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中国科学院上海有机化学研究所 主办

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Chinese Journal of Organic Chemistry

(YOUJI HUAXUE)

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目 次

* 通讯联系人.

研究简报

亮点述评

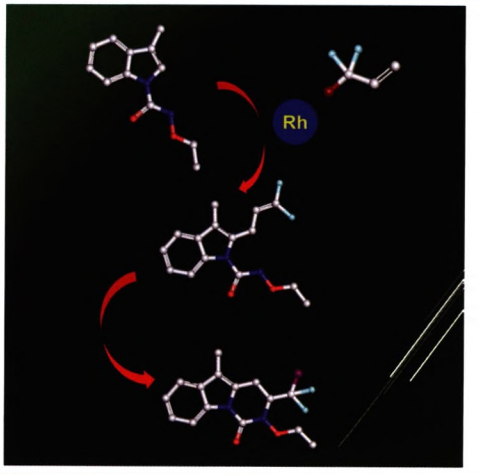
Chinese Journal of Organic Chemistry

Vol. 40 No. 6 June 2020

Cover Picture: Electrocatalytic Synthesis of 2,5-Disubstituted 1,3,4-Oxadiazoles

The electrocatalytic synthesis of non-symmetric 2,5-disubstituted 1,3,4-oxadiazole derivatives via the reaction of aldehydes and hydrazides is reported by Li, Wang, Hao, and Jiang on page 1540. By means of sus-tainable characteristics of electrocatalysis, the reaction could be triggered by *in-situ*-generated *N*-centered radical species under mild conditions, enabling [3+2] annulation to construct 1,3,4-oxadiazole scaffolds without additional oxidants.

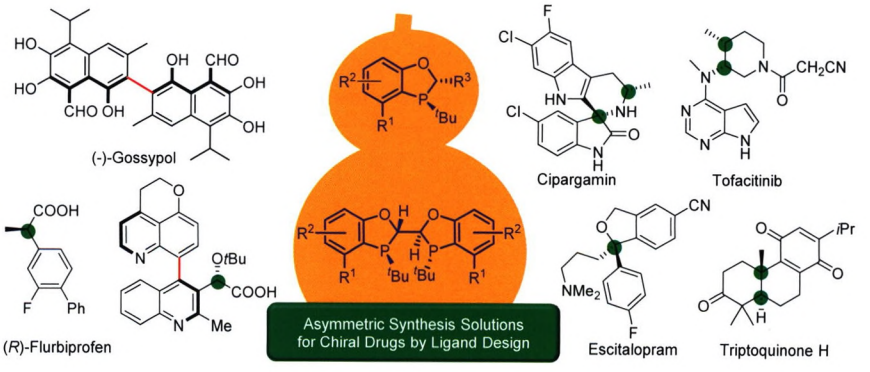
Inside Cover: Cp*Rh(III)-Catalyzed C—H 3,3-Difluoroallylation of Indoles and *N*-Iodosuccinimide-Mediated Cyclization for the Synthesis of Fluorinated 3,4-Dihydropyrimido-[1,6-*a*]-indol-1(2*H*)-one Derivatives



The synthesis of fluorinated 3,4-dihydropyrimido-[1,6-*a*]- indol-1(2*H*)-ones through Cp*Rh(III)-catalyzed C—H 3,3-difluoroallylation and NIS-mediated cyclization is reported by Zhao, Li, Xu and Liu on page 1549. This strategy featured broad synthetic generality, unique versatility and high efficiency, which provided a potential tool for the construction of fluorine-containing heterocycles for drug discovery.

ACCOUNT

Efficient Synthesis of Chiral Drugs Facilated by *P*-Chiral Phosphorus Ligands



The design and development of a series of *P*-chiral mono- and bis-phosphorus ligands based on a benzooxaphosphane backbone and their applications in the synthesis of chiral drugs are summarized.

