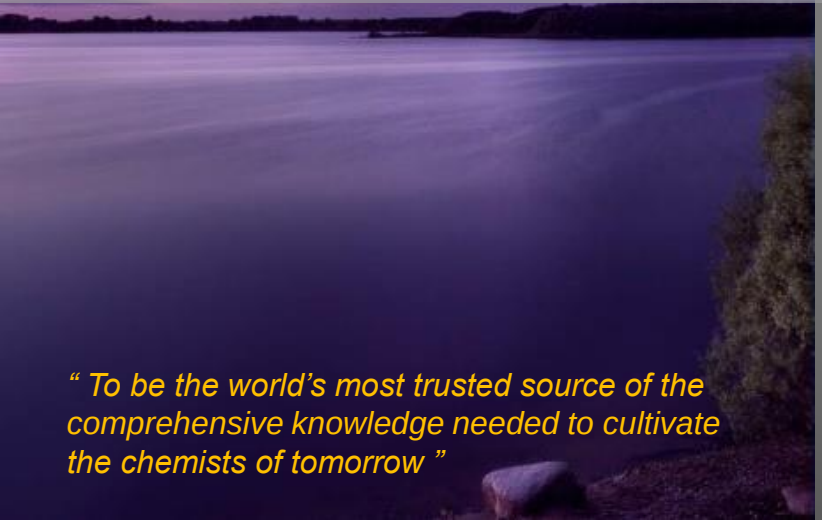
ACS期刊论文投稿与写作



“ To be the world’s most trusted source of the comprehensive knowledge needed to cultivate the chemists of tomorrow ”

1 ACS期刊和平台

2 ACS投稿与写作

3 学术道德和同行评议

主讲人：赵璟

iGroup
中国长煦信息技术咨询（上海）有限公司
iGroup Asia Pacific Ltd.

1　ACS期刊和平台

ACS美国化学会是全球最大的科技学会

- 成立于1876年，至今拥有超过16万名会员
- 众多诺贝尔奖得主和顶尖的研究者
- 为高校和企业提供高品质的科技文献
- 促进化学及相关学科的交流与发展，推动行业进步

ACS期刊简介

- **58种** 高品质的学术期刊
  - 均为 SCI 收录
  - 半数的期刊影响因子IF超过5
  - 在12个化学核心和相关学科具有最高的引用量或影响因子
- 化学领域最高的引用量
  2018年被引用次数超过 340 万
- 被 Journal Citation Report (JCR) 评为
  “化学领域被引用次数最多的期刊”

覆盖广泛的学科领域

普通化学
晶体学
无机化学
有机化学
物理化学
分析化学

高分子科学
材料科学
纳米科学
化学工程
能源与燃料
环境科学

食品科学与技术
农学与林学
理论化学
计算化学
化学信息学
分子生物学

生物化学
生物技术
临床化学
药物化学
药理学和药剂学
毒理学

1870

1875

1879

1880

1885

1905

JOURNAL

OF THE

AMERICAN CHEMICAL SOCIETY.

VOLUME I.

PUBLICATION COMMITTEE:

H. ENDEMANN, Editor,
ARNO BEHR,
GIDEON E. MOORE.

ABSTRACTORS:

EDGAR EVERHART,

STEBBINS, JR.,

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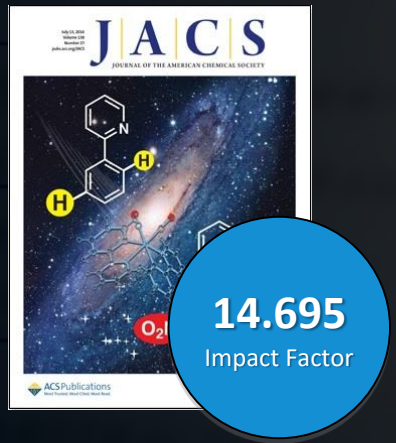


JACS

获得其有史以来最高的影响因子14.695
它是化学领域中获得引用最多的期刊
2018年的被引用次数超过55万
更新频率: Published weekly

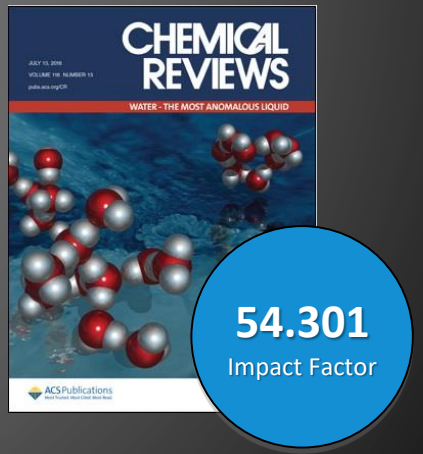
两本综述型期刊

Accounts of Chemical Research

（影响因子21.661）主要对近期的研究进展进行简要总结，对化学及相关领域的基础和应用研究进行简单易懂的概述。

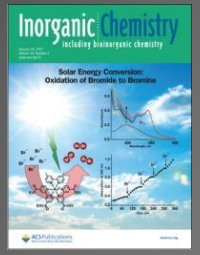
Chemical Reviews

（影响因子54.301）主要发表关于开创性研究的权威综述，这些综述在化学领域中被公认是最全面的。

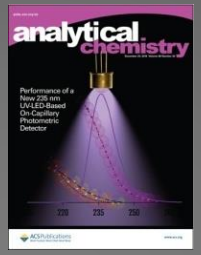


基础化学领域：无机、有机、物化、分析

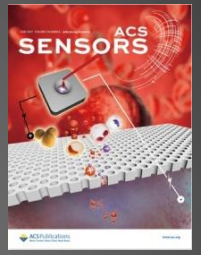
Crystal Growth & Design
IF = 4.153



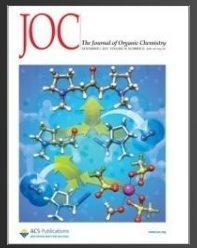
Inorganic Chemistry
IF = 4.850



Analytical Chemistry
IF = 6.350

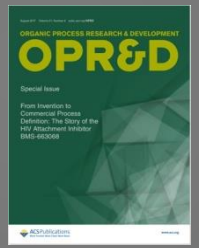


ACS Sensors
IF = 6.944

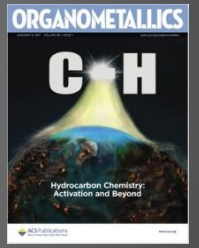


The Journal of Organic Chemistry
IF = 4.745

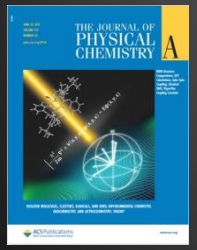
Organic Letters
IF = 6.555



Organic Process Research & Development
IF = 3.327

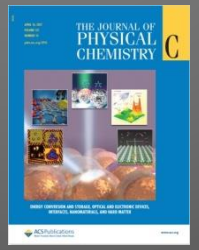


Organometallics
IF = 4.100

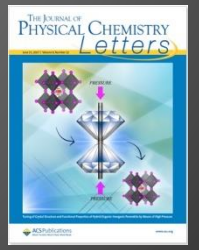


The Journal of Physical Chemistry A
IF = 2.641

The Journal of Physical Chemistry B
IF = 2.923

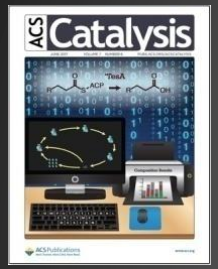


The Journal of Physical Chemistry C
IF = 4.309



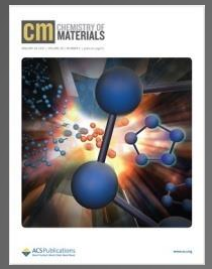
The Journal of Physical Chemistry Letters
IF = 7.329

催化



ACS Catalysis
IF = 12.221

材料

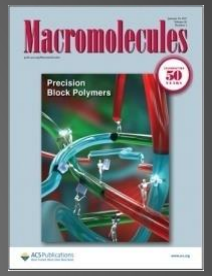


Chemistry of Materials
IF = 10.159

纳米科学

ACS NANO
IF = 13.903

高分子

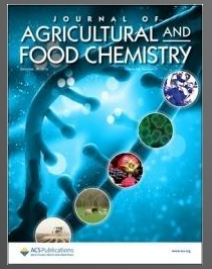


Macromolecules
IF = 5.997

药物化学

Journal of Medicinal Chemistry
IF = 6.054

农业与食品化学



Journal of Agricultural and Food Chemistry
IF = 3.571

化学工程

Industrial & Engineering Chemistry Research
IF = 3.375

环境科学与技术

Environmental Science & Technology
IF = 7.149

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J. Am. Chem. Soc. 2019, 141, 3171
Guo, Zhang, Zh

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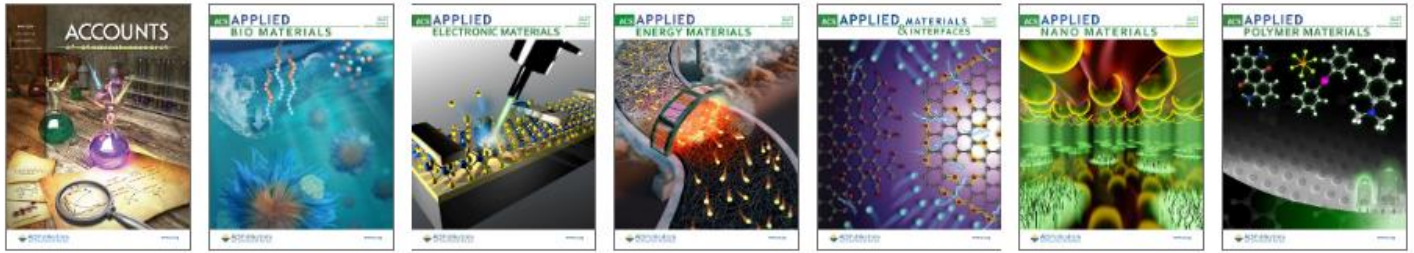

Molecular Optimization Enables over 13% Efficiency in Organic Solar Cells

Wenchao Zhao[†‡], Sunsun Li[†‡], Huifeng Yao[*†‡], Shaoqing Zhang[†‡], Yun Zhang[†‡], Bei Yang[†‡] and Jianhui Hou[*†‡]

