharmacophore as directing group for drug synthesis.

Ren, Qingyun; Nie, Biao; Zhang, Yingjun; Zhang, Ji*

Chin. J. Org. Chem. **2018**, 38(10), 2465

Hydrogen-Bonding Effects in Ruthenium-Catalyzed Olefin Metathesis



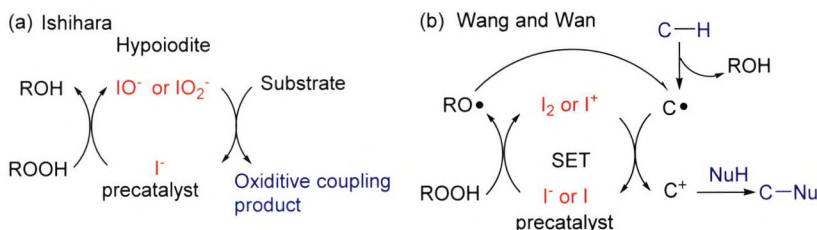
Yan, Tingbin; Liu, Yuehui; Shen, Yuehai*
Chin. J. Org. Chem. **2018**, 38(10), 2491

Development and application of hydrogen bonding-promoted ruthenium-catalyzed olefin metathesis reactions are summarized.

CONTENT

Recent Advances in Oxidative Coupling Reaction Catalyzed by Low-Valence Iodine

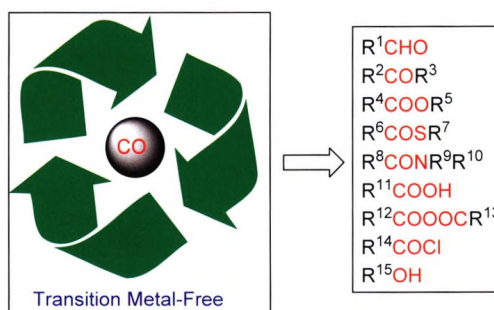
Yan, Yizhe*; Cui, Chang; Li, Zheng
Chin. J. Org. Chem. **2018**, 38(10), 2501



In recent years, low-valence iodine-catalyzed oxidative coupling reaction has made rapid progress, providing an effective method for the construction of C—C, C—O, C—N, C—S, C—P and other chemical bonds. The research progress on low-valence iodine-catalyzed oxidative coupling from 2010 to now is summarized, and the outlook of this field is also prospected.

Research Progress in Transition-Metal-Free Carbonylation Reactions

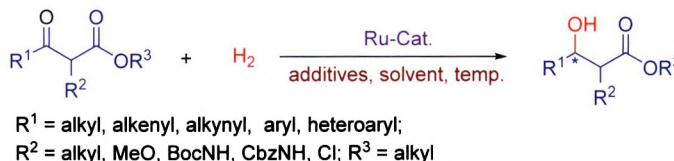
Xu, Fangning; Han, Wei*
Chin. J. Org. Chem. **2018**, 38(10), 2519



In recent years, developing transition-metal-free systems for the carbonylation has attracted highly attention from many researchers. The recent research progress of transition-metal-free carbonylations for the synthesis of aldehydes, ketones, esters, amides, acids, anhydrides, acyl chloride, and alcohols is reviewed. And the development and application prospects for transition-metal-free carbonylation are also discussed.

Progress in Ruthenium-Catalyzed Asymmetric Hydrogenation of β -Keto Esters

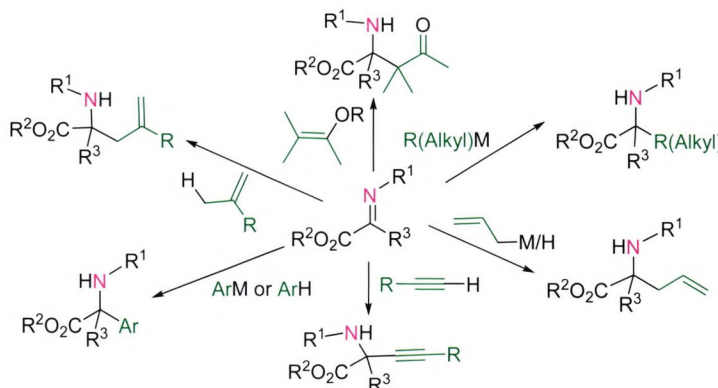
Chen, Shuqi; Yang, Wen; Yao, Yongqi; Yang, Xin; Deng, Yingying; Yang, Dingqiao*
Chin. J. Org. Chem. **2018**, 38(10), 2534



The recent research progress in ruthenium-catalyzed asymmetric hydrogenation of β -keto esters is reviewed. Great attention was paid to the influences of chiral ligands, substrate structures, solvents and additives on the homogeneous asymmetric hydrogenation, as well as the influences of support materials and additives on the heterogeneous asymmetric hydrogenation. Moreover, the possible mechanisms are also discussed.