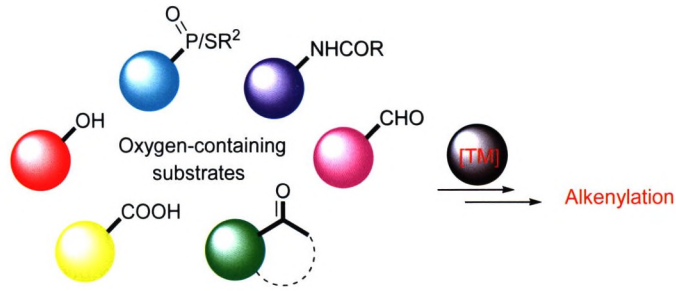
Xu, Ronghua; Yang, He*; Tang, Wenjun*

Chin. J. Org. Chem. **2020**, *40*(6), 1409

CONTENT

REVIEWS

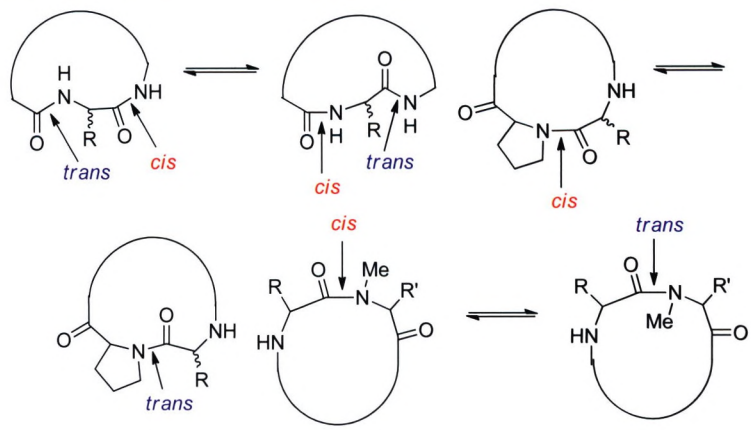
Recent Advances in Transition Metal-O Weak Coordinated C(sp^2)—H Direct Alkenylation Reaction



The transition metal-catalyzed C(sp^2)—H alkenylation of substrates containing hydroxy, aryl ether, aldehyde, carbonyl, carboxyl, amide, phosphoric acid and sulfonic acid and their derivatives groups is reviewed, and its future development trends are prospected.

Yin, Biao; Fu, Manlin; Zhu, Qing*
Chin. J. Org. Chem. **2020**, *40*(6), 1461

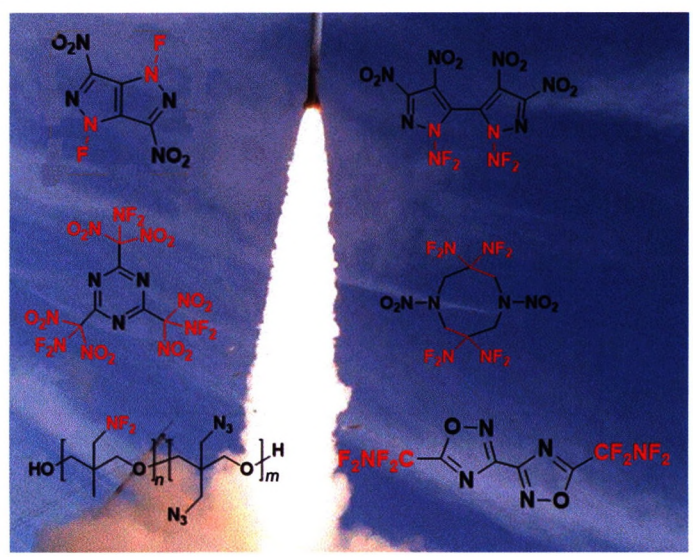
Research Progress on *cis-/trans*-Isomerization of Cyclic Peptide



The characteristics of *cis*- and *trans*-structures in cyclic peptide, such as non-*N*-unsubstituted, proline-containing, and *N*-methylated residues of cyclic peptide are focused. The research progress on *cis*- or *trans*-structure in above cyclic peptides and their analogs is discussed.

Huang, Jing; Yang, Yihua*; Feng, Juan; Li, Junzhang; Liu, Shouxin*
Chin. J. Org. Chem. **2020**, *40*(6), 1473

Progress in Synthesis and Properties of High Energy Density Compounds Regulated by N—F Bond



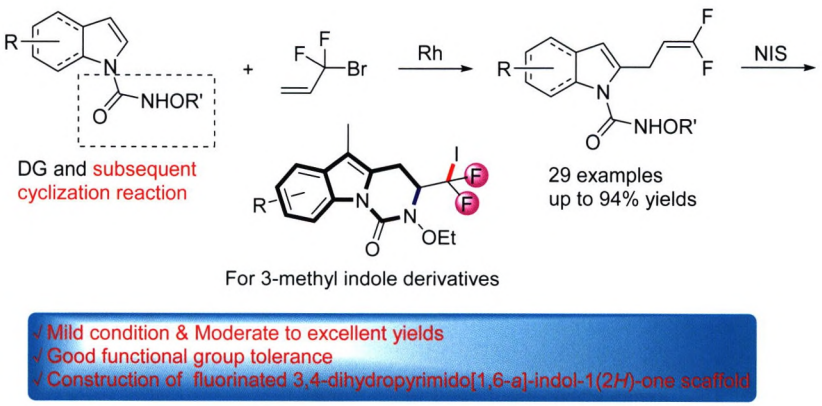
The recent developments of N—F bond and difluoramino (NF_2) energetic derivatives are reviewed. The construction methodologies of N—F bond and difluoroamino groups as well as the synthetic routes to their energetic derivatives are emphatically reviewed. Moreover, the physicochemical and energetic properties of some typical compounds are briefly introduced.