Hide Author Information

† Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Polymer Physics and Chemistry, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

‡ University of Chinese Academy of Sciences, Beijing 100049, China

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标题和作者

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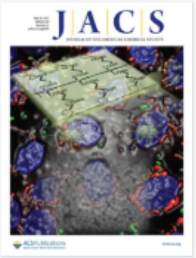

Journal of the American Chemical Society

Cite This: J. Am. Chem. Soc. 2017, 139, 21, 7148-7151

Publication Date: May 17, 2017

https://doi.org/10.102

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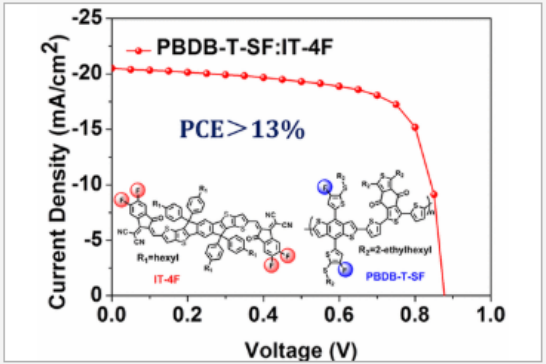
Supporting Information

Abstract

A new polymer d… mole… free organic solar cells (OSCs) were designed and synthesized. The influences of fluorination on the absorption spectra, molecular energy levels, and charge mobilities of the donor and acceptor were systematically studied. The PBDB-T-SF:IT-4F-based OSC device showed a record high efficiency of 13.1%, and an efficiency of over 12% can be obtained with a thickness of 100–200 nm, suggesting the promise of fullerene-free OSCs in practical applications.

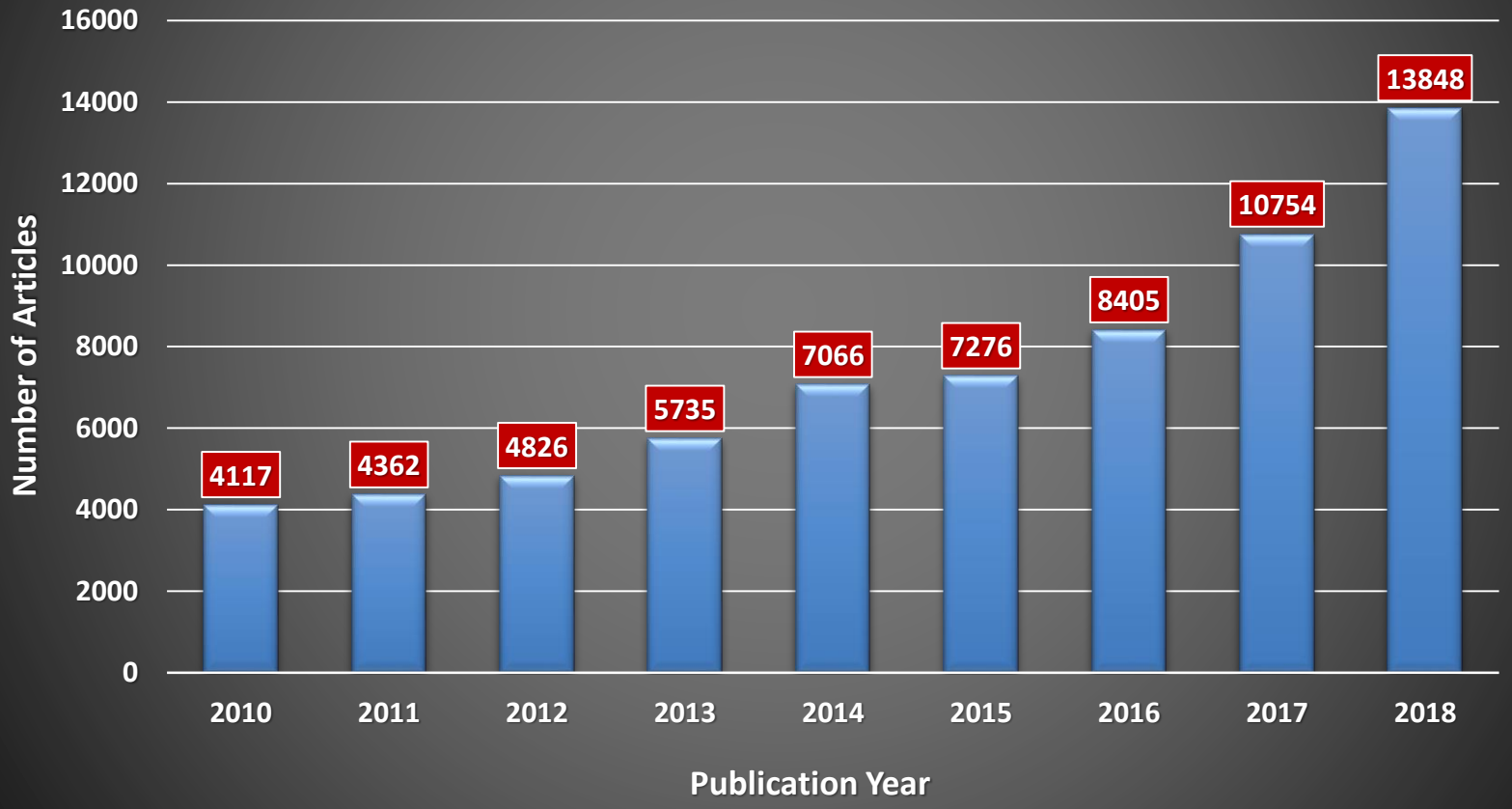
Abstract 摘要



2 ACS期刊投稿

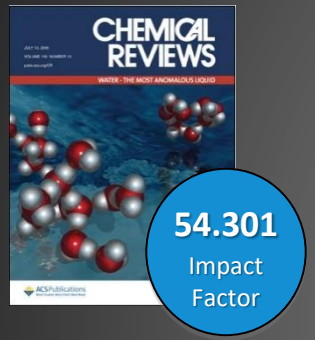
SCI科技论文写作

中国作者在 ACS 期刊的发文数量（2010 - 2018）



高影响因子的ACS期刊

发表所有化学相关的学科领域的著作，要求是其研究工作达到最高水准和新颖性



54.301 Impact Factor

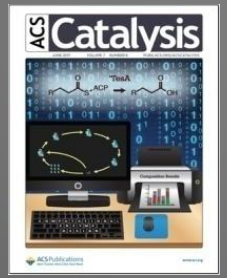
21.661 Impact Factor

14.695 Impact Factor

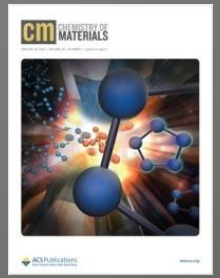
12.837 Impact Factor

ACS NANO
IF = 13.903

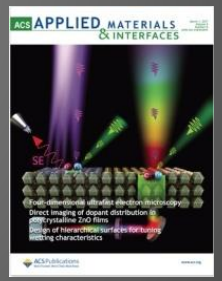
NANO Letters
IF = 12.279



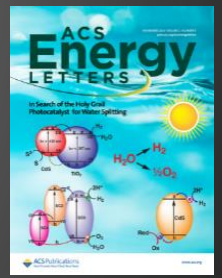
ACS Catalysis
IF = 12.221



Chemistry of Materials
IF = 10.159



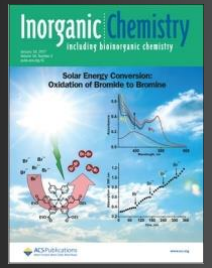
ACS Applied Materials & Interfaces
IF = 8.456



ACS Energy Letters
IF = 16.331

多学科的“合理科学”期刊

要求该研究在科学上是有效的，但不要求对重要性或新颖性进行主观评价。大多数的期刊都有一个更窄的主题范围并强调重要性，投稿时能了解该稿件是否适合该期刊



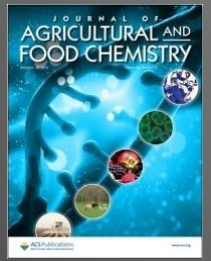
Inorganic Chemistry
IF = 4.850

The Journal of Organic Chemistry
IF = 4.745

Organic Letters
IF = 6.555

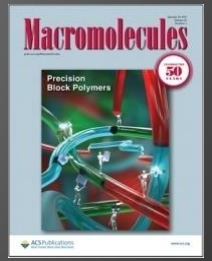
Analytical Chemistry
IF = 6.350

Journal of Medicinal Chemistry
IF = 6.054



Journal of Agricultural and Food Chemistry
IF = 3.571

Environmental Science & Technology
IF = 7.149



Macromolecules
IF = 5.997

ACS期刊投稿流程

第一步：选择　你想投稿的期刊

期刊投稿指南　**Author Guidelines**
期刊范围　　**Journal Scope**

第二步：了解　学术道德 / 出版政策

学术道德指南　Ethical Guidelines
期刊出版协议　Copyright and Permissions
资金提供来源　Funder Reporting Requirement

第三步：写作　准备你的稿件

投稿模板　　Document Templates
格式和语言　Writing Style and Language
文章架构　　Manuscript Components
投稿信　　Cover Letter
图表　　Graphics

第四步：提交　使用在线投稿平台

注册和登录 ACS Paragon Plus 投稿平台
在投稿平台内完成稿件上传
同行评议　Peer Review

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ASAP Publication
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出版信息确认
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Journal Guidelines And Templates

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Guidelines for Authors

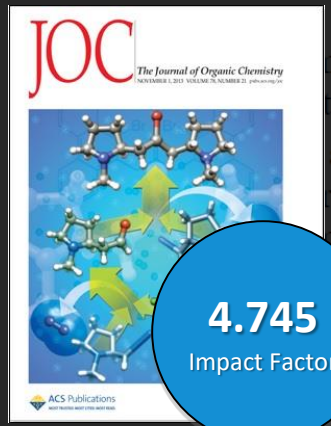
Updated January 2018

1 Scope and Editorial Policy

1.1 Scope of the Journal

The Journal of Organic Chemistry (JOC) welcomes original contributions of fundamental research in all theory and practice of organic chemistry. In selecting manuscripts for publication, the emphasis on the quality and ... as well as the breadth of interest to the ... community.