Synthesis of Chiral α -Amino Acid Derivatives by Asymmetric Addition of α -Imino Ester

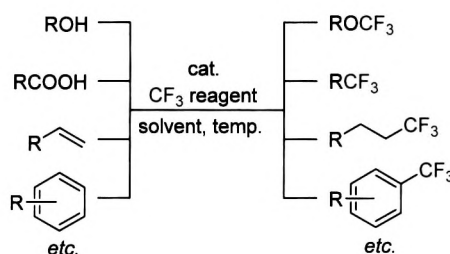
Bi, Jili; Ma, Ransong; Yang, Jinhui*
Chin. J. Org. Chem. **2018**, 38(10), 2553



This review describes the development of such method on the view of reaction types and different kinds of nucleophiles. Specifically, the reactions include allylation reaction, arylation reactions, Mannich reactions, alkenylation reactions, alkynylation reactions and alkylation reactions are introduced, together with the associated reaction mechanisms and recent developments. A prospect on this research field is also given.

Recent Advances in Transition Metal-Promoted Trifluoromethylation Reactions

Chen, Donghan; Yang, Wen; Yao, Yongqi;
Yang, Xin; Deng, Yingying; Yang, Dingqiao*
Chin. J. Org. Chem. **2018**, 38(10), 2571

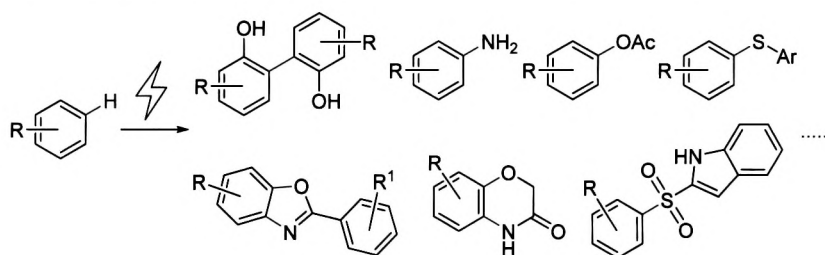


the possible mechanisms of some parts of reactions are also discussed.

Recently, transition metal-promoted trifluoromethylation has been developed rapidly. Starting with the types of transition metal that promote the trifluoromethylation reactions, the research progress of trifluoromethylation promoted by silver, iron, palladium, nickel, rhodium and cobalt in recent years is reviewed. Moreover,

Progress in Electrochemical C—H Functionalizations of Aromatic Compounds

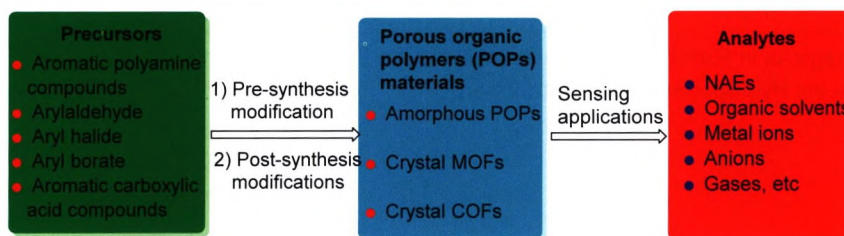
Wu, Yaxing; Xi, Yachao; Zhao, Ming*;
Wang, Siyi
Chin. J. Org. Chem. **2018**, 38(10), 2590



Carbon-hydrogen bonds are extensive and basic chemical bonds existed in organic compounds. Certain C—H activation reactions with chemoselectivity and regioselectivity can also be achieved by the optimization of electrode materials, electrolytes, and solvents. Various reactions focusing on the electrochemical functionalizations of C—H bonds in aromatic compounds are mainly reviewed.

Synthesis and Fluorescent Sensing Application of Porous Organic Polymer Materials

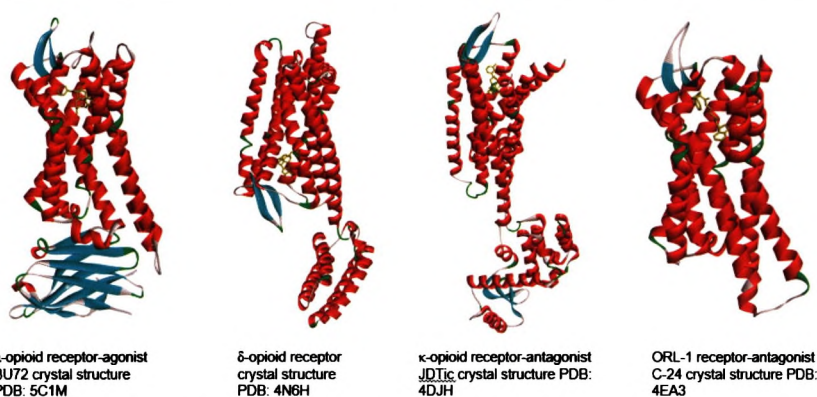
Pang, Chuming; Luo, Shihe; Hao, Zhifeng*;
Gao, Jian; Huang, Zhaohao; Yu, Jiahai;
Yu, Simin; Wang, Zhaoyang*
Chin. J. Org. Chem. **2018**, 38(10), 2606



In this paper, according to the different types of porous organic polymer materials (POPs), namely the amorphous porous organic polymer materials, crystal porous metal organic framework materials containing coordination bond, and crystal covalent organic framework materials, the new progress of the POPs fluorescence materials in recent years is reviewed. Especially, the design and synthesis based on functional organic molecules, and their fluorescence sensing applications, are introduced in details.

