

ACS 数据库学术资源的探索与应用

主讲人：赵璟 ACS数据库培训师

Monday, October 30, 2023

广东石油化工学院



1. ACS 数据库学术资源介绍
2. ACS 数据库平台功能和科研应用
3. ACS 期刊投稿和审稿知识





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ACS Publications 数据库学术资源介绍



ACS Is the World's Largest Scientific Society

- **ACS**美国化学会，成立于**1876**年
- **140**多个国家，超过**15**万名会员
- 出版高品质的专业科学期刊
- 促进化学及相关学科的交流与发展



ACS Is the World's Largest Scientific Society



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IN 140+ COUNTRIES

我们的愿景

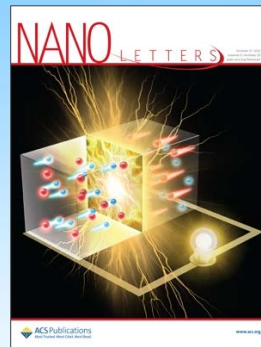
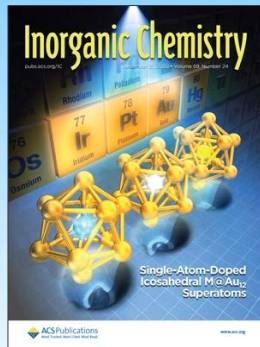
通过化学的变革力量改善人们的生活

我们的使命

推动更广泛的化学企业及其从业者为全球及其人民的生活从中获益

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ACS 美国化学学会出版超过 75 种高品质的科学期刊，共 130 多万篇期刊文章，总被引次数超过 440 万，是化学领域里被引用次数最多的期刊。

---- JCR 期刊引证报告

WE COVER EVERY ASPECT OF CHEMISTRY

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



15.0
Impact
Factor

1905

JOURNAL

OF THE

AMERICAN CHEMICAL SOCIETY.

VOLUME I.

PUBLICATION COMMITTEE:

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Journal of the American Chemical Society 美国化学会志

Impact Factor: 15.0 | Citations: 580,144



2022 IMPACT FACTOR

15.0

美国化学会志 **JACS** 出版于 1879 年，是美国化学会的第一本期刊，也是美国化学会出版社的旗舰期刊。

化学领域获得引用最多，影响力最大的综合类化学期刊，出版化学各个领域里顶尖的基础研究论文。

每年出版大约 2500 篇研究型、通讯和观点型的科研文章。期刊每周出版一期，提供了化学领域必不可少的研究结果，受到全球化学科研工作者的广泛关注。

Chemical Reviews 化学评论

Impact Factor: 62.1 | Citations: 231,674



2022 IMPACT FACTOR

62.1

Chemical Reviews 是最受推崇同时也是排名最高的期刊之一，涵盖了化学学科所有的研究领域，为有机化学，无机化学，物理化学，分析化学，理论化学和生物化学各领域的重要研究提供全面，权威，关键和可读性强的综述文章。

除了综述文章以外，期刊定期出版权威专题，重点关注新兴研究领域的单一主题或方向。

期刊收录研究方向：化学，化学综合

材料研究述评/化学研究述评

■ Accounts of Materials Research

主要发表在某一材料科学分支内相关基础、应用或工程研究领域内的具有作者团队自己研究特色的述评文章，或者前瞻性观点。

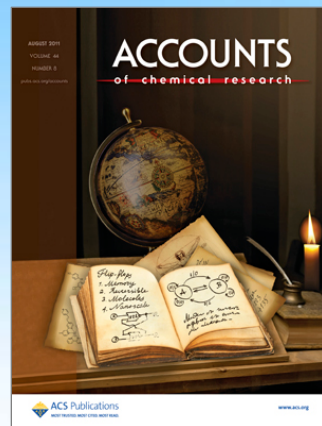
期刊收录研究方向：材料科学



*Accounts of
Materials Research*

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14.6



*Accounts of
Chemical Research*

IMPACT FACTOR

18.3

Organic-Inorganic Chemistry 有机与无机化学

■ The Journal of Organic Chemistry

有机化学领域的旗舰型期刊。

■ Organic Letters

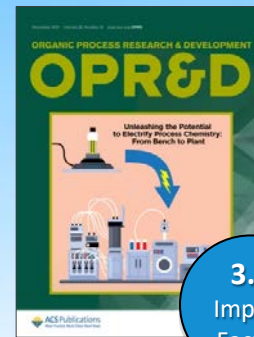
有机化学快报期刊，也是有机化学领域被引用次数最多的期刊。



3.6
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5.2
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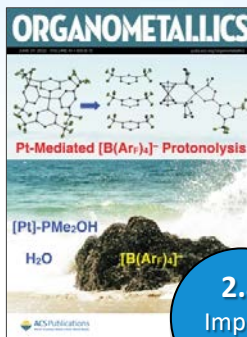
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■ Inorganic Chemistry

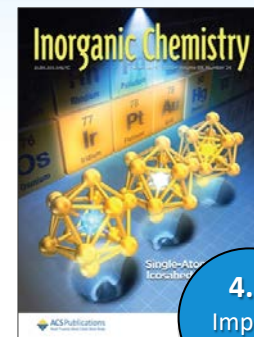
无机化学领域被引用次数最多的期刊。

■ Crystal Growth & Design

晶体学领域被引用次数最多的期刊。



2.8
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Physical Chemistry 物理化学

■ The Journal of Physical Chemistry A

■ The Journal of Physical Chemistry B

■ The Journal of Physical Chemistry C

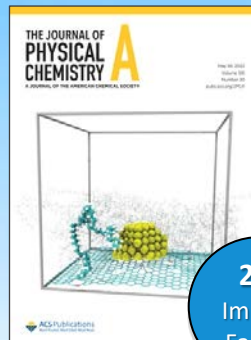
JPC A: 分子、离子、自由基、团簇和气溶胶物理化学的实验、理论和计算研究。

JPC B: 生物物理、生物化学、生物材料和软物质领域的实验、理论和计算研究。

JPC C: 纳米、低维和块状材料物理化学的实验、理论和计算研究;界面的化学转变;以及能量转换和储存。

■ The Journal of Physical Chemistry Letters

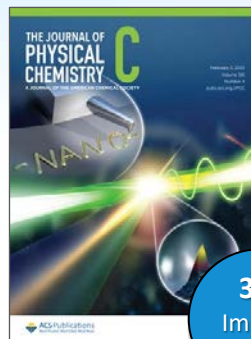
JPCL: 物理化学领域的快报类期刊。



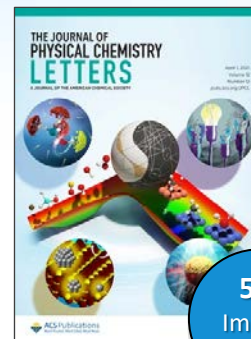
2.9
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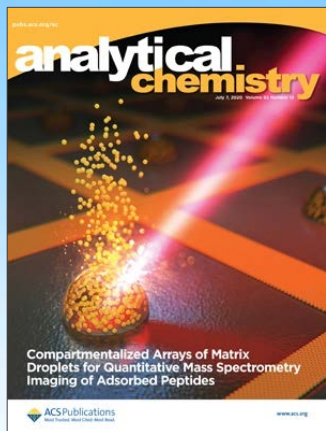


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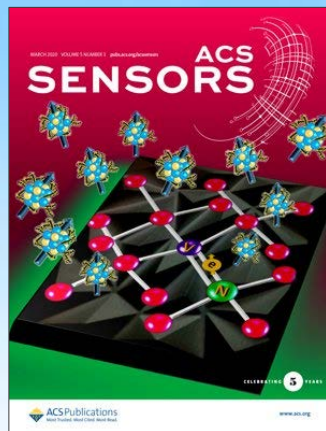
Measurement Science 测量科学