... and other ... synthesis manuscripts are expected to demonstrate substantive ... transformation methods, or shortened routes to target structures. Manuscripts illustrating ... methods ... of previously reported ... different class of reaction substrates, reagents, or catalysts. Natural products isolation and ... shou... synthetic pathways. Manuscripts with a major component of biology, analytical ... materials ... te novelty in the organic chemistry portion of the work being reported.



4.745
Impact Factor

JOC期刊范围：

有机化合物的全合成，多步合成，短路径靶向结构合成

新合成方法需要展现全新的思路概念

天然产物的分离和鉴定报道新的化合物骨架特点和分析鉴定方法的进展

SCI 科技论文基本结构

前段

中段

后段

稿件模板 Template for Submission of Manuscripts to American Chemical Society Journals

TITLE (Word Style "BA_Title"). The title should accurately, clearly, and concisely reflect the emphasis and content of the paper. The title must be brief and grammatically correct. The space above the title is provided for the Journal logo. Do NOT delete this space.

AUTHOR NAMES (Word Style "BB_Author_Nam
substantial contributions to the work, even if th
Use first names, initials, and surnames (e.g., Joh
names (e.g., J. Robert Smith). Do not use only in
causes indexing and retrieval difficulties and in
not include professional or official titles or acad
nated with an asterisk as the author to whom c

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conducted. If the present address of an author differs fro
and give the Present Address under Author Information.
names to address(es).

*KEYWORDS (Word Style "BG_Keywords"). If you are submi
significant keywords to aid the reader in literature retriev*

ABSTRACT: (Word Style "BD_Abstract"). All manuscripts n
state the problem or purpose of the research, indicate the
findings, and point out the major conclusions. Abstract leng

TEXT (Word Style "TA_Main_Text"). For full instructions, please see the journal's Instructions for Authors. Do not modify the font in this or any other section, as doing so will not give an accurate estimate of the formatting for publication and final length of the paper.

FIGURES (Word Style "VA_Figure_Caption"). Each figure must have a caption that includes the figure number and a brief description, preferably one or two sentences. The caption should follow the format "Figure 1. Figure caption." All figures must be mentioned in the text consecutively and numbered with Arabic numerals. The caption should be understandable without reference to the text. Whenever possible, place the key to symbols in the artwork, not in the caption. To insert the figure into the template, be sure it is already sized appropriately and paste before the figure caption. For formatting double-column figures, see the instructions at the end of the template. Do NOT modify the amount of space before and after the caption as this allows for the rules, space above and below the rules, and space above and below the figure to be inserted upon editing.

SCHEMES (Word Style "VC_Scheme_Title"). Groups of reactions that show action are called schemes. Schemes may have brief titles describing their contents. The title should follow the format "Scheme 1. Scheme Title". Schemes may also have footnotes (use Word Style "FD_Scheme_Footnote"). To insert the scheme into the template, be sure it is already sized appropriately and paste after the scheme title. For formatting double-column schemes, see the instructions at the end of the template. Do NOT modify the amount of space before and after the title as this allows for the rules, space above and below the rules, and space above and below the scheme to be inserted upon editing.

CHARTS (Word Style "VB_Chart_Title"). Groups of structures that do not show action are called charts. Charts may have brief titles describing their contents. The title should follow the format "Chart 1. Chart Title". Charts may also have footnotes (use Word Style "FC_Chart_Footnote"). To insert the chart into the template, be sure it is already sized appropriately and paste after the chart title. For formatting double-column charts, see the instructions at the end of the template. Do NOT modify the amount of space before

标题，摘要，图片，语言

Title 起一个引人注目的标题

简明，包含本研究最核心的信息，通常是名词性的结构

CONCISE，Contains relevant information

避免

- 难以理解的缩写
- 复杂的语法或用语
- 难以证实的断言或者主观的词语， 比如 “first” and “only”等
- 把标题写成设问句

TOPIC - focussed （What is it about ? ）

RESULT - focussed （What did we find ? ）

方法：组合重要的字段　　科学意义：需要读者去体会

Mechanism of Catalytic Oxidation of Styrenes with Hydrogen Peroxide in the Presence of Cationic Palladium(II) Complexes
J. Am. Chem. Soc., 2017, 139 (36), pp 12495–12503　催化氧化的机理研究

Radical Route to 1,4-Benzothiazine Derivatives from 2-Aminobenzenethiols and Ketones under Transition-Metal-Free Conditions
Org. Lett., 2016, 18 (24), pp 6424–6427　某种化合物的新合成方法

11-Step Total Synthesis of Pallambins C and D
J. Am. Chem. Soc., 2016, 138 (24), pp 7536–7539　某个天然物的全合成

Cu and Cu-Based Nanoparticles: Synthesis and Applications in Catalysis
Chem. Rev., 2016, 116 (6), pp 3722–3811　综述文献 Review Article

Abstract 摘要

ACS Abstract Guide 摘要文字的若干组成部分

Objective/Sensing Issue | How this was addressed | Findings

Example of an abstract for a conceptual paper

A challenge for sensors detecting ultralow amounts of analyte is that for reliable sampling, large volumes of samples must be analyzed. The implication of large volumes is slow response times. **Herein, we introduce the concept of utilizing conductive gold-coated magnetic nanoparticles (Au@MNPs) as 'dispersible electrodes', which serve as the active element in the selective capture and direct electro-analytical quantification of analytes. The Au@MNPs are modified with self-assembled monolayers containing a peptide for the selective detection of Cu^{2+}. The particles scavenge any Cu^{2+} in solution and are then magnetically drawn back to the macroelectrode where the Cu^{2+} is detected amperometrically.** This concept reduces response times and decreases detection limits by bringing the sensor to the analyte rather than the conventional paradigm of the analyte finding the sensor. The higher sensitivity and lower detection limit is shown to be because all the analyte in the sample is collected, while the shorter response times are because by dispersing the Au@MNPs in solution, the diffusional pathlength of the analyte is drastically reduced.

Graphics 图片

- Be clear, precise
- Informative
- Support your text
- Use color
- Original
- Unpublished

TOC Graphics

TOC作图要求：

- 简单，信息丰富
- 直观地描述研究工作

Article

Mechanism of Catalytic Oxidation of Styrenes with Hydrogen Peroxide in the Presence of Cationic Palladium(II) Complexes

Katherine L. Walker†§, Laura M. Dornan†‡§, Richard N. Zare†, Robert M. Waymouth*†, and Mark J. Muldoon*‡

† Department of Chemistry, Stanford University, Stanford, California 94305, United States

‡ School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, Northern Ireland, BT9 5AG, United Kingdom