Recent Topics in Research and Development of Opioid Drugs

Pan, Chenling; Meng, Ha; Wang, Liangliang;
Shen, Yuehai*; Zuo, Zhili*; Wang, Guanlin;
Chang, Kwen-jen
Chin. J. Org. Chem. **2018**, 38(10), 2625



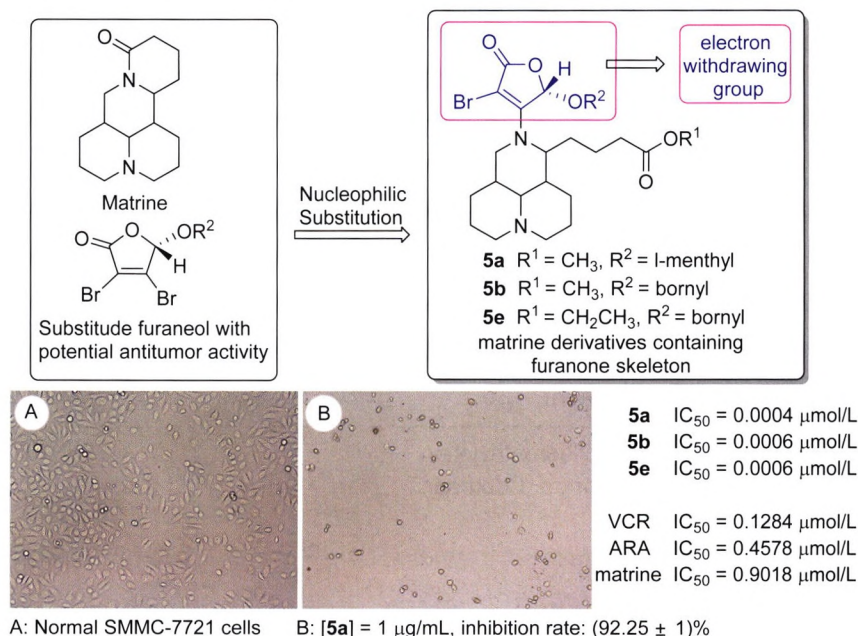
Pain, Substance Abuse, Gastrointestinal Disorders, Cough, Depression, Parkinson's Disease, et al.

Recent reports on several topics in the study of small molecule opioid drugs are summarized.

CONTENT

ARTICLES

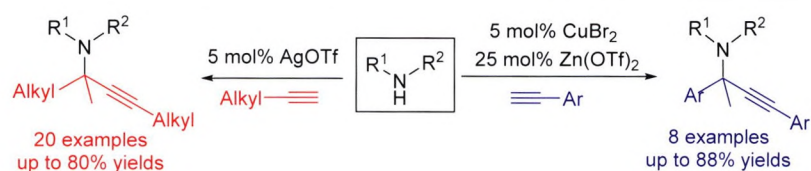
Synthesis of Novel Matrine Derivatives Containing Furanone Skeleton and Preliminary Evaluation of Their Anticancer Activity *in Vitro*



Ma, Fuli; Zhang, Jiao; Li, Ming; Yu, Jiaying; Luo, Wei; Li, Xueqiang*; Wei, Mengxue*
Chin. J. Org. Chem. **2018**, 38(10), 2633

A series of novel matrine derivatives with furanone-modified scaffold were designed and synthesized from matrine and 5-hydroxyl-3,4-dibromo-2-(5*H*)-furanone. Methyl 3-(2-((*S*)-4-bromo-2-(((1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl)oxy)-5-oxo-2,5-dihydrofuran-3-yl)dodecahydropyrido[3,2,1-ij][1,6]naphthyridin-1-yl)propanoate (**5a**) possessed best inhibitory activity against SMMC-7721 cell lines with the IC_{50} value of 0.0004 µmol/L at 24 h, showing markedly higher inhibitory activity *in vitro* than positive control drugs vincristine (0.1284 µmol/L) and cytosine arabinoside (0.4578 µmol/L) as well as the parent compound matrine (0.9018 µmol/L).

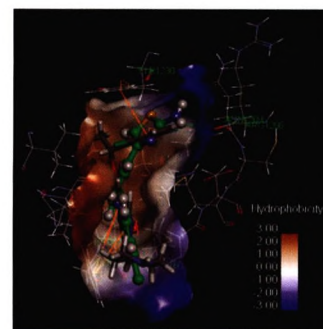
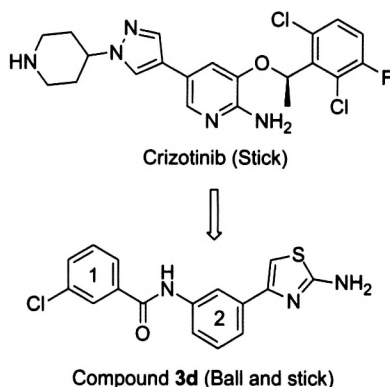
Selective Synthesis of Quaternary Carbon Propargylamines from Amines, Alkynes, and Alkynes under Neat Condition



Wang, Zheng; Yang, Liu; Liu, Huilan; Tan, Yingzhi; Bao, Wenhui; Wang, Ming; Tang, Zilong; He, Weimin*
Chin. J. Org. Chem. **2018**, 38(10), 2639

An efficient protocol for the synthesis of quaternary carbon propargylamines via a one-pot tandem reaction of amines, alkynes, and alkynes under neat condition was developed.