*Analytical
Chemistry*

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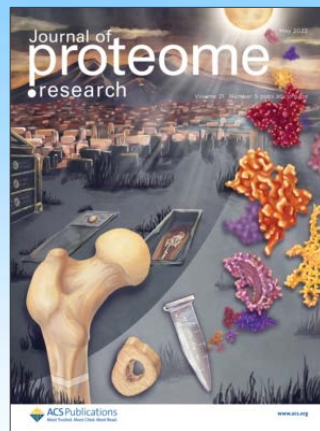
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*ACS
Sensors*

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*Journal of Proteome
Research*

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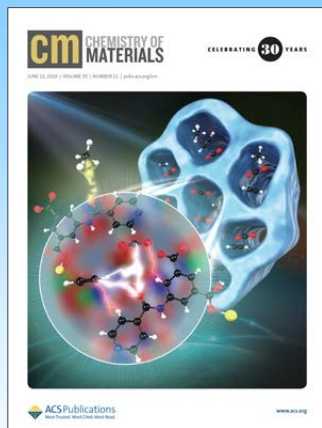


*Journal of the American
Society for Mass
Spectrometry*

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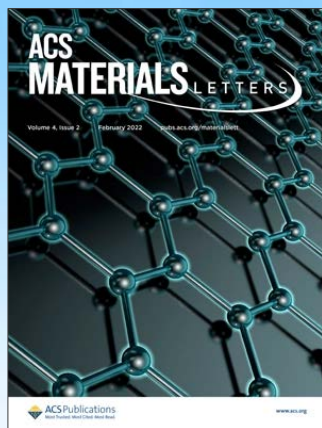
Materials Science & Engineering 材料科学与工程



*Chemistry of
Materials*

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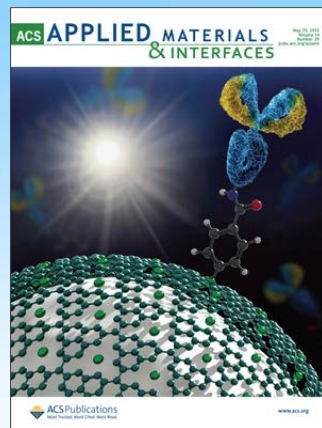
8.6



*ACS Materials
Letters*

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*ACS Applied
Materials &
Interfaces*

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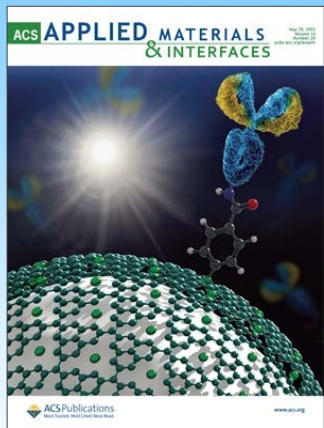


ACS Catalysis

IMPACT FACTOR

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Applied Materials Science & Engineering 应用材料系列期刊



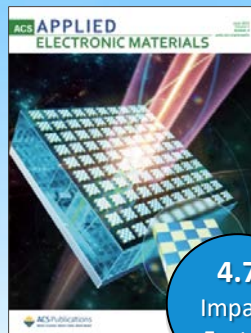
ACS Applied
Materials &
Interfaces

IMPACT FACTOR

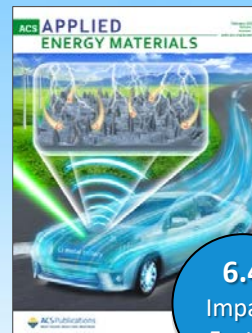
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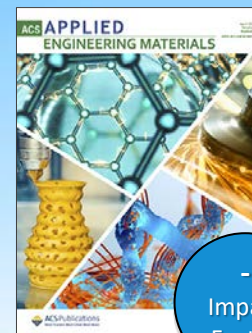
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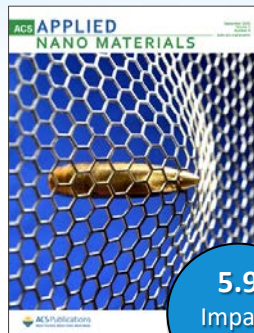
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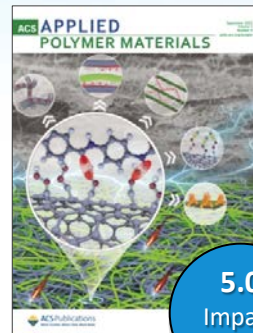
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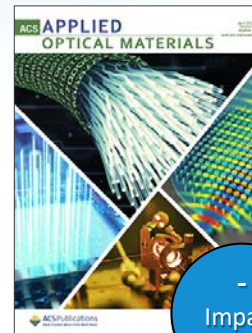
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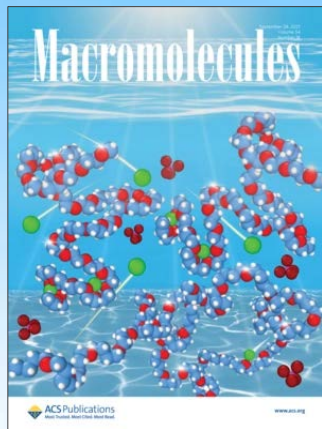


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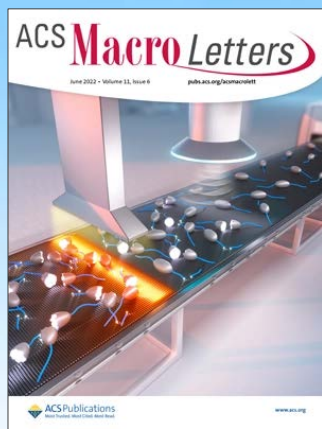
Polymer Science 高分子科学



Macromolecules

IMPACT FACTOR

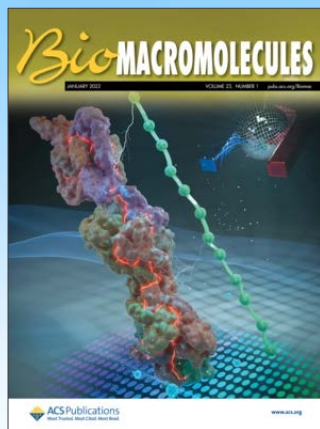
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ACS Macro Letters

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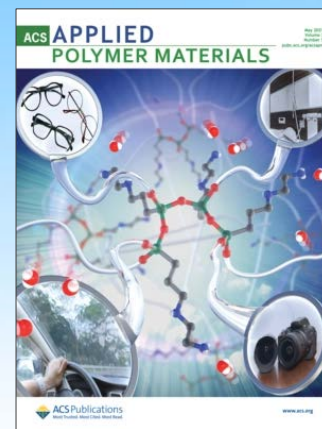
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Biomacromolecules

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ACS Applied Polymer Materials

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Nanoscience and Nanotechnology 纳米科学与技术

■ ACS NANO

出版了关于纳米结构 (纳米材料和组件、纳米器件和自组装结构) 的合成、组装、表征、理论和模拟、纳米生物技术、纳米制造、纳米科学和纳米技术的方法和工具以及自组装和定向组装的综合文章。

■ NANO LETTERS

快速报告在纳米科学和技术所有领域的基础、应用和新兴研究成果的期刊。

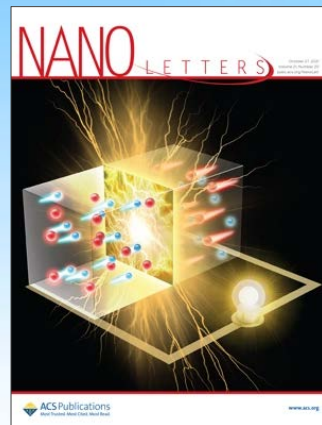
符合其范围的主要标准之一是至少融合两个不同领域或学科。



ACS Nano

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Nano Letters

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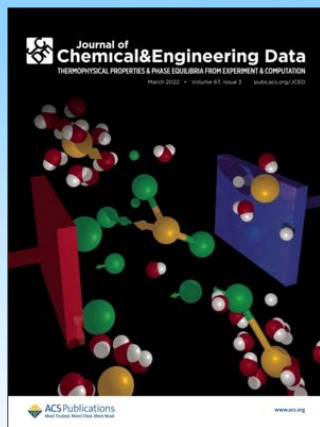
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Energy and Transportation 化工与能源