Zhai, Lianjie; Zhang, Junlin; Zhang, Jiarong; Wu, Minjie; Bi, Fuqiang*; Wang, Bozhou*
Chin. J. Org. Chem. **2020**, *40*(6), 1484

CONTENT

ARTICLES

Cp*Rh(III)-Catalyzed C—H 3,3-Difluoroallylation of Indoles and *N*-Iodosuccinimide-Mediated Cyclization for the Synthesis of Fluorinated 3,4-Dihydropyrimido-[1,6-*a*]-indol-1(2*H*)-one Derivatives



Zhao, Sen; Li, Chunpu; Xu, Bin*; Liu, Hong*
Chin. J. Org. Chem. **2020**, *40*(6), 1549

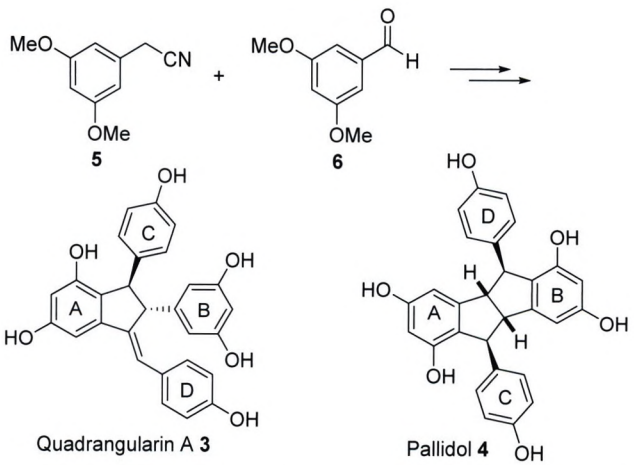
An efficient approach to novel fluorinated 3,4-dihydropyrimido[1,6-*a*]-indol-1(2*H*)-one scaffold has been developed using a Rh-catalyzed C—H 3,3-difluoroallylation of indoles and *N*-iodosuccinimide (NIS)-mediated cyclization strategy.

Mechanism of Synthesis of Phosphinecarboxamides by Reaction of Sodium Phosphaethynolate Anion and Amines under Acid-Free Conditions: Density Functional Theory Investigation

Li, Zhifeng; Wang, Wenpeng; Wang, Xicun; Quan, Zhengjun*
Chin. J. Org. Chem. **2020**, *40*(6), 1563

The reaction of 2-phosphaethynolate anion and primary amines for phosphinecarboxamides synthesis using mechanochemistry has been studied using IR, ^{13}C NMR and ^{31}P NMR spectra, and the reaction occurred under grinding, mild and acid-free conditions at room temperature. In this paper, a comprehensive mechanistic density functional theory (DFT) of B3LYP/6-31G(d,p) study reveals that H shift can be aided/catalyzed with solvents and further the activation free energies barrier can be dramatically decreased, which is responsible for the higher yield of the product in the experiment.

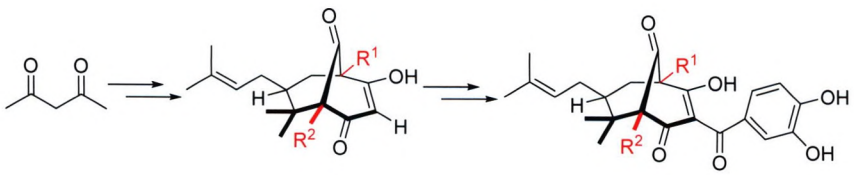
Study on the Total Synthesis of Resveratrol Dimers Quadrangularin A and Pallidol



Han, Jilai; Tang, Meilin; Sun, Xun*
Chin. J. Org. Chem. **2020**, *40*(6), 1571

A effective approach to quadrangularin A (**3**) and pallidol (**4**) has been established from the inexpensive materials of 3,5-dimethoxybenzaldehyde (**5**) and 3,5-dimethoxybenzaldehyde (**6**).

Synthesis and Anti-tumor Activity of Novel Garcinol Analogs

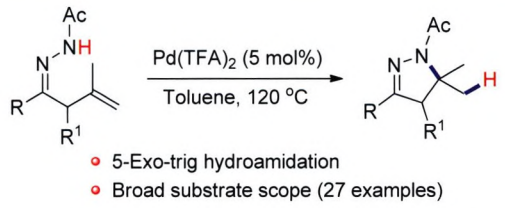


Zhou, Huiyuan; Wu, Yanlin; Huang, Dianhong; Zhang, Mingting; Chen, Huanming; Qian, Mingcheng; Zhao, Shuai; Zhang, Xinyan*; Chen, Xin*
Chin. J. Org. Chem. **2020**, *40*(6), 1578

Three novel garcinol derivatives, in which the bulky side chains at the C8 position and C4 position of garcinol were replaced with smaller allyl group or isoprenyl group, were synthesized through a 9-step procedure starting from acetylacetone. The methyl thiazolyl tetrazolium (MTT) results indicated that the title compounds were moderately lower than that of garcinol on cell proliferation of oral cancer cell lines.