Design, Synthesis, and Biological Evaluation of Novel 2-Amino-4-phenylthiazole Derivatives as c-Met Inhibitors

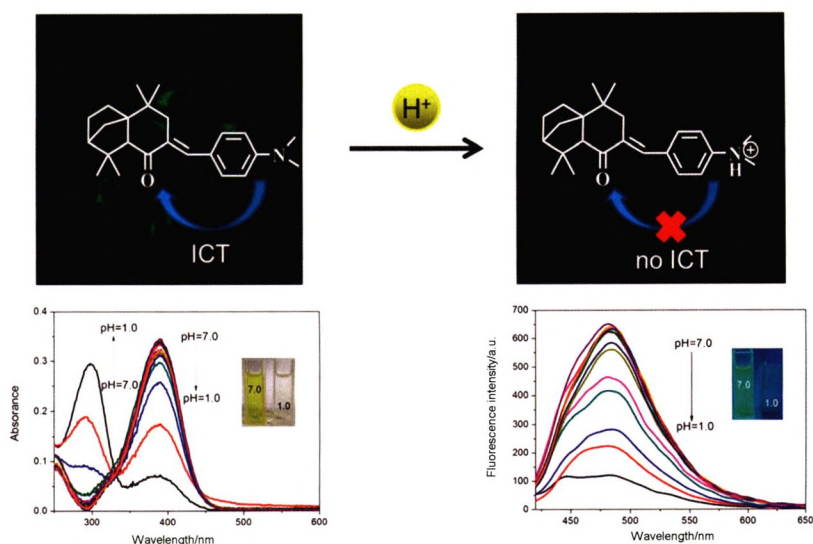


Zhang, Zhihua; Chen, Yu; Wu, Hongmei; Cui, Bo; Xiong, Wulin; Lin, Tenghui; Lin, Rongnan; Guo, Yu*
Chin. J. Org. Chem. **2018**, 38(10), 2648

Novel 2-amino-4-phenylthiazole derivatives were synthesized as potential c-Met inhibitors.

CONTENT

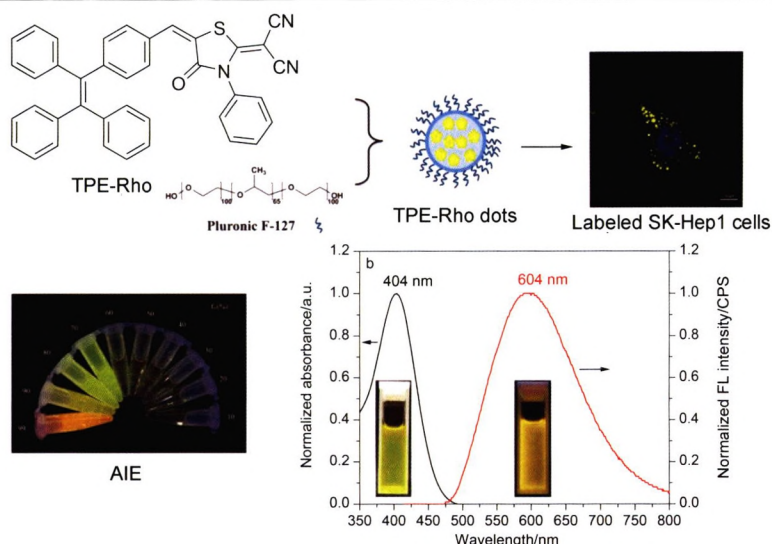
A Novel Fluorescent pH Probe Based on Isolongifolanone and Its Application in Bioimaging



Zhang, Yan; Wang, Zhonglong; Tao, Yu; Xu, Xu; Fang, Hua; Wang, Shifa*
Chin. J. Org. Chem. **2018**, 38(10), 2693

A novel fluorescent pH probe based on isolongifolanone and its application in bioimaging.

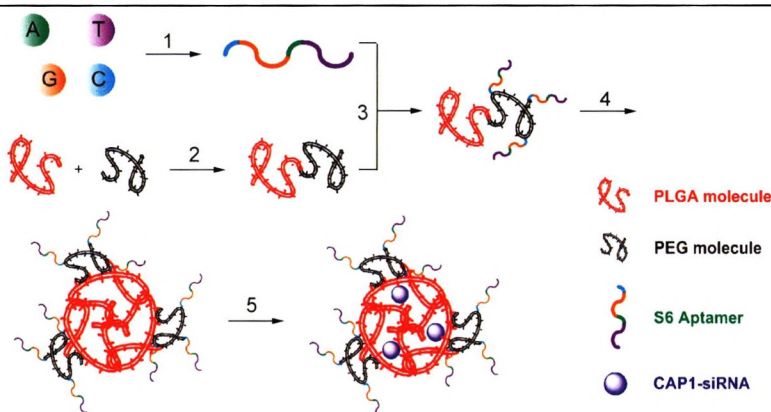
Synthesis and Live Cell Imaging of Tetraphenylethene-Based Fluorescent Nano-probes



