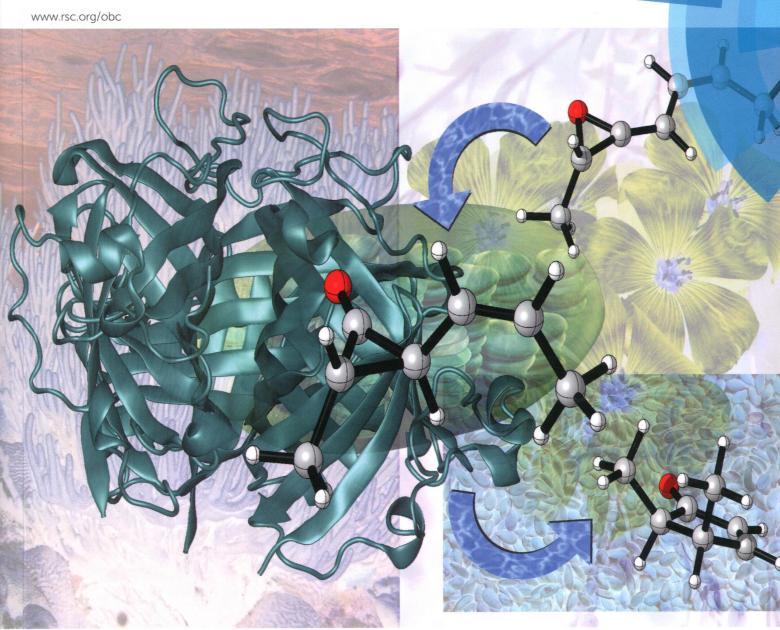
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# Organic & Biomolecular Chemistry



ISSN 1477-0520



#### **PAPER**

Ángel R. de Lera *et al.*A unifying mechanism for the rearrangement of vinyl allene oxide geometric isomers to cyclopentenones

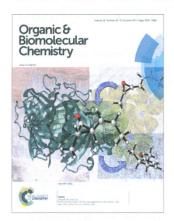
### Organic & Biomolecular Chemistry

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#### IN THIS ISSUE

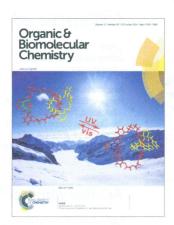
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#### Cover

See Ángel R. de Lera *et al.*, pp. 7694–7701.

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#### Inside cover

See Sheng Hua Liu, Jun Yin *et al.*, pp. 7702–7711.

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#### **PERSPECTIVE**

#### 7655

### 1,3-Halogen migration as an entry to aryl coppers from an unintuitive starting material

R. J. Van Hoveln, S. C. Schmid and J. M. Schomaker\*

Cu-catalyzed 1,3-halogen migration provides a unique way to generate reactive aryl copper species for arene functionalizations.

#### REVIEW

#### 7659

Evolution of a strategy for preparing bioactive small molecules by sequential multicomponent assembly processes, cyclizations, and diversification

James J. Sahn, Brett A. Granger and Stephen F. Martin\*

Multicomponent assembly processes are key steps in the synthesis of diverse polycyclic heterocycles with a broad array of biological activities.

Федеральное государственное бюджетное учреждение науки Центральная научная библиотека Уральского отделения Российской академии наук (ЦНБ УрО РАН)

### The first synthesis of the antiangiogenic homoisoflavanone, cremastranone

Bit Lee, Halesha D. Basavarajappa, Rania S. Sulaiman, Xiang Fei, Seung-Yong Seo\* and Timothy W. Corson\*

The homoisoflavanone cremastranone is synthesized for the first time and shown to block human retinal endothelial cell angiogenesis *in vitro*.

#### 7678

## Iron-catalyzed direct difunctionalization of alkenes with dioxygen and sulfinic acids: a highly efficient and green approach to $\beta$ -ketosulfones

Wei Wei, Jiangwei Wen, Daoshan Yang, Min Wu, Jinmao You and Hua Wang\*

A novel and efficient iron-catalyzed direct difunctionalization of alkenes with sulfinic acids and dioxygen for the synthesis of  $\beta$ -ketosulfones has been developed.