*Industrial &
Engineering
Chemistry Research*

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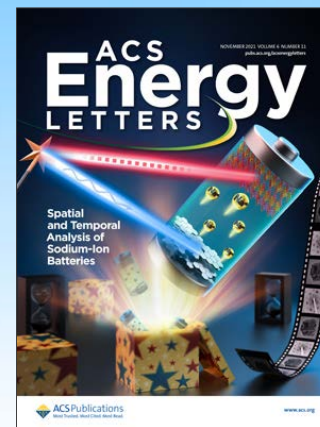
*Journal of Chemical
& Engineering Data*

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Energy & Fuels

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ACS Energy Letters

IMPACT FACTOR
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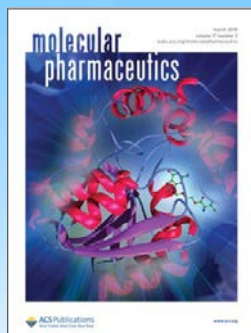
Pharmaceuticals 药物化学



药物化学领域的
顶级期刊



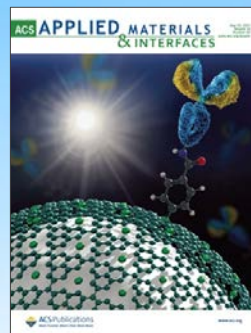
药物化学快报



分子药剂学



药物制剂



界面现象&应用



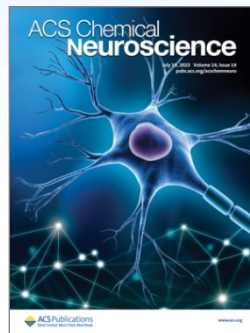
天然产物研究



毒理学



药学与转化科学

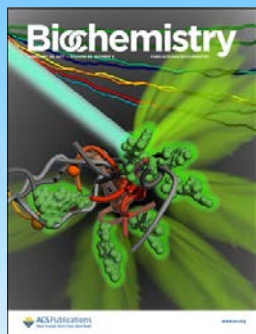


化学神经科学



传染病研究

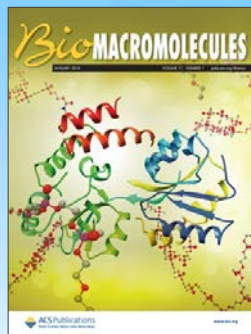
Biotechnology 生物技术



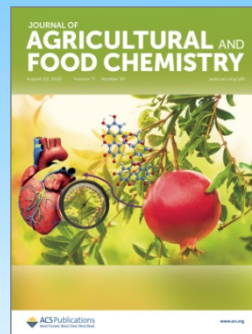
生物化学



生物共轭化学



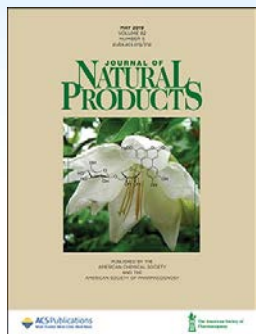
生物大分子



农业&食品科学



生物材料



天然产物研究



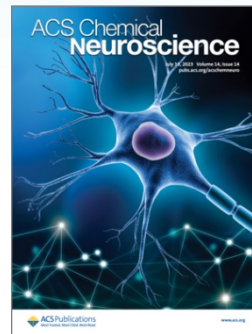
蛋白质组学



合成生物学

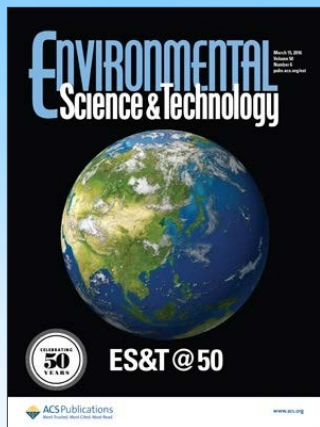


化学生物学



化学神经科学

Environmental Science 环境科学与技术



*Environmental
Science &
Technology*

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11.4



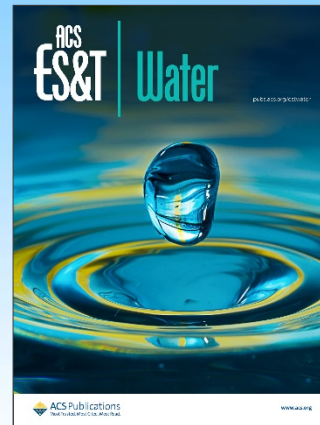
*Environmental
Science &
Technology Letters*

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*ACS ES&T
Engineering*

IMPACT FACTOR
7.1



*ACS ES&T
Water*

IMPACT FACTOR
5.3



*ACS Earth and
Space Chemistry*

IMPACT FACTOR
3.4

Education, Healthcare & Safety 化学教育, 健康与安全

Journal of Chemical Education

化学教育期刊 JCE 创刊于1924年, 是世界上首屈一指的化学教育期刊杂志。

作为化学教育领域和机构的期刊资源, 内容通常涉及了化学课程内容, 化学实验设计, 教学方法和化学教育学。

ACS Chemical Health & Safety

期刊内容包括化学品安全与风险评估, 安全教育及培训, 安保流程, 实验室及化学品储存布局, 紧急响应和计划, 有害材料, 新生污染物, 法规要求和执行, 人为因素, 法规更新解释, 实验室事故及教训。



Journal of Chemical Education

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ACS Chemical Health & Safety

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超星发现

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ACS 数据库主页 pubs.acs.org

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B

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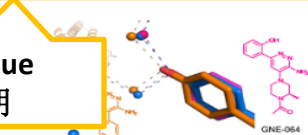
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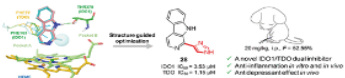
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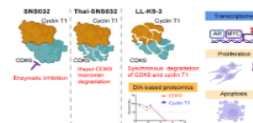
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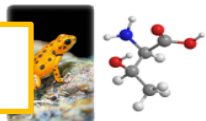


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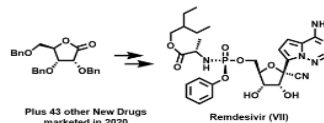
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AND	A AND B AND C 等同于 A B C	同时包含字段 A B C 的数据 用于 查准 ，缩小范围，空格默认为“AND”
OR	A OR B OR C 至少含有其中一个字段	至少包含 A B C 其中一个字段的数据 用于 查全 ，检索同义词
NOT	A B NOT C 排除某个特定的字段	检索同时包含字段 A 和 B，但不包含 C 用于 排除 ，当不需要字段 C 出现
符号	举例	意义和作用
*	cata*	零个或多个字符 ：catalysis, catalyzed, ...
?	palla?ium	只代表一个字符 ：palladium
“ ”	“A B”	精确检索某个特定词组 如果没有“ ”，相当于 A AND B

Case Study 检索案例：钯催化偶联反应

**NOBEL PRIZE
IN CHEMISTRY 2010**
颁发给三位化学家
理查德·赫克
根岸英一
铃木章

钯催化偶联反应是偶联反应的一个大类，以金属钯化合物作为催化剂，它是均相催化剂的研究和应用的活跃领域。

C&EN
news of the week
OCTOBER 11, 2010 EDITED BY WILLIAM G. SCHULZ & LAUREN K. WOLF

NOBEL PRIZE IN CHEMISTRY
AWARDS: Three chemists share prize for palladium-catalyzed cross-couplings

NOBEL LAUREATES garner medals minted in gold, but it was work with another noble metal—palladium—that earned three chemists the big prize this year. Richard F. Heck, Ei-ichi Negishi, and Akira Suzuki were jointly awarded the 2010 Nobel Prize in Chemistry “for palladium-catalyzed cross-couplings in organic synthesis.” Along with their medals, the three chemists will also share \$1.5 million.