Xia, Qi; Chen, Zikang; Zhang, Zhide; Liu, Ruiyuan*
Chin. J. Org. Chem. **2018**, 38(10), 2700

An AIE organic fluorescent probe (TPE-Rho) was designed and synthesized, and an amphiphilic polymer material was used to wrap it into a nano-fluorescence probe (TPE-Rho dots). The optical properties of TPE-Rho dots were studied

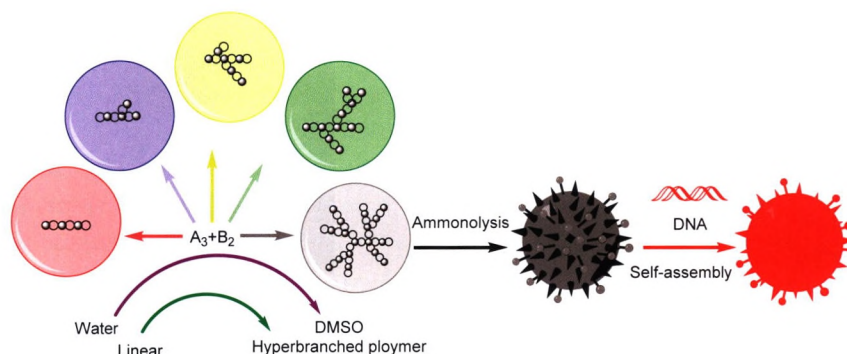
Preparation of Poly(lactic-co-glycolic acid)/Polyethylene Glycol Nanoparticles with Surface-Modified Aptamer S6 and Its Application on Carrier siRNA



Liu, Yang; Xie, Shuanshuan; Zeng, Jie; Tan, Min; Song, Xiaolian; Zhu, Jun*; Wang, Changhui*
Chin. J. Org. Chem. **2018**, 38(10), 2706

Aptamers S6 and poly(lactic-co-glycolic acid)/polyethylene glycol (PLGA-PEG) copolymers were synthesized to obtain a targeted nanocarrier. Finally, the complex was characterized and its role in inhibiting the invasiveness of tumor cells was verified.

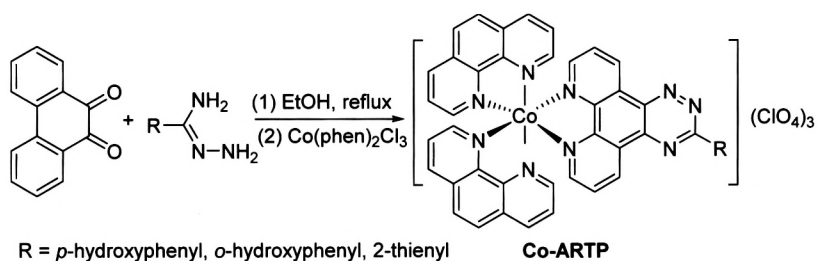
Poly(amido amine)s with Different Branched Architecture: Synthesis, Reactivity and Their Application in Gene Delivery



Poly(amido amine)s with diverse topographical structures are promising candidates for gene delivery and drug carriers. A series of poly(amido amine)s (PAAs) with the same repeating units, however, different degree of branching, were successfully prepared by Michael addition polycondensation of *N,N*-methylenebis(acrylamide) and *L*-cysteine methyl ester hydrochloride in a water/dimethyl sulfoxide co-solvent. The obtained disposed cationic PAAs exhibit good DNA condensation capacities.

Zhang, Wei; Yao, Zijian; Deng, Wei*
Chin. J. Org. Chem. **2018**, 38(10), 2713

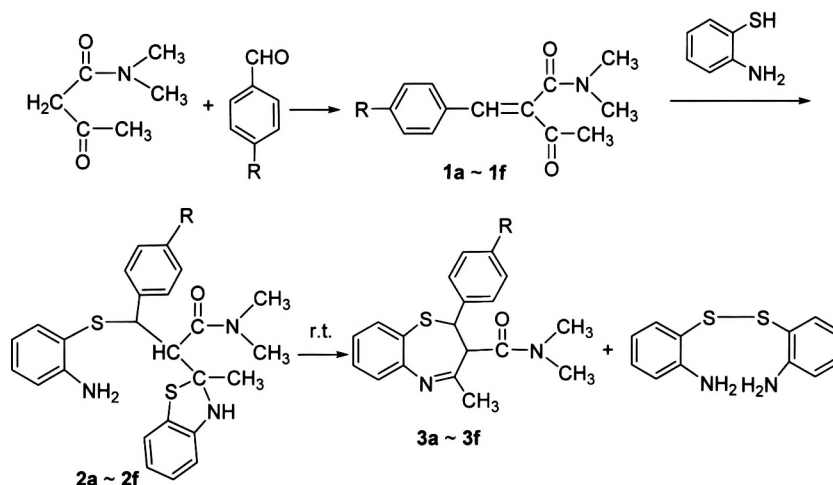
Synthesis and Bioactivities of Novel 1,2,4-Triazine Skeleton Phenanthroline Derivatives and the Fluorescent Recognition on DNA Using Three Novel Co(III) Complexes



Zhang, Chenglu*; Li, Yizheng; Li, Jingyi; Li, Yilin; Gong, Rongqing; Wang, Huayu
Chin. J. Org. Chem. **2018**, 38(10), 2720

Novel 1,2,4-triazine skeleton phenanthroline derivatives **ARTP** were synthesized. They behave high inhibitory activities against Cdc25B and three Co(III)-complexes were synthesized and expected to be the DNA fluorescence probes.