J. Am. Chem. Soc., **2017**, *139* (36), pp 12495–12503

DOI: 10.1021/jacs.7b05413

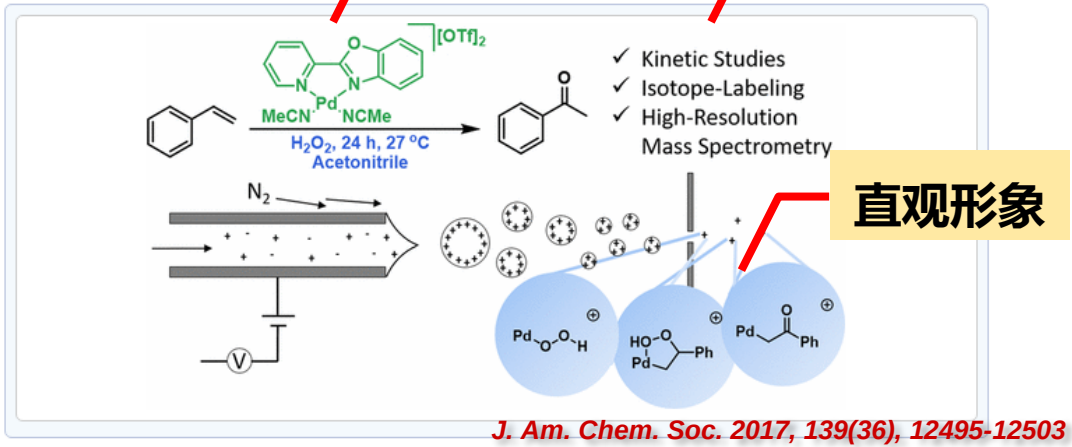
Publication Date (Web): August 29, 2017

*waymouth@stanford.edu, *m.j.muldoon@qub.ac.uk

主要步骤

主要方法

Abstract

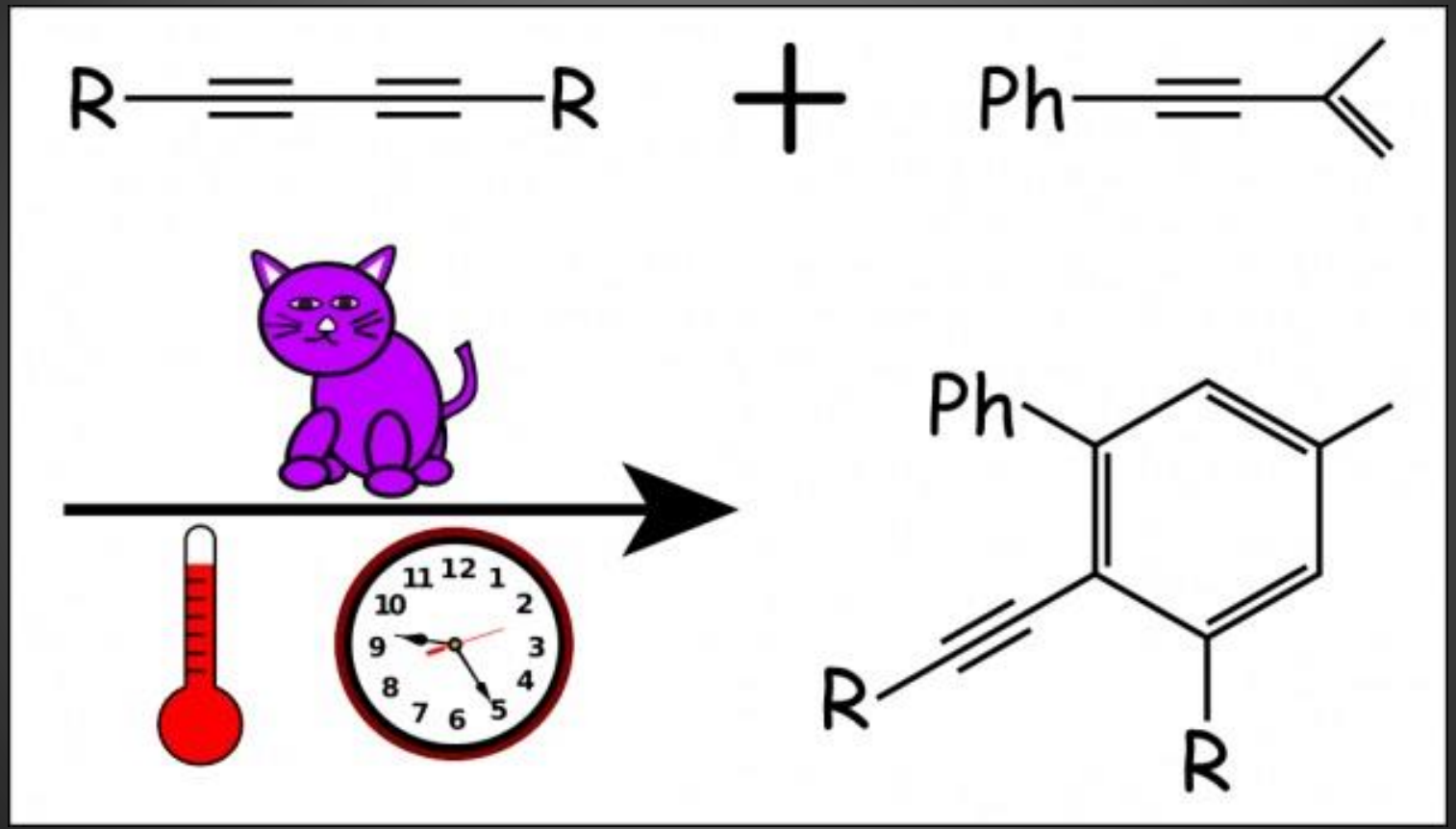


直观形象

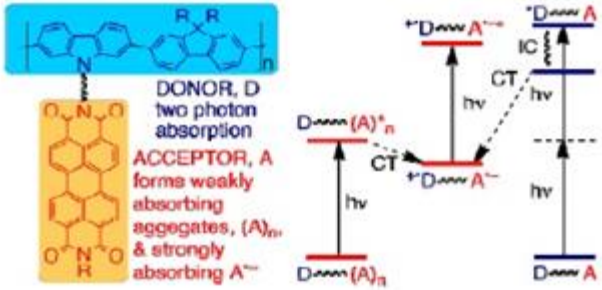
J. Am. Chem. Soc. 2017, 139(36), 12495-12503

您能理解到这个TOC图片是关于室内植物的大气丙酮吸收吗？

不鼓励使用漫画或卡通化的图片（猫：代表了一种催化剂？？？）

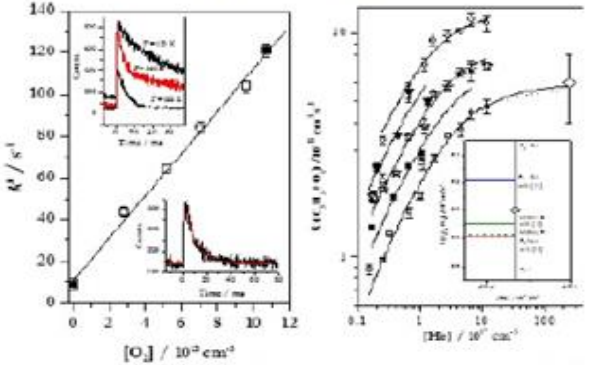


GOOD GRAPHICS



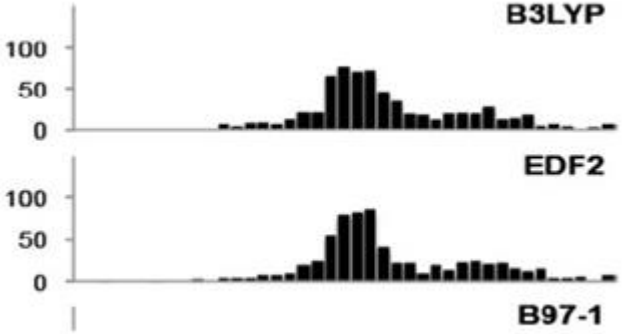
This graphic has a good balance of images and description. All of the type is crisp and easy to read.

POOR GRAPHICS

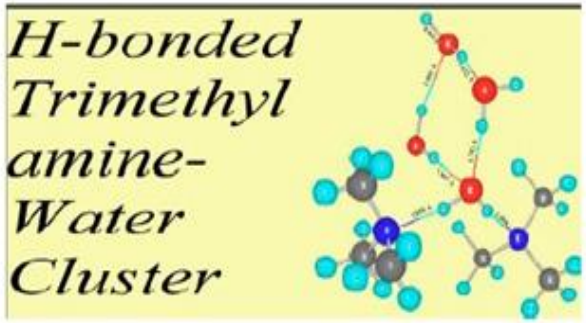


Graphic is very cluttered and most of the fonts are too small or faint to be readable.

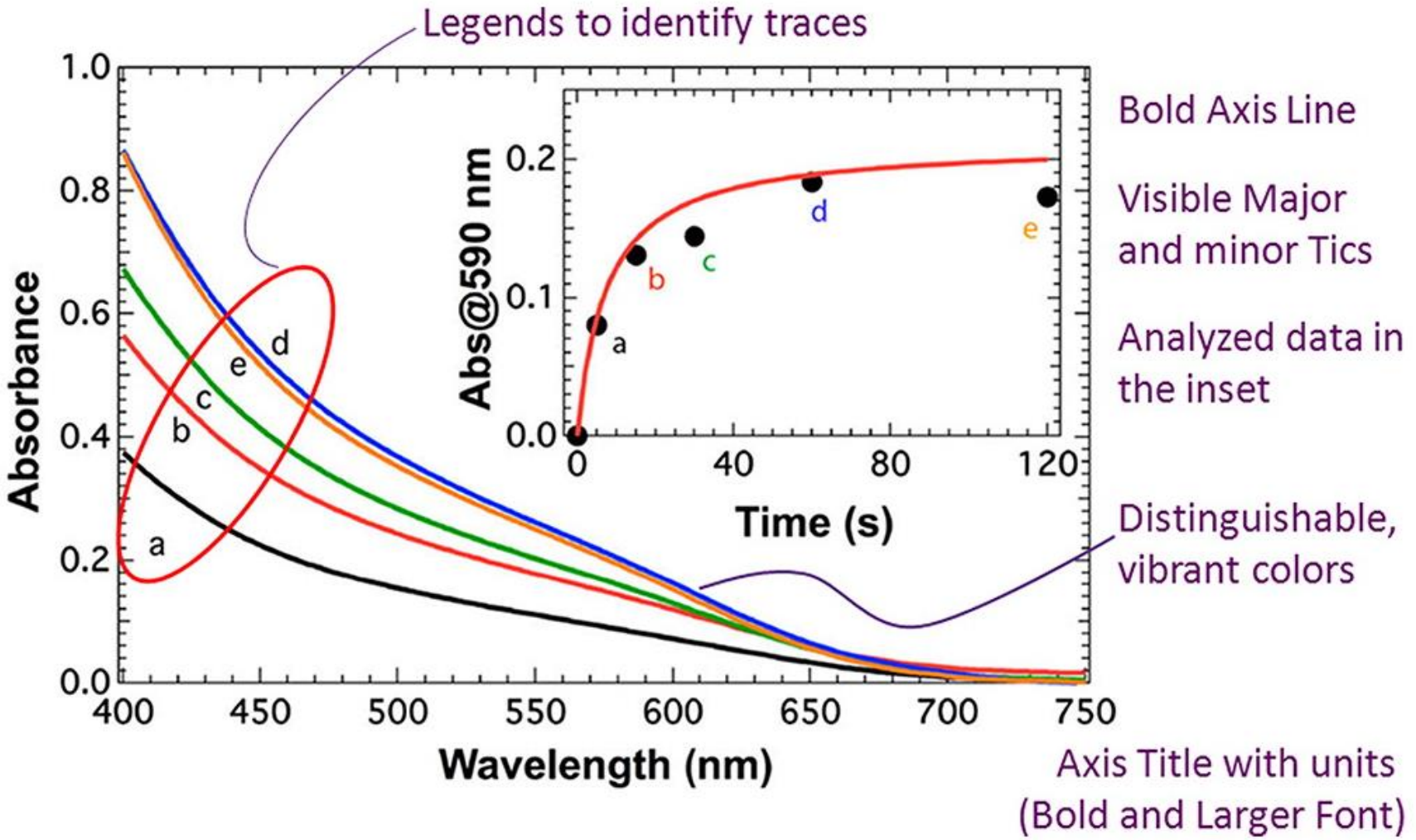
POOR GRAPHICS



Graphic is uninteresting and not informative.



The font is too big, the image says nothing about the article, and the type on the image is unreadable.