Palladium-catalyzed cross-coupling reactions, in which the metal is used to catalyze the formation of carbon-carbon bonds, are widely used to make complex molecular structures. They have been employed to make materials, pharmaceuticals, and other biologically active compounds.

VERSATILITY Heck, Negishi, and Suzuki couplings have been used to make various fine chemicals.

Me = methyl

Heck reactions
DVS-bis-BCB (electronic resin monomer)

Negishi coupling
Serotonin agonist

Suzuki coupling
Boscaldil (fungicide)

“This is a very exciting day for organic chemistry,” comments Stephen L. Buchwald, a chemistry professor at Massachusetts Institute of Technology. “This is a well-deserved award that is long overdue. It is hard to overestimate the importance of these processes in modern-day synthetic chemistry. They are the most used reactions by those in the pharmaceutical

uses Pd to wed an aryl halide with an olefin. “It’s turned out to be something of value to the chemistry community,” Heck says of the reaction that bears his name.

In 1977, Negishi, who is now 75 and the Herbert C. Brown Distinguished Professor of Organic Chemistry at Purdue University, used Pd to catalyze couplings of organoboron reagents with organohalides. Two years later, Suzuki, who is 80 and currently a chemistry professor at Japan’s Hokkaido University, began developing a Pd-catalyzed coupling of organoboron compounds with organohalides.

“The key word here is versatility,” said Negishi, when describing his chemistry to reporters during an early-morning phone call on the day of the announcement. “One of our dreams is to be able to synthesize any organic compound of importance, whether it is a medically important compound or important from the point of view of materials science.”

He likened Pd-catalyzed cross-couplings to the Grignard reaction, a carbon-carbon bond-forming reaction developed by Victor Grignard, the 1912 Nobel Laureate in Chemistry. “The Grignard reaction made possible the synthesis of a wide variety of organic com-

pounds,” Negishi told reporters. “We came up with a totally different method that not only complements but also surpasses in versatility Grignard chemistry.”

“The award recognizes fundamental chemistry at its best,” says American Chemical Society President and Purdue University professor Joseph S. Francisco. “The beauty of this work is that these cross-couplings are

Heck
Negishi
Suzuki

Chem. Eng. News 2010, 88, 41, 7

赫克反应

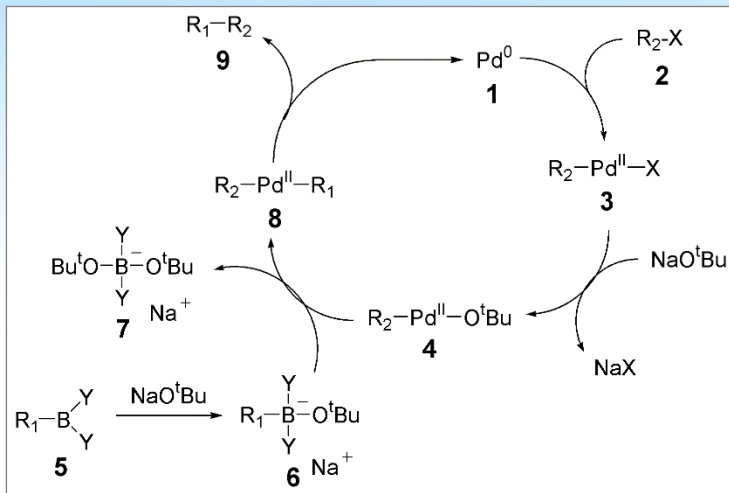
Heck Reaction

根岸英一反应

Negishi Reaction

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Suzuki-Miyaura Reaction



Suzuki Mechanism

Case Study 检索案例：钯催化偶联反应

NOBEL PRIZE
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颁发给三位化学家
理查德·赫克
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OCTOBER 11, 2010 EDITED BY WILLIAM G. SCHULZ & LAUREN K. WOLF

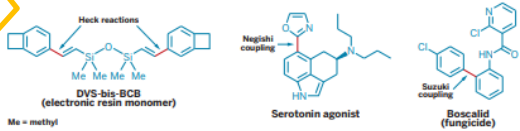
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Negishi coupling
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Suzuki coupling
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Heck



Negishi



Suzuki

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Chem. Eng. News 2010, 88, 41, 7

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反应产生盐或盐样产物:
卤化锌, 卤化锡, 卤化硅

例如:

Heck 反应: 烯烃与芳卤偶联

Suzuki 反应: 芳卤与烷基硼酸偶联

Stille 反应: 卤代烃与有机锡偶联

Hiyama 偶联反应: 卤代烃与有机硅偶联

Sonogashira 偶联反应: 芳卤与炔烃偶联

Negishi 偶联反应: 卤代烃与有机锌偶联

Buchwald-Hartwig 胺化反应: 芳卤与胺偶联

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Search: Palladium-Catalyzed Cross-Coupling

Diarylmethanol
Derivatives
With
Diborylmethane
作为反应底物

Article

Palladium-Catalyzed Cross-Coupling Reaction of Diarylmethanol Derivatives with Diborylmethane

Kento Asai, Masahiro Miura, and Koji Hirano*

The Journal of Organic Chemistry 2022, 87, 11, 7436-7445 (Article)

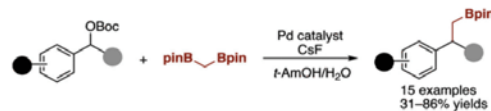
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DOI: 10.1021/acs.joc.2c00715

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Palladium-Catalyzed Cross-Coupling of *N*-Sulfonylaziridines with Boronic Acids

Megan L. Duda and Forrest E. Michael*

Journal of the American Chemical Society 2013, 135, 49, 18347-18349 (Communication)

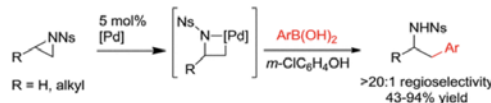
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Thioacetates
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作为反应底物

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Palladium-Catalyzed Cross-Coupling of Benzyl Thioacetates and Aryl Halides

Krista M. Wager and Matthew H. Daniels

Organic Letters 2011, 13, 15, 4052-4055 (Letter)

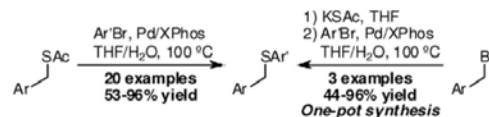
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Palladium-Catalyzed Cross-Coupling Reactions of Organoboron Compounds

Norio, Miyaura and Akira, Suzuki

Chemical Reviews 1995, 95, 7, 2457-2483 (Article)

Publication Date (Print): November 1, 1995

DOI: 10.1021/cr00039a007

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Ligand-Controlled Regioselectivity in Palladium-Catalyzed Cross-Coupling Reactions

Franziska Schoenebeck* and K. N. Houk*

Journal of the American Chemical Society 2010, 132, 8, 2496-2497 (Communication)

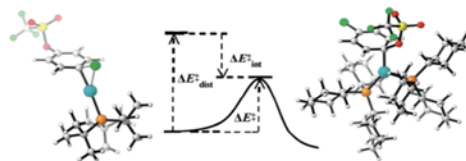
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C(sp³)-H 芳基化

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Garrett P. R. Freure, Eric A. Skrotzki, Jean-Danick E. Lavertu, and Stephen G. Newman*

ACS Catalysis 2021, 11, 19, 12258-12263 (Letter)

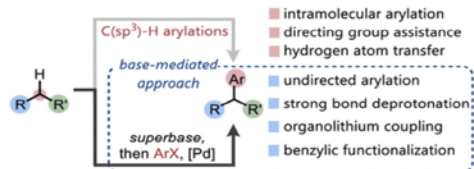
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ABSTRACT