NOTES

Synthesis and Antimicrobial Activity of 2-Substituted-phenyl-3-*N,N*-dimethylformamido)-4-methyl-1,5-benzothiazepine

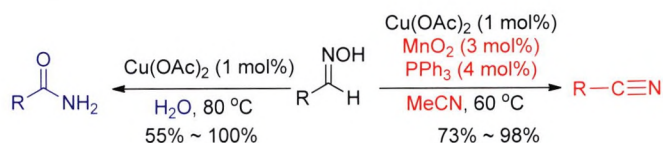
Xu, Tongxiu; Wang, Yan; Tian, Keqing; Wang, Ranran; Yan, Jingyi; Zhang, Ping*
Chin. J. Org. Chem. **2018**, 38(10), 2731

2-Substituted-phenyl-3-(*N,N*-dimethylformamido)-4-methyl-1,5-benzothiazepine (**3a~3f**) were designed and synthesized. **3a~3f** were dynamic control products and had obvious inhibitory effect on fungi and bacteria, especially for *Cryptococcus neoformans* and *Escherichia coli*.

CONTENT

Copper-Catalyzed Selectivity-Switchable Dehydration/Beckmann Rearrangement Reactions of Aldoxime

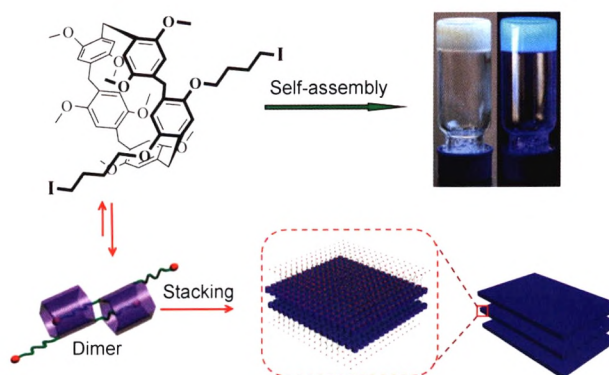
Fan, Xin; Yi, Rong; Wang, Fang; Zhang, Xu*; Xu, Qing; Yu, Lei*
Chin. J. Org. Chem. **2018**, 38(10), 2736



Copper could well catalyze the dehydration reaction of aldoximes to organonitriles in nitrile solvent by using MnO_2 as the co-catalyst and PPh_3 as the ligand. In contrast, instead of organonitriles, the Cu-catalyzed reactions of the aldoximes in water led to amides, which were the products of the Beckmann rearrangements.

Preparation and Properties of Supramolecular Organogel Based on Iodine-Functionalized Pillar[5]arene

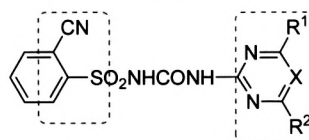
Chen, Jinfa; Liu, Xi; Han, Bingbing; Ding, Jindong; Zhang, Youming; Lin, Qi; Yao, Hong; Wei, Taibao*
Chin. J. Org. Chem. **2018**, 38(10), 2741



A iodine-functionalized pillar[5]arene was designed and synthesized. It can form a stable supramolecular organogel in cyclohexanol, and phase transition temperature is approximately 96 °C. The experiment results showed that a sheet-like structure was formed in self-assembly process of iodine-functionalized pillar[5]arene.

Synthesis and Biological Activity of 2-Cyanobenzenesulfonylurea Derivatives

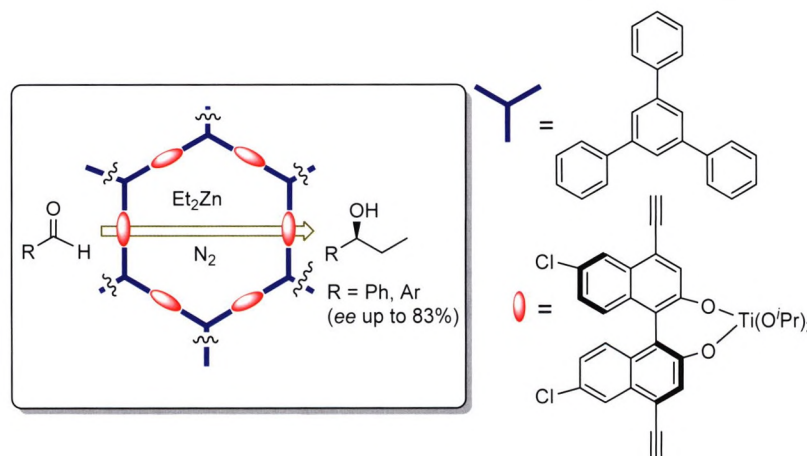
Chen, Wei; Li, Yuxin; Li, Yonghong; Yu, Shujing; Xiong, Lixia; Li, Zhengming*
Chin. J. Org. Chem. **2018**, 38(10), 2747



A series of 2-cyanobenzenesulfonylurea derivatives were designed and synthesized for studying their multi-bioactivity. The bioassay results indicated that some of the title compounds showed excellent *in vitro* antibacterial activity and insecticidal activity.