CONTENT

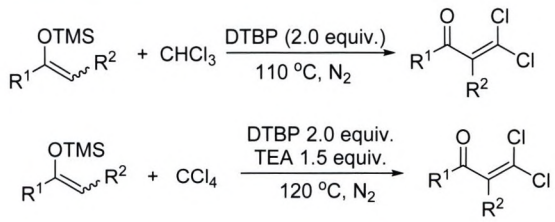
Palladium-Catalyzed *5-exo-trig* Hydroamidation of *β,γ*-Unsaturated Hydrazones for Synthesis of Dihydropyrazoles



Wang, Xucai; Chen, Ming; Zhang, Wei; Zhang, Yaodu; Ren, Zhihui; Guan, Zhenghui*
Chin. J. Org. Chem. **2020**, *40*(6), 1618

A novel and efficient palladium-catalyzed 5-*exo-trig* hydroamidation of *β,γ*-unsaturated hydrazones for the synthesis of dihydropyrazoles was developed. The reaction employs readily available starting materials, tolerates a wide range of functional groups, and produces a series of valuable dihydropyrazoles in good to high yields.

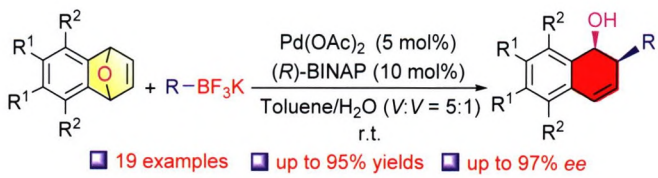
Synthesis of *β,β*-Dichloro-*α,β*-unsaturated Ketones by Trichloromethyl Radical Addition/Elimination of Enol Silyl Ethers



Using di-*tert*-butyl peroxide (DTBP) as oxidant, chloroform or carbon tetrachloride as trichloromethyl radical source and reaction solvent, enol silyl ethers derived from aryl ketone was transferred to *β,β*-dichloro-*α,β*-unsaturated ketone by trichloromethyl radical addition/elimination. The conditions are mild with avoiding the use of metal catalysts, and the substrate of enol silicone ether has good universality.

Ge, Haochen; Du, Keying; Sheng, Weijian*
Chin. J. Org. Chem. **2020**, *40*(6), 1625

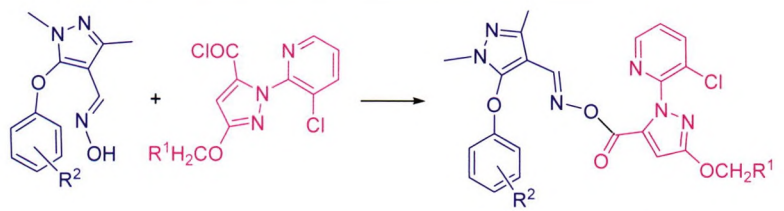
Palladium-Catalyzed Asymmetric Ring-Opening Reactions of Oxabenzonorbornadienes with Potassium Trifluoroborate Salts



Tao, Pingfang; Huang, Jun; Liu, Yuzhao; Wei, Guangming; Wang, Yifei; Wei, Xiansheng; Huang, Guobao*; Li, Xiuying*
Chin. J. Org. Chem. **2020**, *40*(6), 1630

A new, versatile and highly efficient palladium(II)-catalyzed asymmetric ring-opening reaction of oxabenzonorbornadienes with a wide range of potassium trifluoroborate salts was developed.

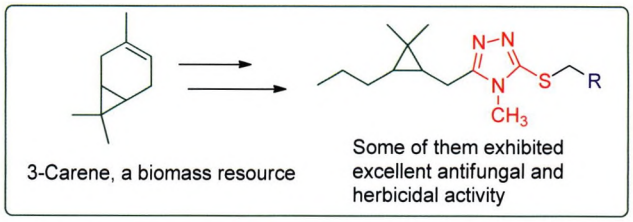
Synthesis and Bioactivities of Novel Pyrazole Oxime Derivatives Containing a *N*-Pyridylpyrazole Moiety



Xun, Xiao; Ni, Yadan; Li, Jinfeng; Ding, Ying; Zhang, Min; Wang, Yang; Hu, Lanping*; Zhou, Huanyu; Yang, Bing*; Shi, Jian; Gao, Lei; Dai, Hong*
Chin. J. Org. Chem. **2020**, *40*(6), 1638

A series of novel pyrazole oxime compounds containing a *N*-pyridylpyrazole moiety were synthesized, and their bioactivities were evaluated.