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Patrick Pfaff, Kusal T. G. Samarasinghe, Craig M. Crews*, and Erick M. Carreira*

Cite this: ACS Cent. Sci. 2019, 5, 10, 1682–1690
Publication Date: September 17, 2019
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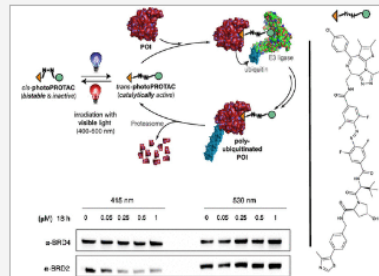
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Abstract
摘要

Off-tissue effects are persistent issues of modern inhibition-based therapies. By merging the strategies of photopharmacology and small-molecule degraders, we introduce a novel concept for persistent spatiotemporal control of induced protein degradation that potentially prevents off-tissue toxicity. Building on the successful principle of bifunctional all-small-molecule Proteolysis Targeting Chimeras (PROTACs), we designed photoswitchable PROTACs (**photoPROTACs**) by including *ortho*-F₄-azobenzene linkers between both warhead ligands. This highly bistable yet photoswitchable structural component leads to reversible control over the topological distance between both ligands. The *azo-cis*-isomer is observed to be inactive because the distance defined by the linker is prohibitively short to permit complex formation between the protein binding partners. By contrast, the *azo-trans*-isomer is active since it can engage both protein partners to form the necessary and productive ternary complex. Importantly, due to the bistable nature of the *ortho*-F₄-azobenzene moiety employed, the photostationary state of the **photoPROTAC** is persistent, with no need for continuous irradiation. This technique offers reversible on/off switching of protein degradation that is compatible with an intracellular environment and, therefore, could be useful in experimental exploration of biological signaling pathways—such as those crucial for oncogenic signal transduction. Additionally, this strategy may be suitable for therapeutic intervention to address a variety of diseases. By enabling reversible activation and deactivation of



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引言

Materials & Methods

材料和方法

Results

结果

Discussion

讨论

Conclusion

结论

Abbreviations

缩写

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作者信息

Acknowledgment

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参考文献

Introduction

Proteins reshape their function in response to environmental changes through allosteric process in which two distinct sites within a protein or protein complex are functionally regulated enzymes. effector binding at a distal site alters the thermodynamic and/or kinetic reaction at the active site. (3) The transfer of chemical information between the two sites is mediated by structural (4) and/or dynamical (5) changes that generally make accessible conformation characteristic of the enzyme active state. (6,7) To attain such a catalytic binding finely tunes the enzyme dynamic conformational ensemble by reshaping the relative conformational states and/or the time scales of structural fluctuations and conformational bidirectional communication between distal sites occurs at the ternary complex, i.e., when substrate are bound at their respective sites, and propagates through dynamic network interactions. (9,10) Capturing the time evolution of the allosteric activation of enzymes at ternary complex involves deciphering the interplay of fast and slow conformational dynamics substrate binding. (11) The transient nature of both the ternary complex and the allosteric undergoing turnover hampers the structural and dynamic characterization of allosteric identification of functionally relevant states. (12-17) It is therefore not surprising that this remains hidden for several enzymes.

Allosteric regulation operating in the model enzyme imidazole glycerol phosphate synthase (IGPS) from *Thermotoga maritima* has been investigated from structural and dynamical perspectives. (18-30) IGPS is a heterodimeric enzyme belonging to class I glutamine amidotransferases (GATase) that encompasses the catalytic interplay between HisH and HisF subunits (Figure 1). HisH catalyzes glutamine hydrolysis producing glutamate and ammonia. The HisF cyclase monomer couples the ammonia produced by HisH, which migrates through an internal tunnel, with N-[(5-phosphoribulose-5-phosphoribulose)formimino]-5-aminoimidazole-4-carboxamide ribonucleotide (PRFAR). The latter also acts as the allosteric effector for the reaction occurring in HisH. The binding of PRFAR, ca. 30 Å far away from the HisH active site, enhances 4500-fold the basal glutaminase activity of IGPS, while the substrate affinity is only moderately altered. (30)

Figure 1



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- Results
- Discussion
- Conclusions
- Methods
- Supporting Information
- Author Information
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Movie S2: accelerated molecular dynamics simulations: sp-Gln substrate binding in the HisH active site (MP4)
Movie S3: accelerated molecular dynamics simulations: sp-Gln substrate binding in IGPS (global view) (MP4)
Movie S4: accelerated molecular dynamics simulations: allosteric activation of IGPS in the ternary complex (MP4)

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Reversible Spatiotemporal Control of Induced Protein Degradation by Bistable PhotoPROTACs

K Pfaff^{1,2}, Kusal T. G. Samarasinghe^{2,3}, Craig M. Crews^{2,3,4} and Erick M. Carreira¹

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²Department of Molecular, Cell, and Developmental Biology, Yale University, New Haven, CT 06511, United States

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⁴Department of Pharmacology, Yale University, New Haven, CT 06511, United States

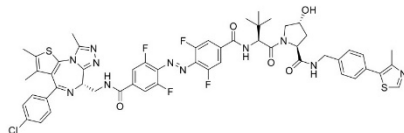
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活化化合物
命名, 编号
结构式
合成步骤

活化化合物
表征分析
Rf, NMR, IR,
ESI-HRMS

(2S,4R)-1-((S)-2-(4-((E)-4-(((S)-4-(4-chlorophenyl)-2,3,3-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl)methyl)carbamoyl)-2,6-difluorophenyl)diazenyl)-3,5-difluorobenzamido)-3,3-dimethylbutanoyl)-4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide (photoPROTAC-1)



JQ-1 amine **18** (10.5 mg, 28.0 μ mol, 1.00 equiv) and acid **S4** (21.4 mg, 28.0 μ mol, 1.00 equiv) were dissolved in anhydrous DMF (0.28 mL, 0.1 M). DIPEA (12 μ L, 85 μ mol, 3.00 equiv) and HATU (11.3 mg, 30.0 μ mol, 1.05 equiv) were added to the reaction mixture at room temperature. After 2 hours, the reaction mixture was quenched by addition of sat. aq. NaHCO₃ and the aq. phase was extracted three times with EtOAc. The combined org. layers were washed with brine and dried over sodium sulfate. Residual DMF and tetramethylurea were removed by lyophilization after freezing in a water/dioxane mixture. The crude product was further purified by flash column chromatography (94% EtOAc/4% iPrOH/2% H₂O) to afford photoPROTAC-1 as an orange oil (16.0 mg, 14.0 μ mol, 51%).

Rf = 0.36 (85% EtOAc/10% iPrOH/5% H₂O).

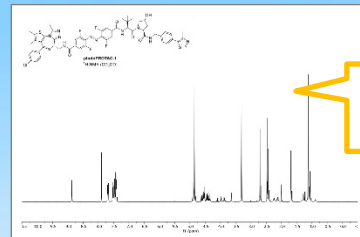
¹H NMR (500 MHz, CD₃OD) δ = 8.87 (s, 1H), 7.70 (dd, J = 5.1, 1.6 Hz, 2H), 7.67 (dd, J = 5.1, 1.6 Hz, 2H), 7.52 (d, J = 8.5 Hz, 2H), 7.48 (d, J = 8.5 Hz, 2H), 7.44 – 7.40 (m, 4H), 4.91 (s, 1H), 4.65 – 4.50 (m, 4H), 3.87 (dd, J = 13.6, 7.0 Hz, 2H), 4.35 (d, J = 15.4 Hz, 1H), 3.98 (d, J = 11.0 Hz, 1H), 3.87 (dd, J = 11.0, 3.8 Hz, 1H), 2.71 (s, 3H), 2.47 (s, 3H), 2.43 (s, 3H), 2.29 – 2.22 (m, 1H), 2.15 – 2.09 (m, 1H), 1.69 (s, 3H), 1.13 (s, 9H).