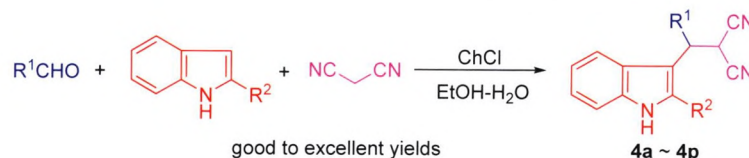
Asymmetric Addition Reaction Catalyzed by 1-(2-Hydroxynaphthalen-1-yl)naphthalen-2-ol Functionalized Porous Organic Polymer

Kong, Shengnan; Qian, Xuefeng; Shu, Mouhai*; Xiao, Wende
Chin. J. Org. Chem. **2018**, 38(10), 2754



A functionalized porous organic polymer POP-BINOL has been prepared and characterized by various techniques. After being treated with $\text{Ti}(\text{O}^i\text{Pr})_4$, the composite material could be used as highly effective and reusable heterogeneous catalyst for asymmetric diethylzinc addition to aldehydes with *ee* value.

Choline Chloride as Catalyst towards the Attractive Yonemitsu Reaction of Benzaldehyde, Indole, and Malononitrile

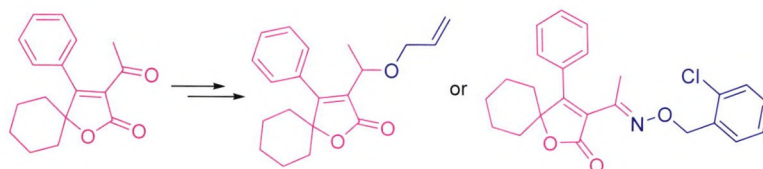


Yang, Zhonghua; Liu, Lanye; Zhao, Yihe; Hong, Yuanlin; Ruan, Hongli; Lü, Chengwei*

Chin. J. Org. Chem. **2018**, 38(10), 2761

A simple and efficient method was developed for the Yonemitsu condensation of indole, benzaldehyde, and malononitrile. Introducing water in reaction system and using choline chloride as cheap and safe catalyst were proved to be efficient to accelerate this multi-component reaction.

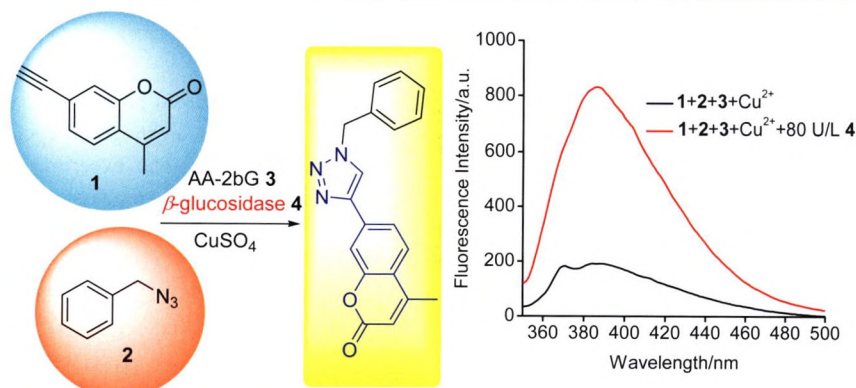
Synthesis and Fungicidal Activity of 3-Acetyl-4-phenyl-1-oxaspiro[4,5]dec-3-en-2-one Derivatives



Guan, Aiyang; Zhao, Yu; Wang, Weiwei; Liu, Xinlei; Wang, Mingan*

Chin. J. Org. Chem. **2018**, 38(10), 2767

A series of novel 3-acetyl-4-phenyl-1-oxaspiro[4,5]dec-3-en-2-one derivatives were synthesized. Their *in vivo* and *in vitro* fungicidal activities were evaluated against phytopathogens, which showed that some of them exhibited excellent inhibition against *P. cubensis* and *P. polysora*.

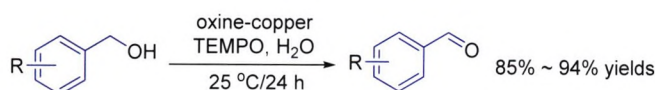
Determination of β -Glucosidase Activity Based on Enzyme-Triggered Click Chemistry

Wang, Longwen; Ma, Jimei*; Cheng, Xin; Li, Zilong; Sun, Linhao; Zeng, Zhen; Jiang, Hong*

Chin. J. Org. Chem. **2018**, 38(10), 2775

A novel and highly sensitive fluorescence method for β -glucosidase activity determination employing enzyme-triggered click chemistry was developed.