Legends to identify traces
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Abs@590 nm
Time (s)
a
b
c
d
e
Bold Axis Line
Visible Major and minor Tics
Analyzed data in the inset
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Grayscale art 600 dpi
Color art 300 dpi

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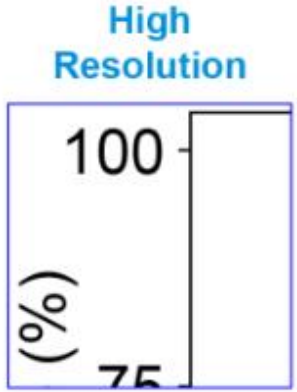
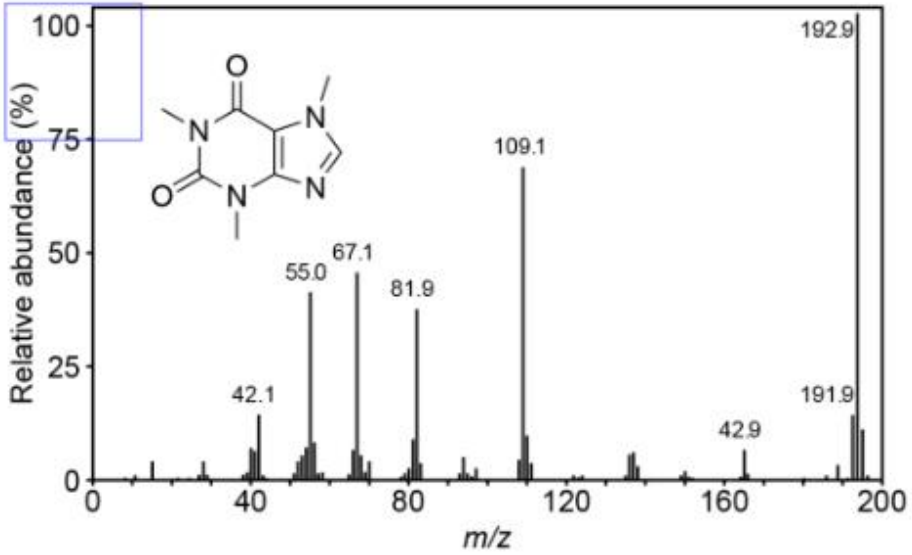
Fonts: Helvetica or Arial



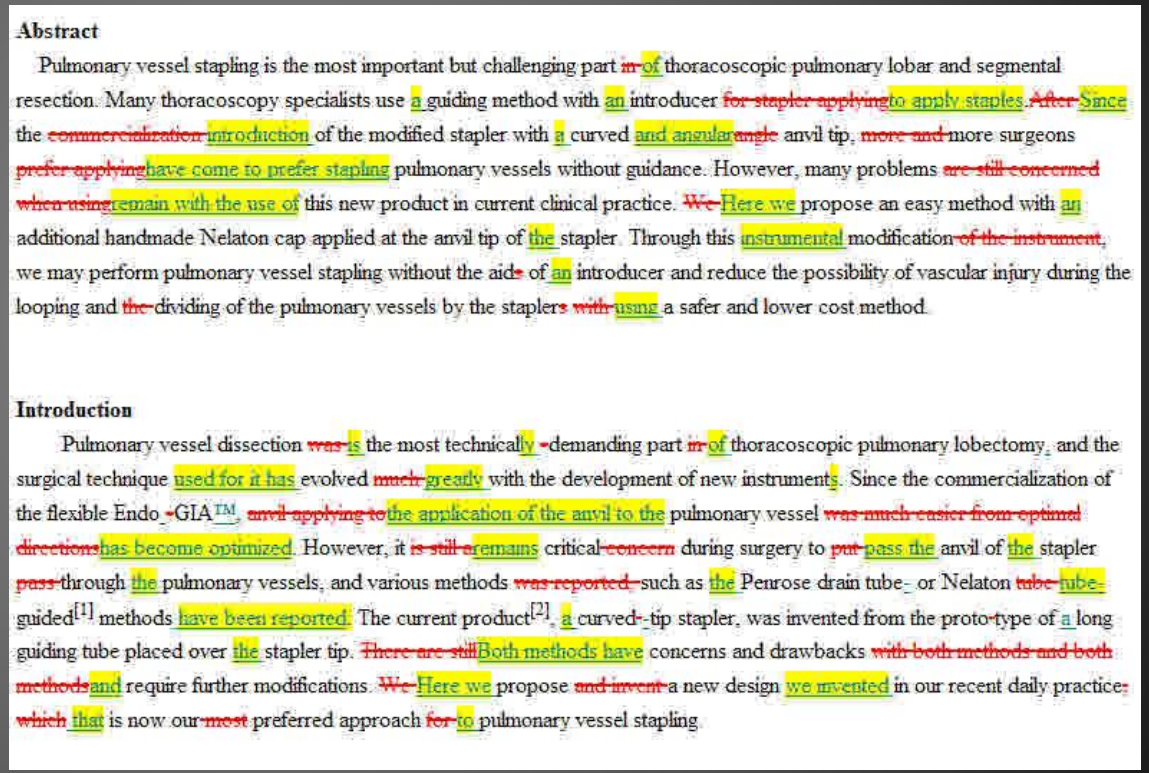


Language and Text 语言文字表述

- 专业词汇的积累
- IUPAC 和 缩写
- 母语和英语的不同
- 不断练习

- 客观表达 避免主观语句
- 逻辑清晰 > 句式复杂

- 自我修改 / 他人修改
- 写作编辑服务
- 论文查重：原创检测



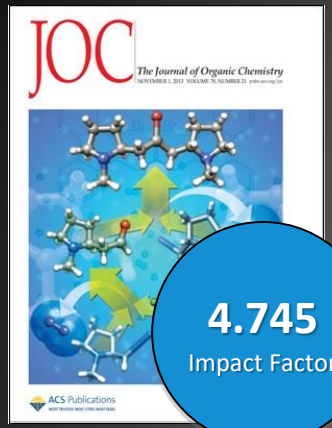
Abstract

Pulmonary vessel stapling is the most important but challenging part ~~in~~ of thoracoscopic pulmonary lobar and segmental resection. Many thoracoscopy specialists use a guiding method with an introducer ~~for stapler applying~~to apply staples. ~~After~~ Since the ~~commercialization~~ introduction of the modified stapler with a curved and ~~angular~~angle anvil tip, ~~more and~~ more surgeons ~~prefer applying~~have come to prefer stapling pulmonary vessels without guidance. However, many problems ~~are still concerned when using~~remain with the use of this new product in current clinical practice. ~~We~~ Here we propose an easy method with an additional handmade Nelaton cap applied at the anvil tip of the stapler. Through this instrumental modification ~~of the instrument~~, we may perform pulmonary vessel stapling without the aid ~~-~~ of an introducer and reduce the possibility of vascular injury during the looping and ~~the~~ dividing of the pulmonary vessels by the staplers ~~with~~ using a safer and lower cost method.

Introduction

Pulmonary vessel dissection ~~was~~ is the most technically ~~-~~demanding part ~~in~~ of thoracoscopic pulmonary lobectomy, and the surgical technique used for it has evolved ~~much~~ greatly with the development of new instruments. Since the commercialization of the flexible Endo ~~-~~GIA™, ~~anvil applying to~~the application of the anvil to the pulmonary vessel ~~was much easier from optimal directions~~has become optimized. However, it ~~is still a~~remains critical ~~concern~~ during surgery to ~~put~~ pass the anvil of the stapler ~~pass~~ through the pulmonary vessels, and various methods ~~was reported~~ such as the Penrose drain tube ~~-~~ or Nelaton ~~tube~~ tube ~~-~~ guided[1] methods have been reported. The current product[2], a curved ~~-~~tip stapler, was invented from the proto ~~-~~type of a long guiding tube placed over the stapler tip. ~~There are still~~Both methods have concerns and drawbacks ~~with both methods and both methods~~and require further modifications. ~~We~~ Here we propose ~~and invent~~ a new design we invented in our recent daily practice ~~which~~ that is now our ~~most~~ preferred approach ~~for~~ to pulmonary vessel stapling

怎样把格式写得更漂亮



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The Journal of Organic Chemistry

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Standard Abbreviations and Acronyms:

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Compound Characterization Checklist:

https://pubs.acs.org/page/joceah/submission/ccc.html

Crystallographic Information File:

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Overview:

https://pubs.acs.org/page/orlef7/submission/authors.html

Author Guidelines:

http://pubsapp.acs.org/paragonplus/submission/orlef7/orlef7_authguide.pdf?

Common Abbreviations & Formatting Checklist:

http://pubsapp.acs.org/paragonplus/submission/orlef7/orlef7_abbreviations_checklist.pdf?

FORMATTING CONVENTIONS

- ☐ Reagents and solvents are lowercase in all text, tables, and graphics:
  - toluene
  - acetone

- ☐ Trade names and proper nouns are capitalized in all text, tables, and graphics:
  - PhenoFluor

- ☐ Compound numbers are **bolded** in all text, tables, and graphics:
  - compound **5**
  - compounds **6a-j**

- ☐ Space before and after mathematical operators:
  - 5 + 7
  - time = 5 h

- ☐ No space between mathematical symbols and numbers:
  - <50
  - 45%
  - 1:9

TABLE FORMATTING

Sample Table

entry	acid	cat. (mol %)	solvent	time (h)	compd	yield (%)
1	**3a**	**2** (5)	CH_2Cl_2	12	**1a**	35
2	**3a**	**6** (20)	MeOH	24	**1b**	72

☐ Column headings:

- Lowercase
- Light gray background shading (select gray 15% in Word)

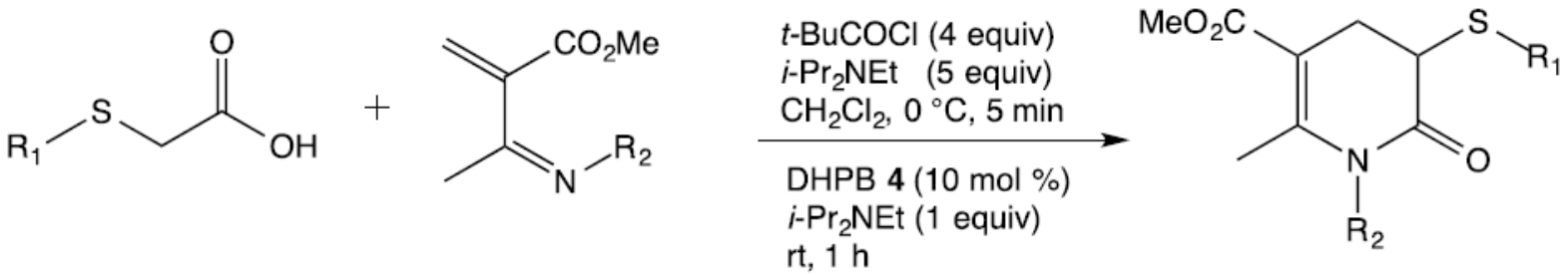
☐ Units of measure next to column headings – acceptable formats:

- Parentheses: yield (%) time (h)
- Comma: yield, % time, h
- Slash: yield/% time/h