¹³C NMR (126 MHz, CD₃OD) δ = 174.4, 172.0, 166.8, 166.7, 166.5, 157.4, 156.1, 155.3, 153.0, 152.2, 149.0, 140.3, 139.2, 138.1, 138.1, 134.3, 133.5, 133.4, 133.3, 133.3, 132.0, 132.0, 131.5, 131.4, 131.3, 130.4, 129.8, 129.0, 113.4, 113.1, 71.1, 60.9, 59.9, 58.2, 56.8, 43.7, 42.9, 39.0, 37.2, 27.1, 15.8, 14.4, 12.9, 11.6.

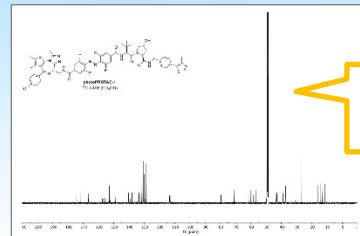
¹⁹F NMR (471 MHz, CD₃OD) δ = -121.4, -121.5.

IR: 3322, 2925, 28855, 1665, 1533, 1427, 1343, 1243, 1090, 1047, 967, 843.

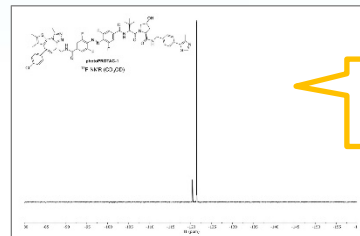
ESI-HRMS: calcd. for C₃₂H₃₅ClF₆N₁₁O₅S₂ [M+H]⁺ 1108.3135, found 1108.3144.



¹H-NMR



¹³C-NMR



¹⁹F-NMR

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- 53. Osuna, S. The Challenge of Predicting Distal Active Site Mutations in Computational Enzyme Design. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2021**, *11*, e1502. DOI: 10.1002/wcms.1502 [Crossref] [CAS] [Google Scholar]
- 54. Douangamath, A.; Walker, M.; Beismann-Driemeyer, S.; Vega-Fernandez, M. C.; Sterner, R.; Wilmanns, M. Structural Evidence for Ammonia Tunneling across the (B₀)₈ Barrel of the Imidazole Glycerol Phosphate Synthase Bionzyme Complex. *Structure* **2002**, *10*, 185–193. DOI: 10.1016/S0969-2126(02)00702-5 [Crossref] [PubMed] [CAS] [Google Scholar]
- 55. Ahuja, L. G.; Taylor, S. S.; Kornev, A. P. Tuning the "Violin" of Protein Kinases: The Role of Dynamics-based Allostery. *IUBMB Life* **2019**, *71*, 685–696. DOI: 10.1002/iub.2057 [Crossref] [PubMed] [CAS] [Google Scholar]
- 56. Ahuja, L. G.; Kornev, A. P.; Mclendon, C. L.; Veglia, G.; Taylor, S. S. Mutation of a Kinase Allosteric Node Uncouples Dynamics Linked to Phosphotransfer. *Proc. Natl. Acad. Sci. U.S.A.* **2017**, *114*, E931–E940. DOI: 10.1073/pnas.1620667114 [Crossref] [PubMed] [CAS] [Google Scholar]

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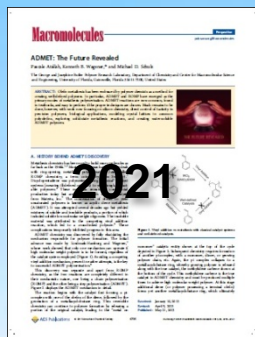
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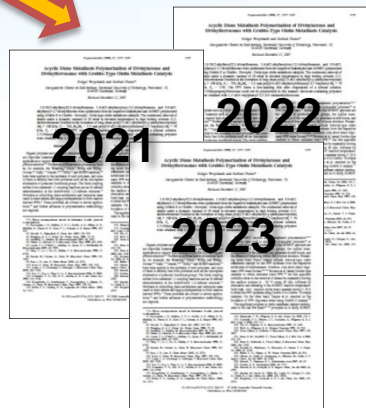
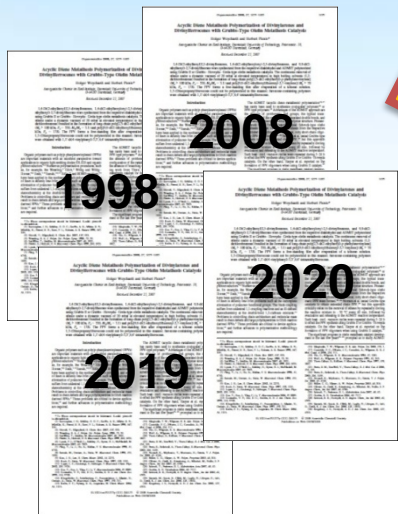


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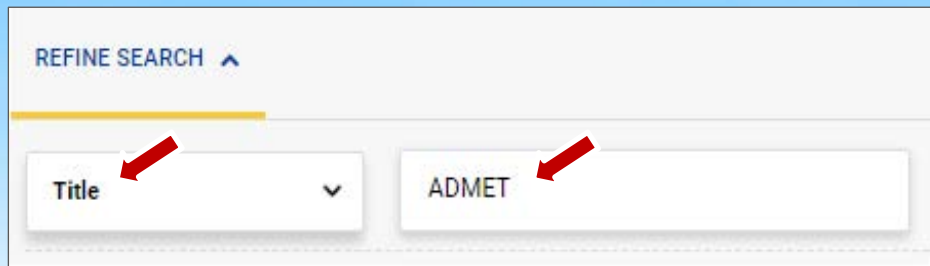
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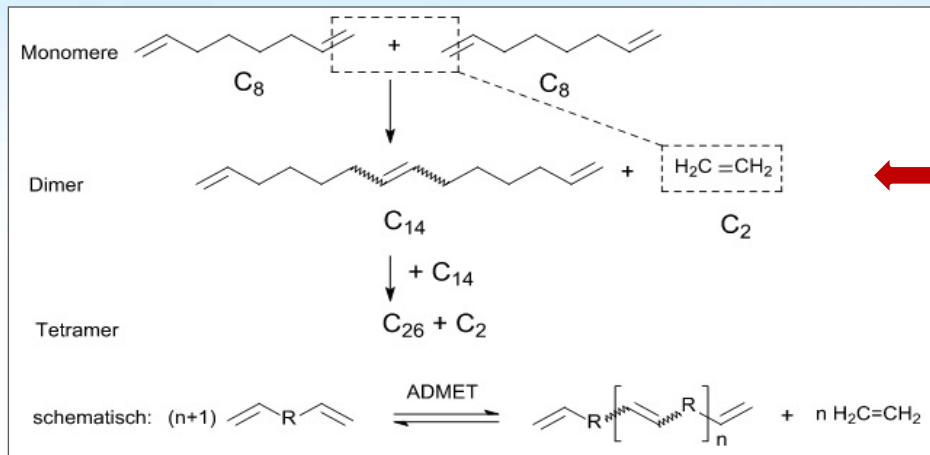
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ADMET: The Future Revealed

Farzad Afshar, Kenneth E. Wagene,* and Michael D. Schick

The George and Cynthia Baker Wilson Research Laboratory, Department of Chemistry and Center for Macromolecular Science and Engineering, University of Florida, Gainesville, Florida 32611-7030, United States

ABSTRACT: Cyclic metathesis has been introduced by polymer chemists as a method for creating well-defined polymers. In particular, ADMET and ROMP have emerged as the primary routes to suitable polynorbornenes. ADMET reactions are now commonly found in textbooks, and easy to perform if the proper techniques are chosen. Much remains to be done, however, with such new living/active chain chemistry, direct control of tacticity in polynorbornene polymer synthesis, controlling crystal lattices in common polynorbornenes, exploring suitable metathesis reactions, and creating noncyclic ADMET polymers.