#### 7682

### Total synthesis and biological evaluation of atrop-O-benzyl-desmethylabyssomicin C

R. Matovic,\* F. Bihelovic, M. Gruden-Pavlovic and R. N. Saicic\*

The desmethyl analogue of abyssomicin C was synthesized. The synthetic analogue retained its antibacterial activity, whereas its cytotoxicity decreased for three orders of magnitude, as compared to the natural product.

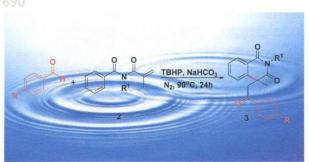
#### 7686

### Catalytic amide allylation of $\alpha$ -ketoesters: extremely high enantioselective synthesis of ester functionalised $\alpha$ -methylene- $\gamma$ -butyrolactones

Masaki Takahashi, Yusuke Murata, Masahiro Ishida, Fumitoshi Yagishita, Masami Sakamoto, Tetsuya Sengoku and Hidemi Yoda\*

A significant breakthrough on the novel amide allylation on the acyclic  $\alpha$ -ketoester systems, achieving extremely high enantioselective synthesis of ester functionalised  $\alpha$ -methylene- $\gamma$ -butyrolactones, is reported.

#### COMMUNICATIONS

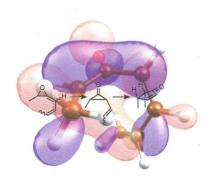


#### Synthesis of isoquinoline-1,3(2H,4H)-dione derivatives via cascade reactions of N-alkyl-N-methacryloyl benzamide with aryl aldehydes

Wannian Zhao, Ping Xie, Min Zhang, Ben Niu, Zhaogang Bian, Charles Pittman Jr. and Aihua Zhou\*

A cascade reaction between N-alkyl-N-methacryloylbenzamide and aryl aldehydes was developed to generate isoquinoline-1,3(2H,4H)-dione derivatives.

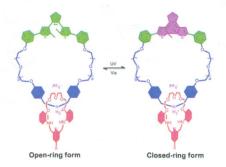
#### **PAPERS**



#### A unifying mechanism for the rearrangement of vinyl allene oxide geometric isomers to cyclopentenones

Adán B. González-Pérez, Alexander Grechkin and Ángel R. de Lera\*

Z-Vinyl allene oxides are predicted to rearrange with high fidelity to stereodefined cyclopentenones through intermediate cyclopropanones.



#### Photo-responsive [2] catenanes: synthesis and properties

Ziyong Li, Fang Hu, Guoxing Liu, Wen Xue, Xiaoqiang Chen, Sheng Hua Liu\* and Jun Yin\*

A series of novel dithienylethene-based macrocycles containing ammonium moieties has been synthesized.



#### Dithienylethene-based rotaxanes: synthesis, characterization and properties

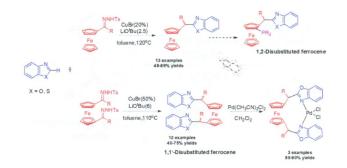
Fang Hu, Juanyun Huang, Meijiao Cao, Zhao Chen, Ying-Wei Yang, Sheng Hua Liu\* and Jun Yin\*

The photochromic materials have been widely applied in many fields.

# Copper-catalyzed direct alkylation of 1,3-azoles with *N*-tosylhydrazones bearing a ferrocenyl group: a novel method for the synthesis of ferrocenyl-based ligands

Qiang Teng, Jianfeng Hu, Li Ling, Ranfeng Sun, Junyang Dong, Shufeng Chen and Hao Zhang\*

A new type of 1,1'-disubstituted ferrocenyl (N,N) bidentate ligand was synthesised *via* CuBr-catalyzed coupling of 1,3-azoles with ferrocenyl ketone-derived N-tosylhydrazones.