☐ No lines

SCHEME FORMATTING

Sample Scheme



1 **3** **5**
83%

- ☐ Font either Arial or Helvetica in structures and text
- ☐ Reagents and conditions are above/below arrows
- ☐ No punctuation at the end of line(s)
- ☐ Acceptable formats for yield:
  - In parentheses after compound name: **4c** (79%)
  - Below compound name without parentheses: **3a** 85%

Cover Letter 投稿信

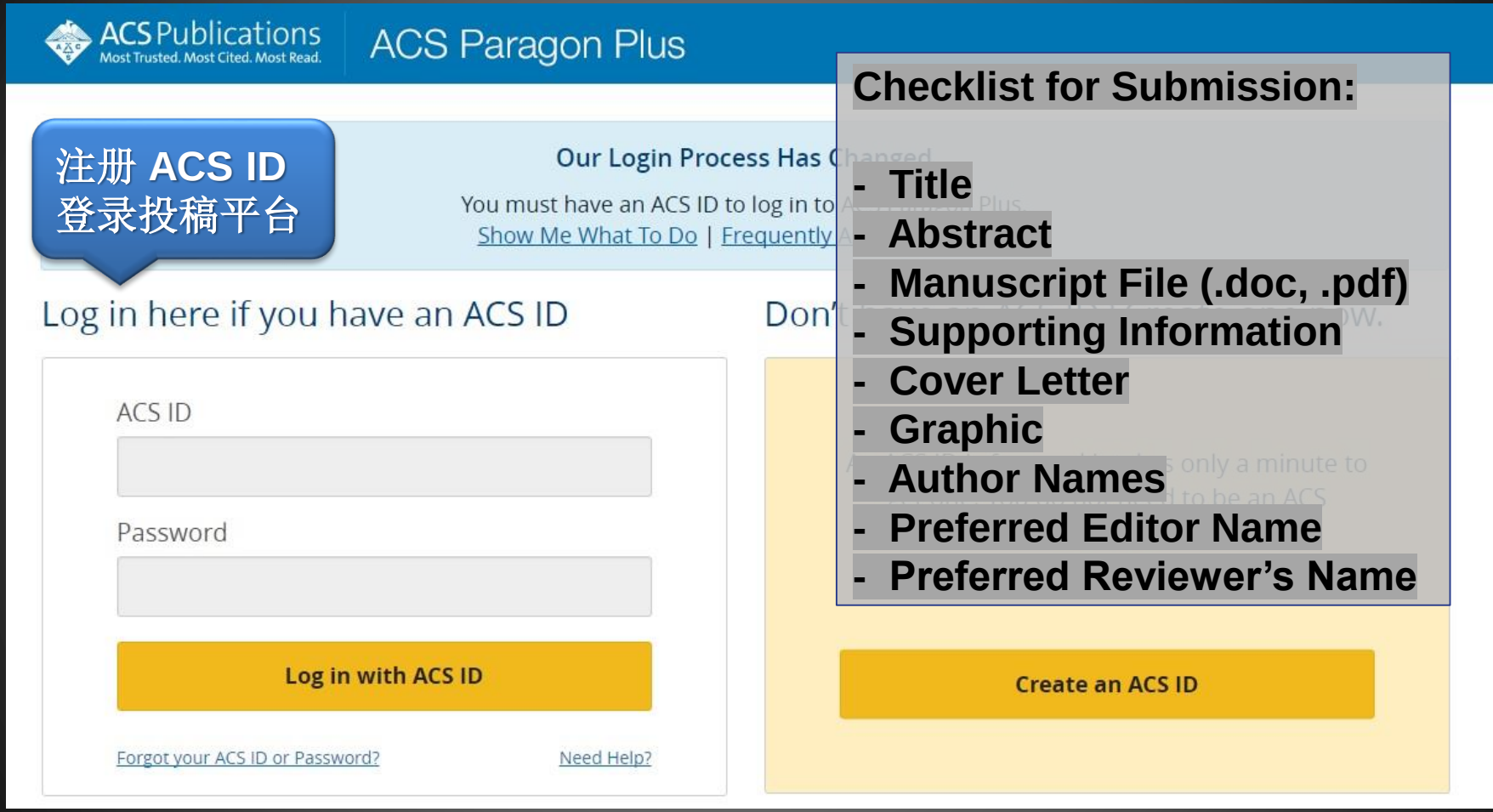
致某位 ACS期刊编辑
Dear Professor *XXX*

标题是什么，并提及投稿的期刊
We wish to submit our manuscript “TITLE” for publication in ACS XXXX Journal.

研究工作的重点和亮点 （a synopsis of the article）
We describe a new, non-natural enzyme-catalyzed reaction, aziridination of olefins via intermolecular nitrene transfer.

We discovered that a variant of cytochrome P450BM3 used in our previous studies of intermolecular sulfimidation also catalyzes aziridination.

We were able to improve this activity more than 50-fold and the enantioselectivity of enzyme-catalyzed aziridination was improved to 99% ee for a range of styrenyl substrates. （有亮点的关键性数据）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Password
Log in with ACS ID
Forgot your ACS ID or Password?
Need Help?
Create an ACS ID
Checklist for Submission:
- Title
- Abstract
- Manuscript File (.doc, .pdf)
- Supporting Information
- Cover Letter
- Graphic
- Author Names
- Preferred Editor Name
- Preferred Reviewer's Name

4 学术道德与同行评议

Most Common Ethical Violations

自我抄袭

Self-plagiarism – reusing your own content

预先公布

Prior publication – journals have policies about what they consider to be published content

一稿多投

Concurrent submissions – submitting the same manuscript to multiple journals at the same time

Most Common Ethical Violations

数据造假或篡改

Data fabrication or falsification – deliberately or unintentionally changing the data to fit the conclusions

有问题的原创作者

Ghost or Gift Authorship – adding authors who did not contribute, or leaving off authors who did

Ways Violations Are Uncovered:

从技术上来说：

CrossCheck

compares manuscript text to published work

Image checking software

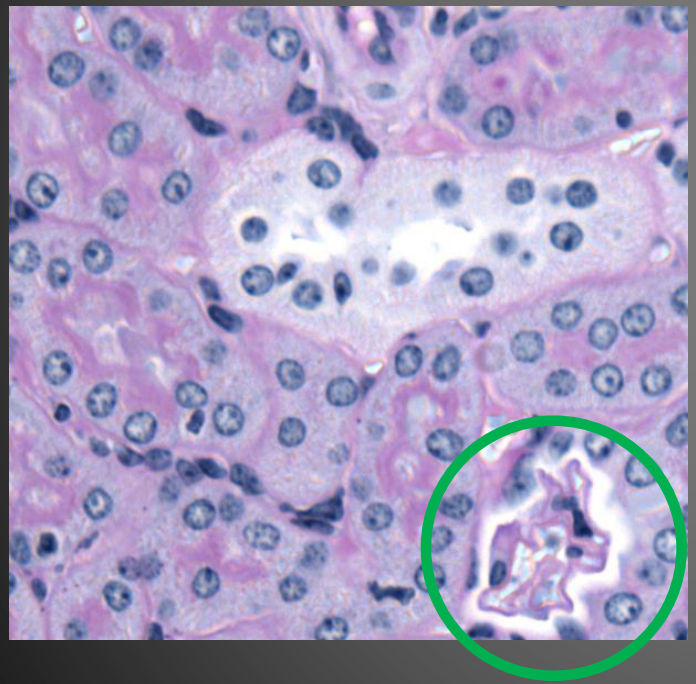
use Photoshop judiciously

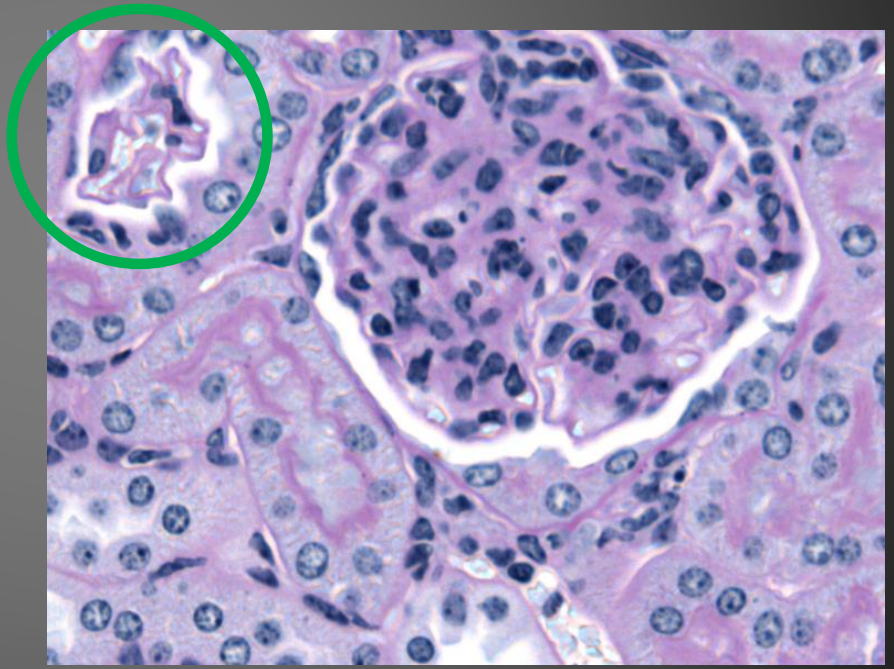
从科学交流上来说：

Social networking (blogs, Facebook, Twitter)