A. HISTORY BEHIND ADMET'S DISCOVERY

Metathesis chemistry has long been used to build macromolecules as far back as the 1940s.^{1,2} Most of the times that this deals with ring-opening metathesis polymerization (also called ROMP chemistry, a term coined by Tim Saegusa).³ Direct metathesis was first proposed using classical metathesis systems (osmium tetroxide) to yield long, linear, isotactic polymers.⁴ These materials were in commercial production but had very poor molecular weight distributions (MWDs).⁵ The combination of olefins to yield controlled polymers is known as cyclic olefin metathesis (COMET). It was attempted several decades ago but yielded mixtures of soluble and insoluble products, a portion of which included odd chain end units and light oligomers. The insoluble material was attributed to the competing ring addition reaction, which led to a crosslinked polymer.⁶ These complications impeded further progress in this area.

ADMET chemistry was discovered by fully elucidating the mechanism responsible for polymer formation. The initial advance was made by Livshits, Harkness, and Wagene,⁷ who first showed that only one mechanism can operate if high molecular weight polymers to be formed regardless of the catalyst system employed (Figure 1). Avoiding a competing ring addition mechanism proved to be an alternative, a key step to successful ADMET polymerizations.⁸

This discovery was separate and apart from ROMP chemistry, as the two reactions are completely different in their mechanistic nature, one being a chain polymerization (ROMP) and the other being a step polymerization (ADMET). Figure 2 displays the ADMET mechanism in detail.

The reaction begins with the catalyst first forming a pi-complex with the olefin of the diene, followed by the generation of a noncyclic olefinic ring. This noncyclic olefinic ring can continue to polymerize to form a portion of the original catalyst, leading to the "closed-loop"




Figure 1. Ring addition to metathesis with classical catalyst systems and well-defined catalyst.

noncyclic" catalyst only chains at the top of the cycle depicted in Figure 2. Subsequent olefinic ring formation of another pi-complex, with a necessary, slow, ring-opening polymer chain exit. Again, the pi-complex collapses to a noncyclic olefinic ring, whereby growing polymer is allowed along with the free catalyst, the noncyclic olefinic chain does at the bottom of the cycle. The noncyclic olefinic chain is the true catalyst in ADMET chemistry and used to produce multiple times to achieve high molecular weight polymers. At this stage additional diene (or polymer possessing a terminal olefin) forms yet another noncyclic olefinic ring, which ultimately

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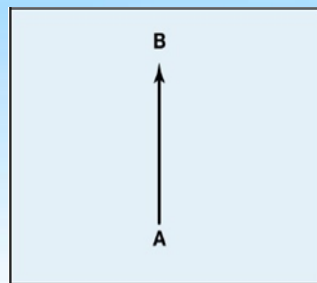
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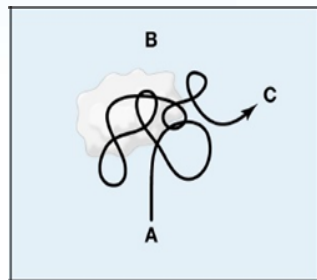
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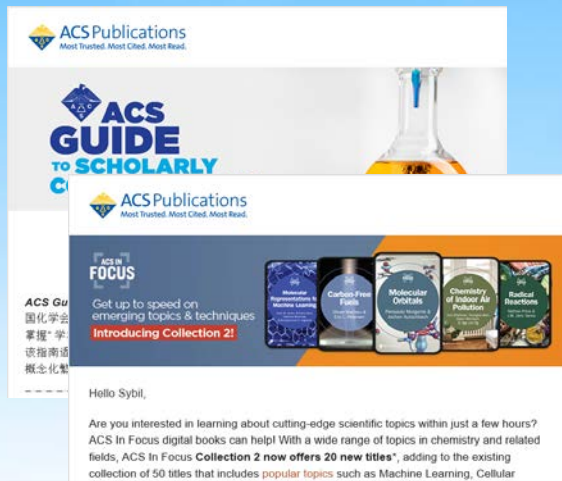
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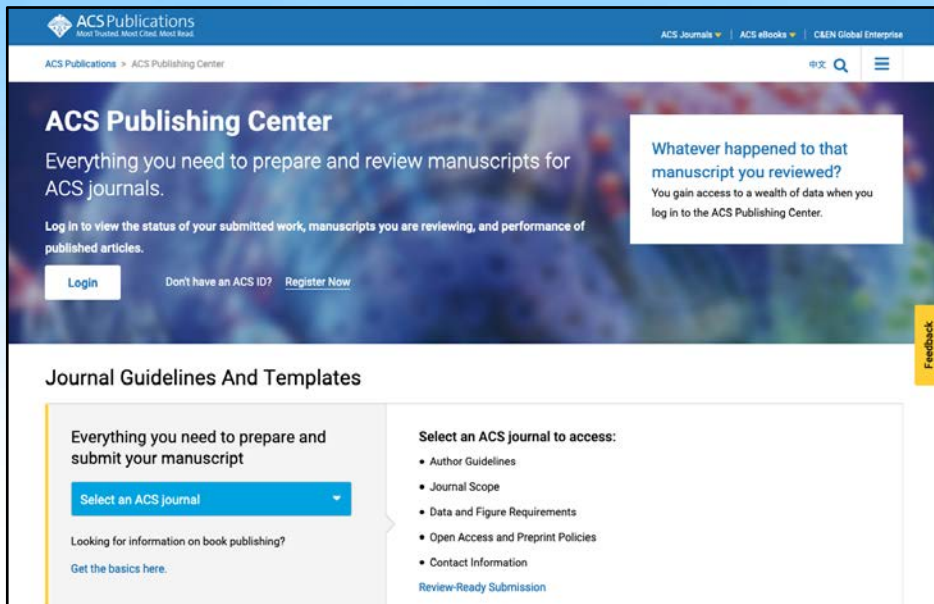
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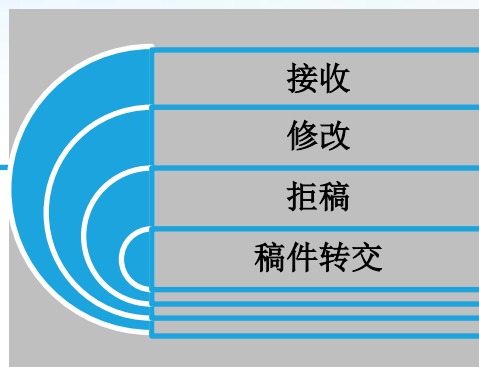
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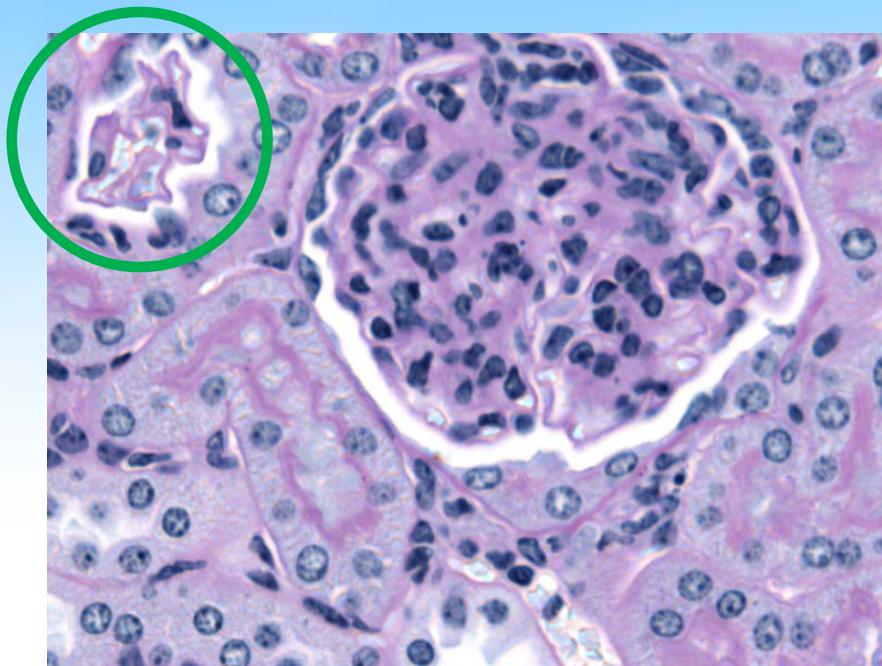
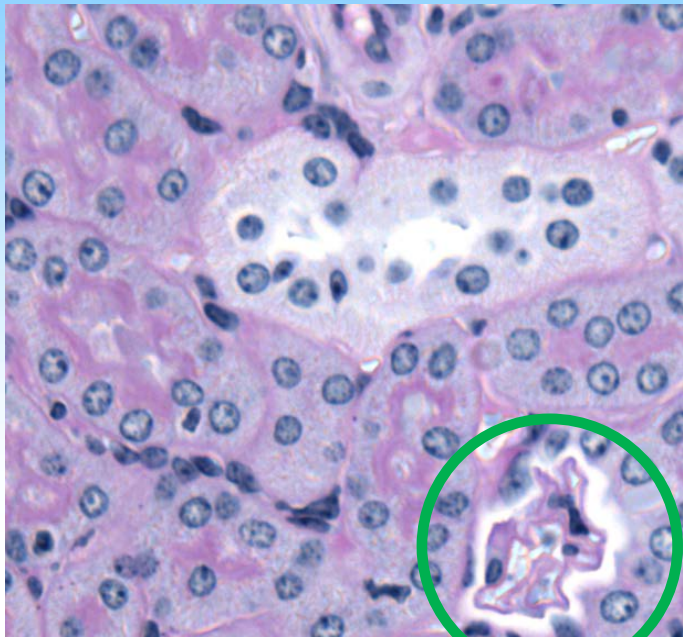
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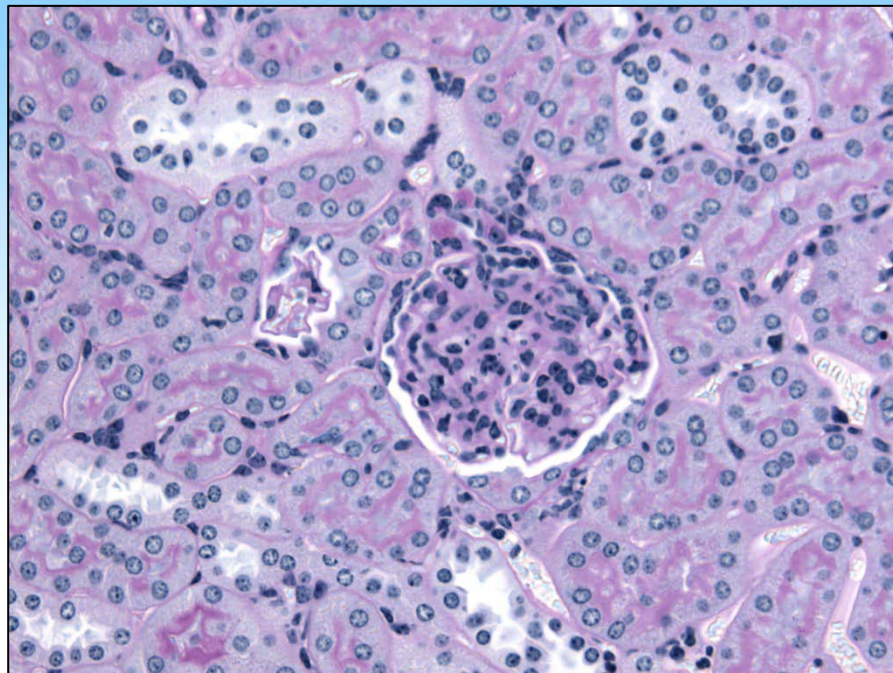