Copper-Catalyzed Aerobic Oxidation Reaction of Benzyl Alcohol in Water under Base-Free Condition

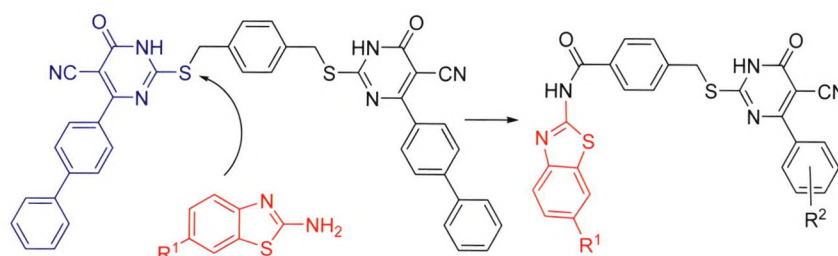


Yang, Xiaojiang; Mao, Jincheng*; Zhang, Heng; Zhang, Yang; Mao, Jinhua

Chin. J. Org. Chem. **2018**, 38(10), 2780

A green and very mild method for the oxidation of benzyl alcohols to aromatic aldehydes with excellent conversions has been developed. The reaction could be carried out directly in air at room temperature and was catalyzed by bis(8-quinolinolato)-copper(II) with 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) as co-catalysts.

Synthesis and Antibacterial Activity Evaluation of the Thiouracil Derivatives Containing Benzothiazole



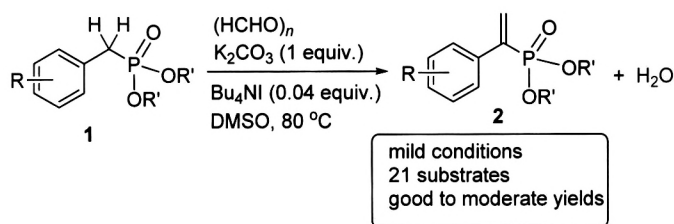
Cui, Penglei; Liu, Na; Chen, Hua*; Li, Xiaoliu*

Chin. J. Org. Chem. **2018**, 38(10), 2784

A series of thiouracil compounds containing benzothiazole were synthesized by modifying the structure of thiouracil compounds with novel antibacterial mechanism.

CONTENT

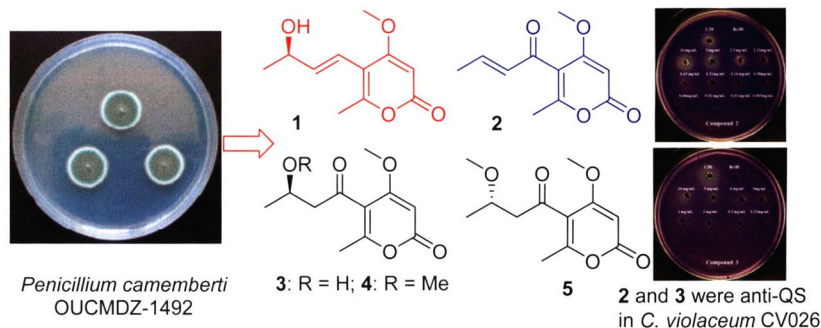
An Efficient Synthesis of 1-Arylvinylphosphonates via Direct Functionalization of C(sp³)—H Bond



Ren, Linjing; Ran, Maogang; Fang, Xuehong; Zhao, Ling; Yao, Qiuli*
Chin. J. Org. Chem. **2018**, 38(10), 2791

An efficient protocol for the preparation of vinyl phosphonates from benzylic phosphonates and paraformaldehyde is achieved under mild conditions in air by direct functionalization of the C(sp³)—H bond adjacent to the phosphonate group. Moderate to high yields can be obtained for a broad scope of substrates.

α -Pyronoids with Quorum Sensing Inhibitory Activity from the Mangrove Fungus *Penicillium camemberti* OUCMDZ-1492



Fan, Yaqin; Zhu, Guoliang; Wang, Yi; Zhu, Xiaocui; Gong, Qianhong; Jia, Qian; Fu, Peng; Zhu, Weiming*
Chin. J. Org. Chem. **2018**, 38(10), 2798

Pyrenocine P (1), a new α -pyronoid, along with four known analogues was isolated from an oligotrophic cultures of the mangrove fungus *Penicillium camemberti* OUCMDZ-1492. Their structures were identified as (*R,E*)-5-(3-hydroxybut-1-en-1-yl)-4-methoxy-6-methyl-2*H*-pyran-2-one (1), pyrenocine A (2), (*R*)-pyrenocine B (3), (*R*)- (–)-pyrenocine E (4) and (*S*)-(+)-pyrenocine E (5), respectively. Compounds 2 and 3 showed potent quorum sensing inhibitory activity in *Chromobacterium violaceum* CV026. In addition, the absolute configurations of compounds 3~5 were determined for the first time.

HIGHLIGHTS

Chin. J. Org. Chem. **2018**, 38(10), 2805

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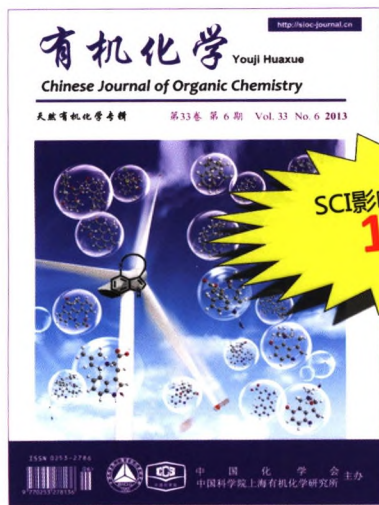
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