Synthesis, Biological Activity and Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) Study of Novel 4-Methyl-1,2,4-triazole-thioethers Containing *gem*-Dimethylcyclopropane Ring

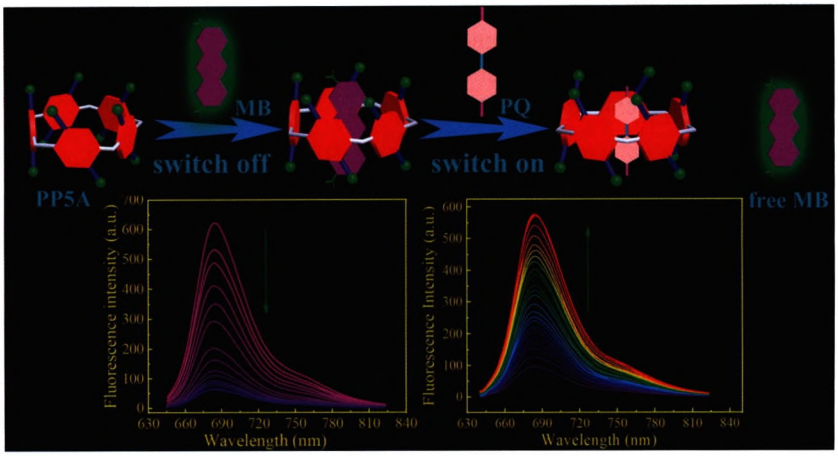


Yu, Youpei; Duan, Wengui*; Lin, Guishan; Kang, Guoqiang; Wang, Xiaoyu; Lei, Fuhou
Chin. J. Org. Chem. **2020**, *40*(5), 1647

Twenty novel 4-methyl-1,2,4-triazole-thioether compounds containing *gem*-dimethyl cyclopropane ring were designed and synthesized. The *in vitro* antifungal and herbicidal activities of the target compounds were preliminarily evaluated.

CONTENT

Competitive Fluorescence Sensing for Paraquat Based on Methylene Blue/Water-Soluble Phosphate Salt Pillar[5]-arene

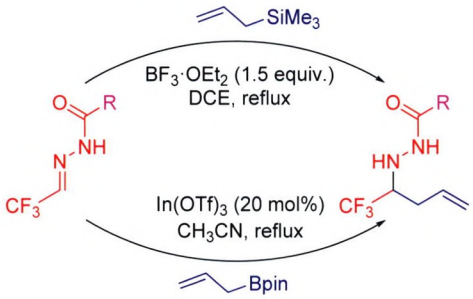


Yang, Yunhan; Bao, Qiulian; Luo, Jianping; Yang, Junli; Li, Canhua; Wei, Keke; Chuan, Yongming; Yang, Lijuan*

Chin. J. Org. Chem. **2020**, *40*(6), 1680

The methylene blue/water-soluble phosphate salt pillar[5]arene (MB/PP5A) inclusion complex was prepared. A competitive fluorescence sensing for detection of paraquat (PQ) based on this inclusion complex was constructed. The inclusion complex probe has the advantages of strong selectivity, simple and fast preparation, wide pH measurement and good anti-interference performance.

Study on Allylation Reactions of Trifluoromethylated Acylhydrazones with Allylsilanes or Allylboronates

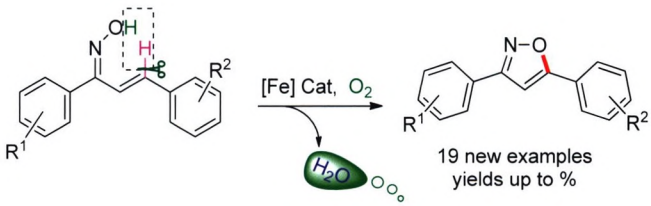


Hu, Yongqin; Huang, Danfeng*; Wang, Kehu; Zhao, Zhuanxia; Zhao, Fangxia; Xu, Weigang; Hu, Yulai*

Chin. J. Org. Chem. **2019**, *39*(6), 1689

Allylation reactions of trifluoromethylated acylhydrazones with allyltrimethylsilane or pinacolyl allylboronate were found to proceed smoothly in the presence of Lewis acid to afford a series of trifluoromethylated homoallylic *N*-acylhydrazines in high yields.

$FeCl_2$-Catalyzed Intramolecular Aerobic Reaction for Construction of Isoxazoles Heterocycle

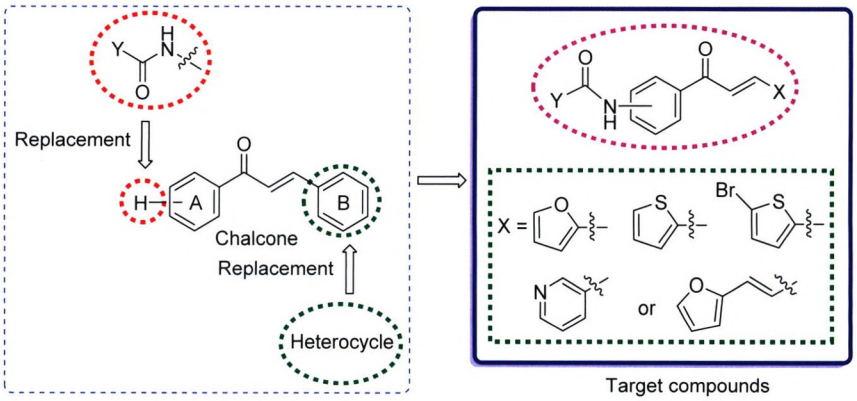


Abdukader, Ablimit*; Wang, Rong; Mamat, Marhaba; Liu, Chenjiang*

Chin. J. Org. Chem. **2020**, *40*(6), 1697

A general produce is developed to synthesize varieties of multi substituted isoxazole derivatives via iron-catalyzed direct aerobic oxidative C—O bond formation.