Most scientists regarded the new streamlined peer-review process as 'quite an improvement.'

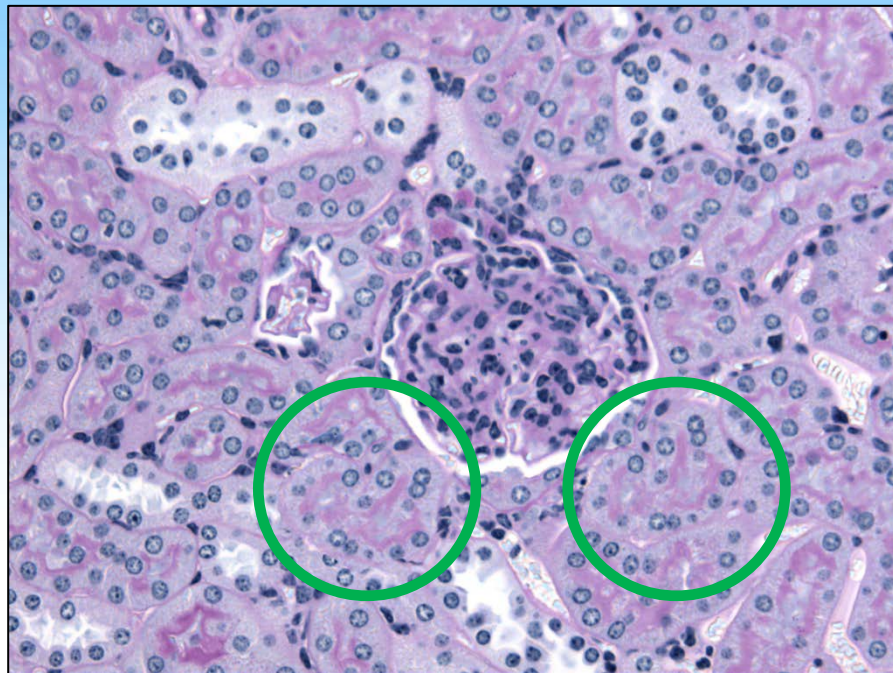
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*** ADDITION / CORRECTION** This article has been corrected. View the notice.

Photocatalytic Gas Phase Reactions


Murielle Schreck and Markus Niederberger*

Cite This: *Chem. Mater.* 2019, 31, 3, 597-618
Publication Date: January 16, 2019
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Correction to Photocatalytic Gas Phase Reactions

Murielle Schreck and Markus Niederberger*

Cite This: *Chem. Mater.* 2019, 31, 4, 1469
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cm CHEMISTRY OF MATERIALS | < Correction to Photocatalytic Gas Phase Reactions > | 🔍 ☰

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 CO₂ 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 ▾

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 CO₂ over Ru/Silicon Nanowire Catalysts with Visible and Near-Infrared Photons. *Adv. Sci.* 2014, *1*, 1400001, DOI: 10.1002/adv.201400001 [[Crossref](#)], [[CAS](#)] [[Google Scholar](#)]

This publication has no figures.

What has been corrected?

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Mechanical Reconfiguration of Stereoisomers
Kelly M. Wiggins[†], Todd W. Hudnall[†], Qilong Shen[‡], Matthew J. Kryger[‡], Jeffrey S. Moore[‡]
and Christopher W. Bielawski^{†*}

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Cite This: *J. Am. Chem. Soc.* 2010, 132, 10, 3256-3257
Publication Date: February 18, 2010
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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 CH₃CN solutions of high-molecular-weight derivatives (M_N > 25 kDa) to sonication at 0 °C resulted in >05%

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Retraction

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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.

撤稿说明

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。



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- B. ACS Nano
- C. Energy & Fuels
- D. Chemical Reviews

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- B. catalyzed
- C. cata*
- D. cata?



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