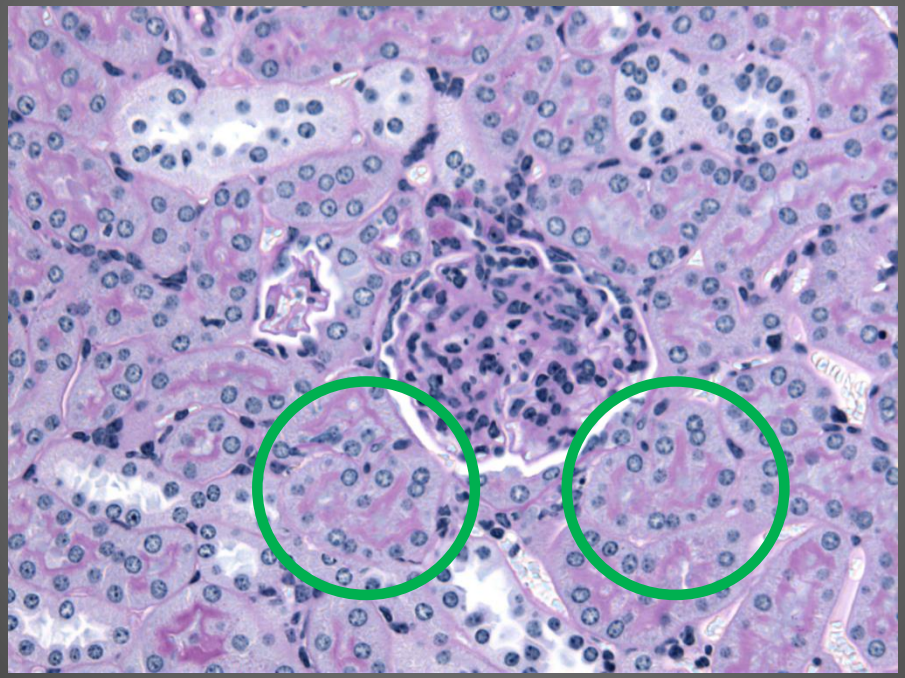
offer new means to question published works in a very public forum

Duplication between images





Duplication within images



Reasons for Retractions：

1. **Further research reveals flaws in data**
   进一步的研究揭示了数据中的缺陷
2. **Irreproducible results**
   无法复制的结果
3. **Incorrect analysis**
   错误的分析
4. **Accidental ethical violations**
   意外违反学术道德
5. **Intentional ethical violations**
   故意违反学术道德

学术道德与出版政策

Correction **Retraction**

更正 撤稿

ADDITION / CORRECTION This article has been corrected. View the notice.

Photocatalytic Gas Phase Reactions

Murielle Schreck and Markus Niederberger*

Cite This: *Chem. Mater.* 2019, 31, 3, 597-618
Publication Date: January 16, 2019
https://doi.org/10.1021/acs.chemmater.8b04444

Article Views 1119 | Altmetric 6 | Citations -

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Chemistry of Materials

ORIGINAL ARTICLE This notice is a correction

Correction to Photocatalytic Gas Phase Reactions

Murielle Schreck and Markus Niederberger*

Cite This: *Chem. Mater.* 2019, 31, 4, 1469
Publication Date: February 12, 2019
https://doi.org/10.1021/acs.chemmater.9b00418

Article Views 436 | Altmetric 6 | Citations -

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PDF (218 KB)

Correction

In our review on photocatalytic gas phase reactions, we should have included in Section 3.2, Specific Examples from Literature, the work of Ozin and co-workers. The topic of this particular section is how to increase the efficiencies of photocatalytic gas phase reactions. Since their first papers in 2014,(1,2) Ozin and co-workers have been significantly contributing to the field of photocatalytic gas-phase reduction of CO_2 to chemicals and fuels, addressing different aspects like selectivity, the role of residual carbon contamination on the sample, influence of illumination, batch vs flow reactors, surface chemistry of the photocatalysts, or photothermal effects.(3−5)

References

ARTICLE SECTIONS Jump To

This article references 5 other publications.

1. O'Brien, P. G.; Sandhel, A.; Wood, T. E.; Jelle, A. A.; Hoch, L. B.; Perovic, D. D.; Mims, C. A.; Ozin, G. A. Photomethanation of Gaseous CO_2 over Ru/Silicon Nanowire Catalysts with Visible and Near-Infrared Photons. *Adv. Sci.* 2014, *1*, 1400001, DOI: 10.1002/advs.201400001 [Crossref], [CAS], [Google Scholar]

This publication has no figures.

Where has been corrected ?

RETURN TO ISSUE | < PREV ARTICLE NEXT >

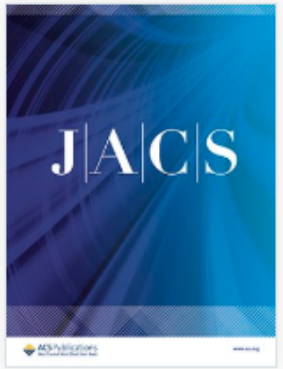
Mechanical Reconfiguration of Stereoisomers

Kelly M. Wiggins[†], Todd W. Hudnall[†], Qilong Shen[‡], Matthew J. Kryger[‡], Jeffrey S. Moore[‡] and Christopher W. Bielawski[*†]

View Author Information

此文由于违反学术道德而撤稿

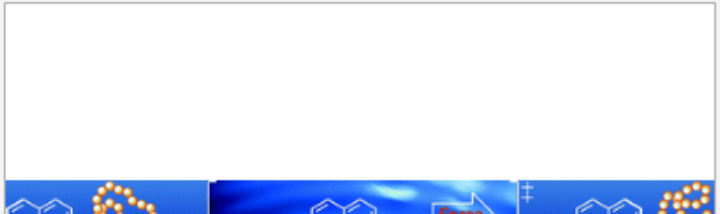
Cite This: *J. Am. Chem. Soc.* 2010, 132, 10, 3256-3257
Publication Date: February 18, 2010
https://doi.org/10.1021/ja910716s



Journal of the American Chemical Society

Abstract

Poly(methyl acrylate) of varying molecular weight was grown from the enantiopure ditopic initiator (*R*)- or (*S*)-1,1′-binaphthyl-2,2′-bis-(2-bromoisobutyrate). Subjecting CH_3CN solutions of high-molecular-weight derivatives (M_N > 25 kDa) to sonication at 0 °C resulted in >95%



Retraction of "Mechanical Reconfiguration of Stereoisomers"

Kelly M. Wiggins, Todd W. Hudnall, Qilong Shen, Matthew J. Kryger, Jeffrey S. Moore and Christopher W. Bielawski*

Cite This: *J. Am. Chem. Soc.* 2015, 137, 9, 3428
Publication Date: March 11, 2015
https://doi.org/10.1021/jacs.5b01988

PDF (122 KB)

Journal of the American Chemical Society

Retraction !!!

Based on an investigation conducted by The Office of Research Integrity at The University of Texas at Austin, it was determined that the data and scientific conclusions of this article are unreliable as a result of scientific misconduct by one of the co-authors affiliated with the University at the time of its publication. The authors retract this article accordingly.

The original paper was published February 18, 2010 (*J. Am. Chem. Soc.***2010**, *132*, 3256−3257. DOI: 10.1021/ja910716s), and retracted March 11, 2015.

This publication has no figures.

JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Retraction

pubs.acs.org/JACS

Retraction of "Mechanical Reconfiguration of Stereoisomers"

Kelly M. Wiggins, Todd W. Hudnall, Qilong Shen, Matthew J. Kryger, Jeffrey S. Moore, and Christopher W. Bielawski*

J. Am. Chem. Soc. **2010**, *132*, 3256−3257. DOI: 10.1021/ja910716s

Based on an investigation conducted by The Office of Research Integrity at The University of Texas at Austin, it was determined that the data and scientific conclusions of this article are unreliable as a result of scientific misconduct by one of the co-authors affiliated with the University at the time of its publication. The authors retract this article accordingly.

The original paper was published February 18, 2010 (*J. Am. Chem. Soc.* **2010**, *132*, 3256−3257. DOI: 10.1021/ja910716s), and retracted March 11, 2015.

Retraction:

基于德克萨斯大学奥斯汀分校诚信研究办公室进行的一项调查，在发表这篇文章时，由于该大学的一名联合作者在科学上的不端行为，因此确定这篇文章的数据和科学结论是不可靠的。作者据此撤回了这篇文章。

Electronic Supporting Information

This paper was retracted on March 11, 2015 (*J. Am. Chem. Soc.* **2015**, *137*, DOI: 10.1021/jacs.5b01988).

Mechanical Reconfiguration of Stereoisomers

Kelly M. Wiggins,[†] Todd W. Hudnall,[†] Qilong Shen,[‡] Matthew J. Kryger,[‡] Jeffrey S. Moore[‡] and Christopher W. Bielawski[*†]

[†] Department of Chemistry & Biochemistry, The University of Texas, Austin, Texas 78712
[‡] Department of Chemistry, University of Illinois at Urbana-Champaign, IL 61801

E-mail: bielawski@cm.utexas.edu

General Considerations. (*S*)-, (*R*)- and *rac*-1,1′-binaphthyl-2,2′-bis-(2-bromo-*iso*butyrate),[1] (*S*)-1,1′-binaphthyl-2-ol-2′-pivalate[2] and (*S*)-1,1′-binaphthyl-2,2′-bis-(pivalate)[2] were prepared following literature procedures. All other chemical reagents were purchased from commercial sources and used without additional purification. All syntheses were performed under an inert atmosphere of nitrogen using standard Schlenk techniques or in a nitrogen-filled drybox. Solvents were dried over 3Å molecular sieves or Al_2O_3 and deoxygenated (via a Q5 catalyst) using a Vacuum Atmospheres Company solvent purification system (Model No. 103991), and then subsequently stored over molecular sieves (3Å) in a drybox. ^{1}H and ^{13}C NMR data were collected on Varian Unity INOVA 400 MHz and Varian Mercury 300 MHz spectrometers. Chemical shifts (δ) are reported in ppm and are referenced downfield from $(CH_3)_4Si$ using the residual solvent peak as an internal standard ($CDCl_3$: 7.24 ppm for ^{1}H and 77.0 ppm for ^{13}C NMR, respectively). Sonication experiments were carried out under argon using a Sonics & Materials VC-505 Liquid Cell Ultrasonic processor operating at 20 kHz and equipped with a 12.8 mm replaceable tip titanium probe. Custom Schlenk cells[3] were fabricated in house. UV–vis spectra were recorded using a Perkin Elmer Instruments Lambda 35 spectrometer. CD spectra were recorded on a Jasco J-815 CD spectrometer. High-resolution mass spectra (HRMS) were obtained with a VG analytical ZAB2-E instrument (CI). Elemental analyses were performed at Midwest Microlab, LLC (Indianapolis, IN). Thermogravimetric analyses (TGA) were performed using a Mettler-Toledo TGA/SDTA851e under an atmosphere of N_2 at a temperature scan rate of 10 °C min^{-1}. Gel permeation chromatography (GPC) was performed on a Viscotek system equipped with a VE 1122 pump, a VE 7510 degasser, two fluorinated polystyrene columns (I-MBHW-3478 and I-MBLMW-3078) thermostated to 30 °C (using a ELDEX CH 350 column heater) and arranged in series.[4] Molecular weight and polydispersity data are reported relative to polystyrene standards in tetrahydrofuran (THF). Optical rotation measurements were obtained using an ATAGO AP300 automatic polarimeter.