Synthesis of Chalcone Derivatives and Studies on Their Inhibitory Activity and Molecular Docking



Xiao, Tingting; Cheng, Wei; Qian, Weifeng; Zhang, Tingting; Lu, Tong; Gao, Yang; Tang, Xiaorong*

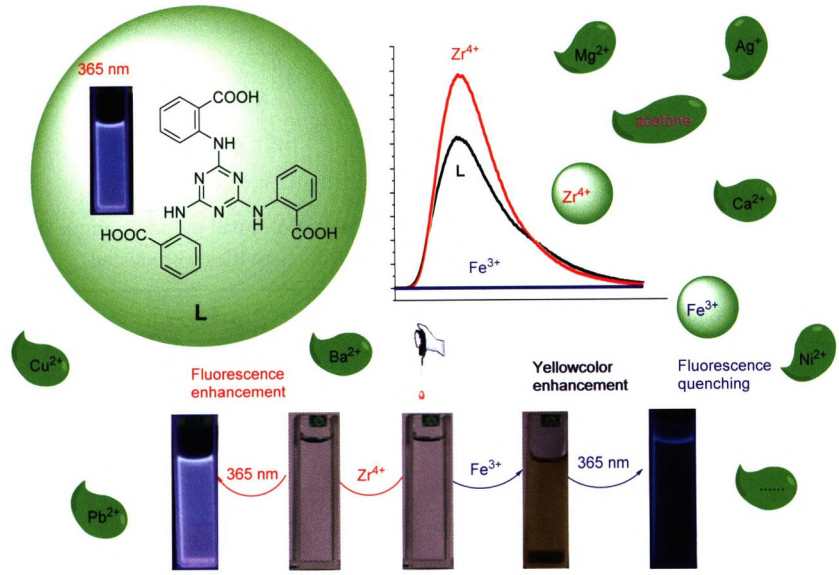
Chin. J. Org. Chem. **2020**, *40*(6), 1704

Twenty nine chalcone derivatives were designed and synthesized. The antifungal activities of all the synthesized compounds were determined against five plant pathogenic fungi namely *Rhizoctonia solani*, *Fusarum graminearum*, *Helminthosporium maydis*, *Sclerotinia sclerotiorum* and *Botrytis cinerea*.

CONTENT

NOTES

Triazine Derivative for Fluorescence Sensing of Zr^{4+}, Fe^{3+} Ions and Acetone

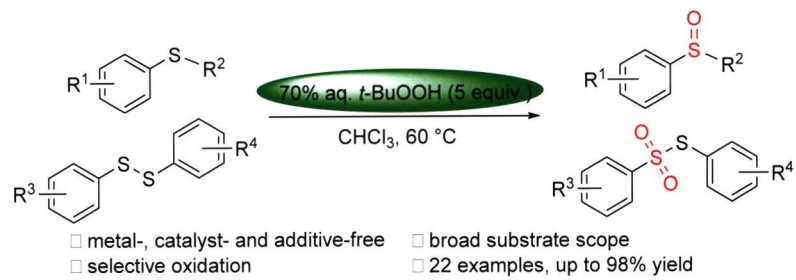


Ma, Xuelin; Han, Limin*; Zhang, Xiaoyong*; Zhang, Yuheng, Wang, Li, Yang, Kun; Ji, Jie

Chin. J. Org. Chem. **2020**, *40*(6), 1745

2,2',2''-(1,3,5-Triazine-2,4,6-triimino)tribenzoic acid (**L**, **H_3TATIB**) fluorescence response chemosensor has been synthesized by one pot reaction and its fluorescent behaviors to transition metal ions were systematically investigated.

Selective Oxidation of Sulfides/Disulfides to Sulfoxides/Thiosulfonates Using *t*-Butyl Hydroperoxide (TBHP) without Catalyst

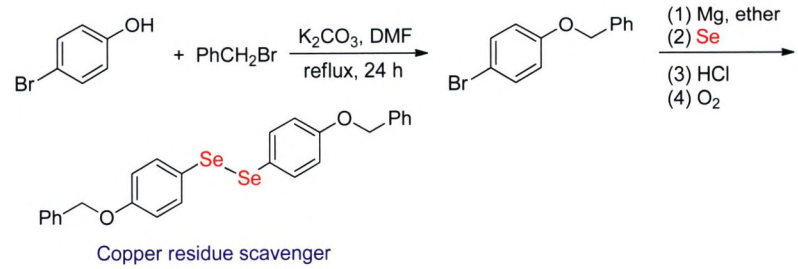


Jiang, Xiaoying; Yao, Chuansheng; Tong, Chuo; Bai Renren; Zhou, Tao; Xie, Yuanyuan*

Chin. J. Org. Chem. **2020**, *40*(6), 1752

A novel and simple method for the selectively oxidation of sulfides to sulfoxides and oxidation of disulfides to thiosulfonates in the presence of a common oxidant *t*-butylhydroperoxide (TBHP) without catalyst and additives.