#### 7728

# Linear synthesis of the branched pentasaccharide repeats of O-antigens from *Shigella flexneri* 1a and 1b demonstrating the major steric hindrance associated with type-specific glucosylation

Jason M. Hargreaves, Yann Le Guen, Catherine Guerreiro, Karine Descroix and Laurence A. Mulard\*

Shigella flexneri serotypes 1b and 1a are Gram-negative enteroinvasive bacteria causing shigellosis in humans.

#### 7750

### Synthesis of a chiral building block for highly functionalized polycyclic ethers

G. Pazos, M. Pérez,\* Z. Gándara, G. Gómez and Y. Fall\*

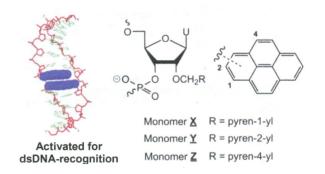
An efficient procedure for preparing enantiopure polycyclic ethers based on the furan singlet oxygen oxidation approach is reported.

#### 7758

# Recognition of double-stranded DNA using energetically activated duplexes with interstrand zippers of 1-, 2- or 4-pyrenyl-functionalized O2'-alkylated RNA monomers

Saswata Karmakar, Andreas S. Madsen, Dale C. Guenther, Bradley C. Gibbons and Patrick J. Hrdlicka\*

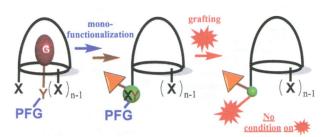
Energetically activated double-stranded probes with interstrand arrangements of intercalator-functionalized nucleotides enable recognition of mixed-sequence DNA with single nucleotide fidelity.



#### An economical and environmentally friendly oxidative biaryl coupling promoted by activated MnO<sub>2</sub>

Jingjing Yang, Shutao Sun, Ziyu Zeng, Hongbo Zheng, Wei Li, Hongxiang Lou and Lei Liu\*

A mild, economical, and environmentally friendly oxidative biaryl coupling by MnO<sub>2</sub> was developed to deliver five- to eight-membered tricyclic products.



#### A versatile strategy for appending a single functional group to a multifunctional host through host-guest covalent-capture

Jean-Noël Rebilly,\* Assia Hessani, Benoit Colasson and Olivia Reinaud

A novel two-step strategy allowed us to selectively monofunctionalize a molecular host (calix[6]arene) with various groups of interest (redox tag, fluorophore, chelating ligand).

#### Exploring functional cyclophellitol analogues as human retaining beta-glucosidase inhibitors

Kah-Yee Li, Jianbing Jiang, Martin D. Witte, Wouter W. Kallemeijn, Wilma E. Donker-Koopman, Rolf G. Boot, Johannes M. F. G. Aerts, Jeroen D. C. Codée, Gijsbert A. van der Marel and Herman S. Overkleeft\*

Of six cyclophellitol analogues, the N-pentylaziridine is the most effective retaining human beta-glucosidase inhibitor considering potency and compound stability.

#### Palladium-catalyzed one pot 2-arylquinazoline formation via hydrogen-transfer strategy

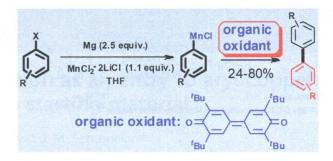
Huamin Wang, Hui Chen, Ya Chen and Guo-Jun Deng\*

2-Arylquinazolines were prepared from nitroarenes and benzyl alcohols or benzyl amines via a hydrogen transfer strategy.

The transition-metal-catalyst-free oxidative homocoupling of organomanganese reagents prepared by the insertion of magnesium into organic halides in the presence of MnCl<sub>2</sub>·2LiCl

Zhihua Peng,\* Na Li, Xinyang Sun, Fang Wang, Lanjian Xu, Cuiyu Jiang, Linhua Song and Zi-Feng Yan

An oxidative homocoupling of organomanganese reagents was performed in one pot without an additional transition-metal catalyst.