(*S*)-1,1′-Binaphthyl-2-(pivalate)-2′-(2-bromo-isobutyrate). To a stirred solution of (*S*)-1,1′-binaphthyl-2-ol-2′-pivalate (180 mg, 0.27 mmol) and triethylamine (0.05 mL, 0.36 mmol) in CH_2Cl_2 (3 mL) cooled to 0 °C was added dropwise 2-bromo-isobutyrylbromide (0.04 mL, 0.35 mmol). The resulting suspension was allowed to slowly warm to ambient temperature and then stirred for an additional 20 h. After diluting the resulting reaction mixture with additional CH_2Cl_2 until the total volume was 20 mL, it was poured slowly into ice cold water (20 mL) and stirred for 30 min. The organic layer was then separated, and the aqueous phase was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with a saturated solution of $NaHCO_3$ (1 × 20 mL), dried over $MgSO_4$, and then passed over a short plug of neutral alumina. The solvent was removed under reduced pressure to afford the desired product as a white powder (120 mg, 0.23 mmol) in 85% yield. m.p. 120–122 °C. ^{1}H NMR ($CDCl_3$, 400.27 MHz): δ 0.72 (s, 9H, *piv*-CH_3), 1.25 (s, 3H, CBr-CH_3), 1.46 (s, 3H, CBr-CH_3), 7.28-7.36 (m, 5H, Ar-*CH*), 7.42-7.50 (m, 3H, Ar-*CH*), 7.91 (t, ^3J = 8.0 Hz, 2H, Ar-*CH*), 7.95 (d, ^3J = 8.8 Hz, 1H,

[1] Doyagüez, E.; Blumenfeld, R. *J. Poly. Sci., Part A* **2004**, *42*, 902.
[2] Cai, D.; Lovers, R. D.; Reider, P. J. *Tetrahedron Lett.* **2002**, *43*, 4003.
[3] Sottos, N. S.; Goodwin, J. W.; Schubert, P. F.; Wang, H. H. *J. Am. Chem. Soc.* **1985**, *103*, 3781.

Sonication of an Ultrahigh Molecular Weight Polymer. It has been previously observed that high molecular weight polymers are subject to degradation upon sonication.[5] Subjecting an ultrahigh molecular weight polymer (M_n = 2.8 MDa, PDI = 1.36; prepared from S_1 (methyl acrylate)$_n$ (S_1)$_n$ = 33,680) to sonication in CH_3CN for 24 h afforded a material with a significantly reduced molecular weight (M_n = 156 kDa, PDI = 1.93; see Figure S10) but a minimal loss in its CD signal intensity. In this case, cleavage events may be occurring in non-chain centered locations along the polymer chains at a rate that is higher than isomerization of the embedded binol moieties.

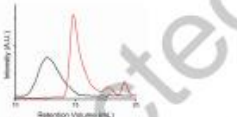


Figure S10. Gel permeation chromatograms of an ultrahigh molecular weight polymer prepared from *R*- and methyl acrylate before (black line; M_n = 2.8 MDa, PDI = 1.36) and after 24 h of being subjected to sonication in CH_3CN (red line; M_n = 156 kDa, PDI = 1.93).

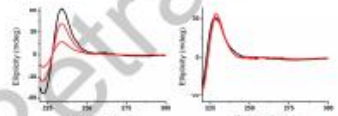


Figure S11. CD spectra of CH_3CN solutions of (A) (*S*)-2,2′-binaphthol (0.05 mg/mL) and (B) (*S*)-1,1′-binaphthyl-2,2′-bis-(pivalate) (0.05 mg/mL) before (black) and after (red) being heated in the melt (240 °C, sand bath) for 1 and 65 h. The former sample showed a 35% loss in CD signal intensity after 1 h and 73% loss after 65 h; no significant change in CD signal intensity was observed in the latter sample even after being heated for 65 h.

[4] Cannon, M. M.; Davis, D. A.; Shen, Q.; Odom, S. A.; Sottos, N. R.; White S. R.; Moore, J. S. *Chem. Rev.* **2009**, *109*, 5750.

Attempts at Thermally Racemizing S_{100K}. The decomposition temperature of S_{100K} was determined to be 364 °C by TGA (Figure S3A). A 50 mL round bottom flask was charged with S_{100K} (100 mg), nitrogen purged Ph_2O (10 mL), and a stir bar, and then fitted with a reflux condenser. After vigorously refluxing the resulting solution under nitrogen in a sand bath thermostated to 270 °C for 72 h, it was poured into excess methanol. The precipitated polymer was isolated by filtration, dried under reduced pressure, and examined by CD spectroscopy in CH_3CN (Figure S3B).

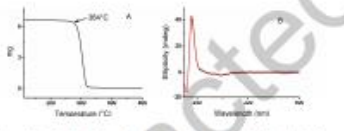


Figure S3. (A) TGA of S_{100K} under nitrogen at a scan rate = 10 °C min^{-1}. (B) CD spectra of S_{100K} in CH_3CN (0.4 mg/mL) before (black) and after (red) being refluxed in Ph_2O for 72 h.

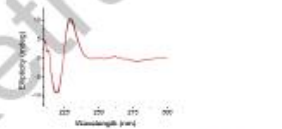


Figure S4. CD spectra of an end-functionalized PMA (M_n = 90.5 kDa, PDI = 1.02), prepared from (*S*)-1,1′-binaphthyl-2-(pivalate)-2′-(2-bromo-isobutyrate) and methyl acrylate in CH_3CN (0.1 mg/mL) before (black) and after (red) being subjected to sonication for 24 h.

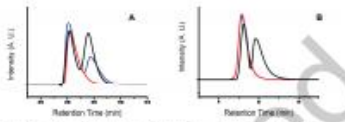


Figure S12. (A) HPLC chromatograms of *rac*-2,2′-binapthol (black), *S*-2,2′-binapthol (red), *S*-2,2′-binapthol after being heated in Ph_2O at 220 °C for 24 under an atmosphere of nitrogen (blue).[6] (B) HPLC chromatograms of *rac*-1,1′-binaphthyl-2,2′-bis-(pivalate) (black), *S*-1,1′-binaphthyl-2,2′-bis-(pivalate) (red), *S*-1,1′-binaphthyl-2,2′-bis-(pivalate) after being heated in Ph_2O at 220 °C for 24 h under an atmosphere of nitrogen (blue). HPLC conditions: Chiralpak OD column (250 x 4.6 mm); solvent: 5%→20% isopropanol in hexanes (v/v); rate: 0.5 mL/min, UV detection: 254 nm.

[5] Moss, L.; Ryabo, D.; Berlan, Z. *J. Org. Chem.* **2003**, *68*, 3677.

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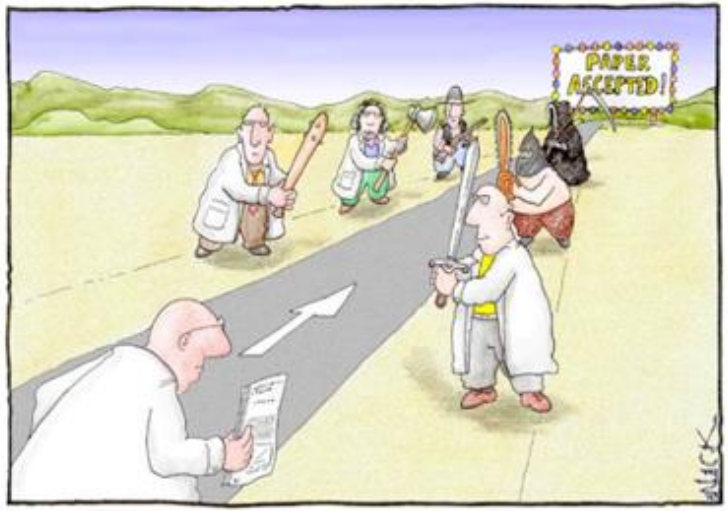

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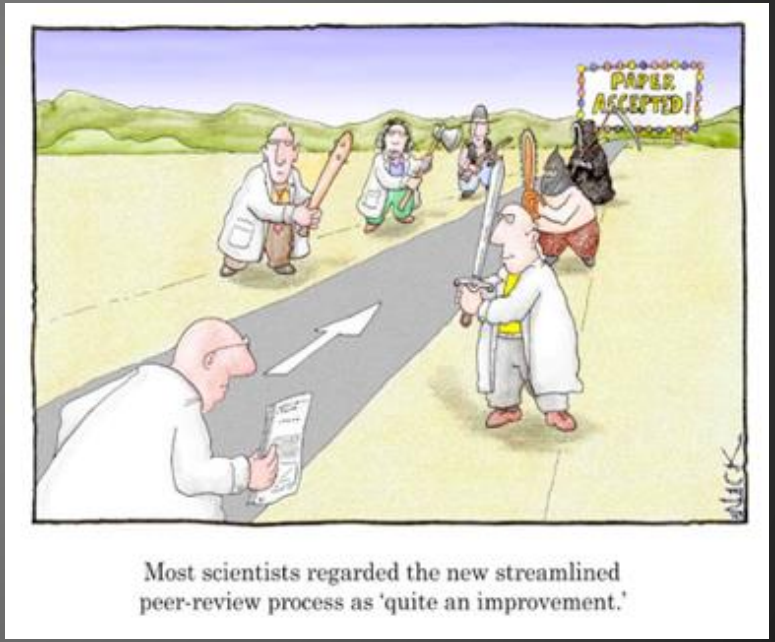

Most scientists regarded the new streamlined peer-review process as 'quite an improvement.'


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