Design and Synthesis of 1,2-Bis(4-(benzyloxy)phenyl)diselane: A Scavenger for Residual Copper

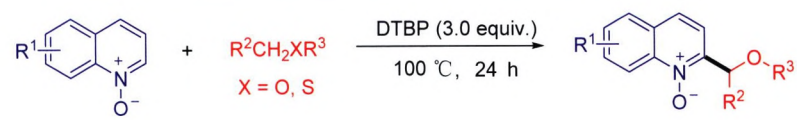


Ge, Yanyu; Kong, Jing; Yang, Chenggen; Yang, Qian; Zhang, Xu*

Chin. J. Org. Chem. **2020**, *40*(6), 1760

The designed and prepared 1,2-bis(4-(benzyloxy)phenyl)diselane showed superior activity in copper pollutant elimination. This work presents a novel method for removing copper residue and may be applied in pharmaceutical industry owing to the safe and metabolizable features of selenium.

Metal-Free C-2 Alkylation of *N*-Oxides with Ethers via Radical Cross-Coupling Reactions



Dong, Daoqing; Li, Guanghui; Chen, Demao; Sun, Yuanyuan; Han, Qingqing; Wang, Zuli*; Xu, Xinming; Yu, Xianyong

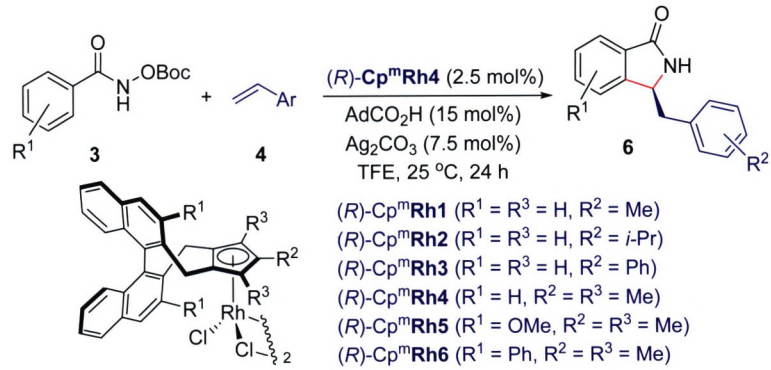
Chin. J. Org. Chem. **2020**, *40*(6), 1766

An efficient method for the C-2 alkylation of quinoline *N*-oxides with ethers via radical cross-coupling reactions has been developed. The desired products with moderate to high yield could be obtained.

CONTENT

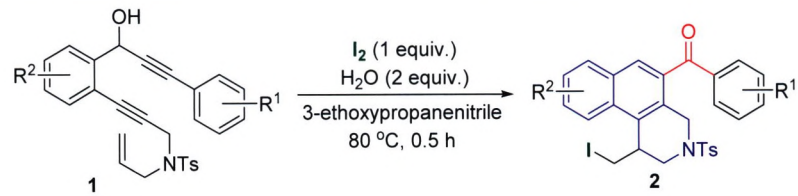
HIGHLIGHTS

Synthesis and Application of Chiral Multisubstituted Cyclopentadienyl Ligands



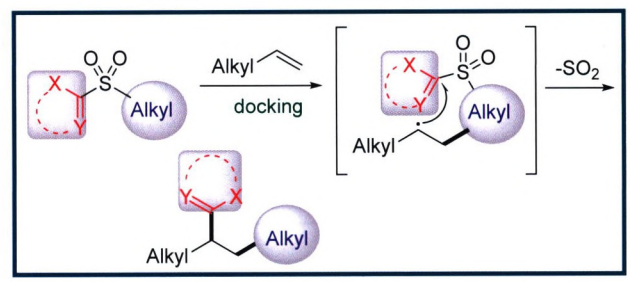
Liang, Hao; Wang, Jun*
Chin. J. Org. Chem. **2020**, *40*(6), 1792

Iodine Promoted Cascade Cycloisomerization of 1-En-6,11-diynes



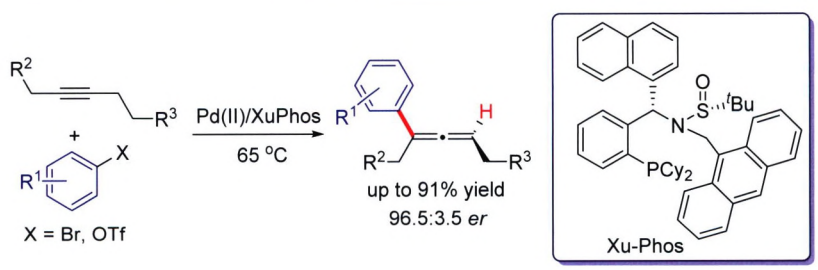
Gao, Pin; Duan, Xinhua*
Chin. J. Org. Chem. **2020**, *40*(6), 1794