#### 7810

Palladium-catalyzed carbonylation of halo arene-cis-dihydrodiols to the corresponding carboxylates. Access to compounds unavailable by toluene dioxygenase-mediated dihydroxylation of the corresponding benzoate esters

Jordan Froese, Jason Reed Hudlicky and Tomas Hudlicky\*

Compounds of high synthetic value were produced in a much more efficient manner than was previously possible through fermentation.

Pd(OAc)<sub>2</sub>, Et<sub>3</sub>N, PPh<sub>3</sub>, ROH
OR<sup>1</sup> CO (1 atm)
OR<sup>1</sup> (6-76%)

$$X = I, Br$$
 $R^1 = H, C(CH_3)_2$ 
 $CO_2R$ 

OR<sup>1</sup>
OR<sup>1</sup>
 $CO_2R$ 

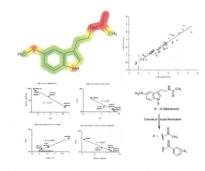
OR<sup>1</sup>
 $CO_2R$ 
 $CO_2R$ 

#### 7820

### Theoretical insight into the antioxidant properties of melatonin and derivatives

Jeffrey R. Johns\* and James A. Platts

Density functional theory calculations on melatonin, metabolites and synthetic derivatives thereof, and a range of other biological antioxidant molecules are presented, with a view to understanding the antioxidant ability of these molecules.

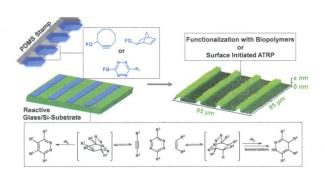


#### 7828

# Surface patterning with natural and synthetic polymers *via* an inverse electron demand Diels—Alder reaction employing microcontact chemistry

Oliver Roling, Artur Mardyukov, Sebastian Lamping, Benjamin Vonhören, Stefan Rinnen, Heinrich F. Arlinghaus, Armido Studer and Bart Jan Ravoo\*

Bioorthogonal ligation methods are the focus of current research due to their versatile applications in biotechnology and materials science for post-functionalization and immobilization of biomolecules.



$$R = \text{aryl, alkyl}$$

$$In \textit{situ C-C bond cleavage and Mannich addition reaction}$$

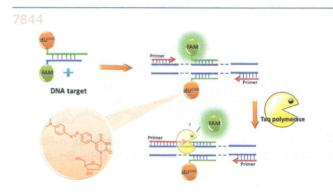
$$R = \frac{\text{CF}_3}{\text{CF}_3} + F_3 \text{C}$$

$$R = \frac{\text{CF}_3}{\text{CF}_3} + \frac{\text{CF}$$

# Generalized access to fluorinated $\beta$ -keto amino compounds through asymmetric additions of $\alpha,\alpha$ -difluoroenolates to CF<sub>3</sub>-sulfinylimine

Chen Xie, Lingmin Wu, Haibo Mei, Vadim A. Soloshonok, Jianlin Han\* and Yi Pan

Asymmetric reactions between CF<sub>3</sub>-containing N-imines and  $\alpha$ , $\alpha$ -difluoroenolates giving  $\beta$ -keto-amino compounds featuring the R-CO-CF<sub>2</sub>-CH(NH<sub>2</sub>)-CF<sub>3</sub> moiety with high yields and diastereoselectivities were developed.

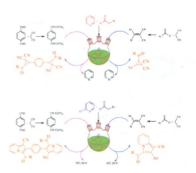


### Synthesis and evaluation of a photoresponsive quencher for fluorescent hybridization probes

Marina Kovaliov, Chaim Wachtel, Eylon Yavin and Bilha Fischer\*

dU<sup>DAB</sup> modified probes are promising probes for gene quantification in real-time PCR detection and as photoswitchable devices.

7859



# Ultrasound-assisted 1,3-dipolar cycloaddition and cyclopropanation reactions for the synthesis of bis-indolizine and bis-cyclopropane derivatives

Mehdi Abaszadeh\* and Mohammad Seifi

We report a new method for the synthesis of bis-indolizine and bis-cyclopropane derivatives under ultrasound irradiation, using a 1,3-dipolar cycloaddition reaction or a cyclopropanation reaction, respectively.