Polarity Umpolung Strategy for the Radical Alkylation of Alkenes



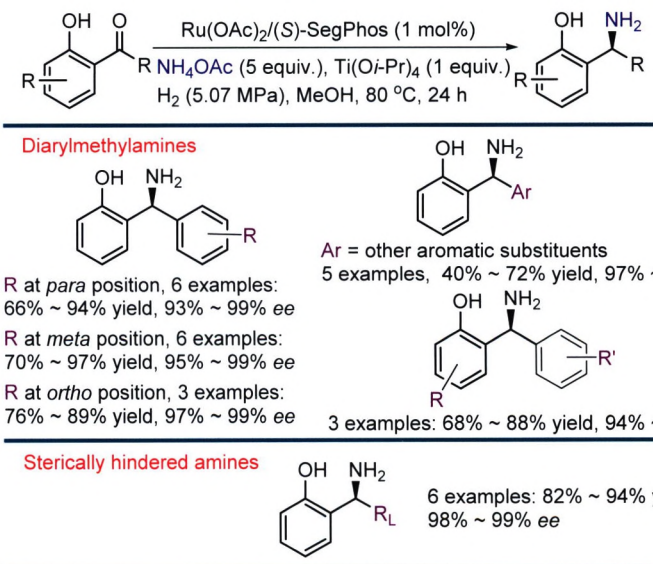
Wei, Rongbiao; Bao, Hongli*
Chin. J. Org. Chem. **2020**, *40*(6), 1797

Synthesis of Enantioenriched Trisubstituted Allenes via Pd-Catalyzed Heck Reaction of Alkynes

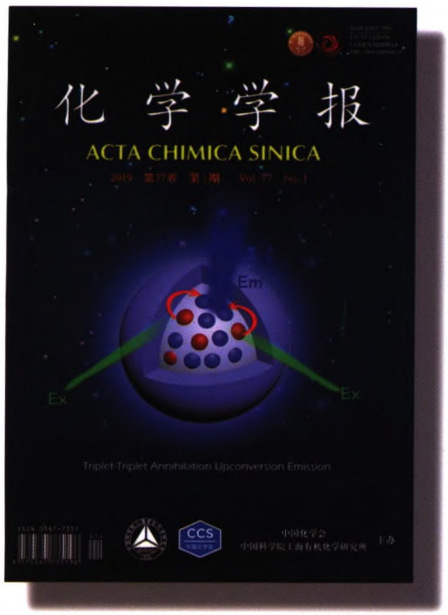


Hou, Xuelong*
Chin. J. Org. Chem. **2020**, *40*(6), 1800

Ruthenium-Catalyzed Direct Asymmetric Reductive Amination for the Synthesis of Chiral Diarylmethylamines and Sterically Hindered Amines



Huang, Haizhou; Chang, Mingxin*
Chin. J. Org. Chem. **2020**, *40*(6), 1802



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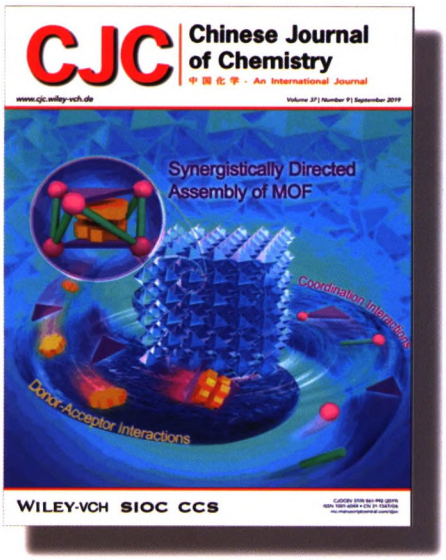

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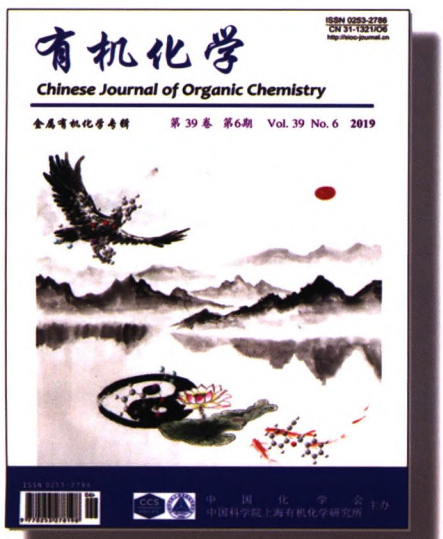

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