ACS Publications
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课程签到码

# ACS Publications：跨学科化学的学术资源

From American Chemical Society (ACS)
CALIS 第二十二届引进数据库培训周

赵璟  iGroup China

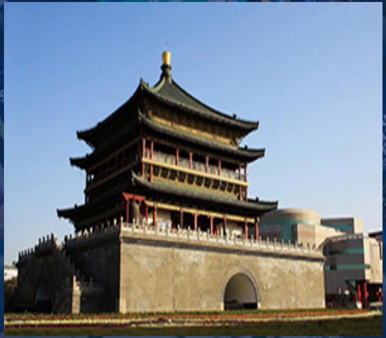
2024 年 5 月 14 日

# 关于 iGroup China

iGroup 成立于 1983 年，在全球 20 多个国家和地区都设有办事处，是亚太地区最大的学术科研资源提供商之一，独家负责各领域科研数据库的销售和服务。

在中国，iGroup China代表ACS（美国化学会）、Science（美国科学促进会）、APS（美国物理学会）、SPIE （国际光学工程学会） 、SAE（国际自动机工程师学会）等四十多家国际学术出版社，助力高校机构、政府机构及企业的研发和创新，帮助科研人员获取有价值的学术文献，了解最新的科学成果。

公司网址：www.igroup.com.cn



# American Chemical Society

课程签到码

**ACS 美国化学会是世界上最大的科技学会之一**

- 成立于 1876 年
- 学会总部位于美国华盛顿特区
- 全球遍布 140 多个国家，超过 15 万会员
- 出版高品质的专业科学期刊

# ACS Publications 数据库出版物资源

https://pubs.acs.org

ACS 数据库出版物资源包含：

- ACS Journals 70 多种电子期刊
- ACS eBooks 1600 多本电子图书
- ACS In Focus 系列电子图书
- C&EN 化学与工程新闻杂志
- 试剂标准手册
- 学术交流指南

全库资源超过 140 万篇文章，涵盖了 20 多个与化学相关的研究领域。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新闻杂志


ACS Reagent Chemicals
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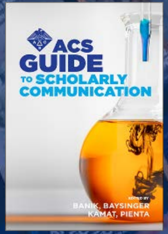


ACS Guide
学术交流指南

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# ACS Journals 学术期刊

*https://pubs.acs.org*

课程签到码

已出版 70 多种高品质的专业科学期刊，发表化学各个领域的前沿研究成果。

ACS 期刊的影响因子中位数为 5.3。

美国化学会志 JACS 保持在化学领域里是被引用次数最多的期刊。

根据 2023 年 JCR Citation Reports：
ACS期刊的总被引用次数超过 440 万。

ACS 的全文访问量来自中国的占比最高。

# WE COVER EVERY ASPECT OF CHEMISTRY

课程签到码

ACS 的很多期刊是跨学科的，涵盖了广泛的研究领域课题的前沿研究成果。研究需要寻求的答案可能不仅限于一种 ACS 期刊。

ACS 期刊涵盖的学科领域包括但不限于：

| | | | |
|---|---|---|---|
| 无机化学 | 物理化学 | 能源 | 农业与食品化学 |
| 有机化学 | 理论与计算化学 | 催化 | 生物与药物化学 |
| 有机金属化学 | 高分子科学 | 材料科学 | 化学工程与工业化学 |
| 分析化学 | 化学教育 | 纳米科学 | 地球、空间与环境化学 |

# Journal of the American Chemical Society

Impact Factor: 15.0 | Citations: 580,144

课程签到码


**Editor-in-Chief**
Erick M. Carreira
from ETH Zürich

美国化学会志 **JACS** 创刊于1879年，是美国化学会的第一本期刊，是学会的旗舰刊。

JACS 期刊每年发表大约2500篇科研文章，每周出版一期。它是化学领域里被引用次数最多的跨学科化学期刊，发表化学各个领域里顶尖的基础和应用研究成果。

**期刊收录研究方向：化学，化学综合**

Indexed in: CAS, SCIE, Scopus, PubMed, etc.

# Chemical Reviews

Impact Factor: 62.1 | Citations: 231,674

课程签到码


2022 IMPACT FACTOR

**62.1**

**Chemical Reviews** 是世界杰出的期刊之一，涵盖化学学科所有的研究领域，它为有机化学，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。

**Chemical Reviews** 是化学期刊大类里影响因子最高的期刊。

**期刊收录研究方向：化学，化学综合**

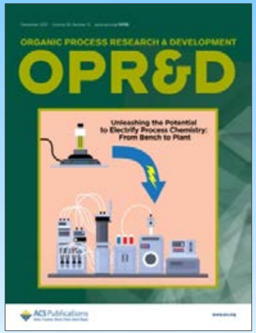
Indexed in: CAS, SCIE, Scopus, PubMed, etc.

# Basic Science of Chemistry 化学的基础科研领域

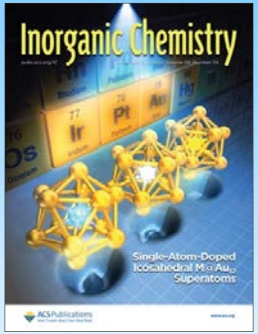
课程签到码


有机化学

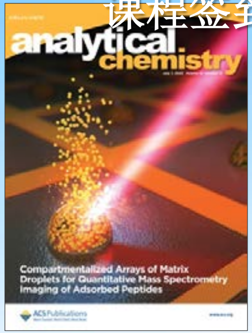

有机快报




有机工艺



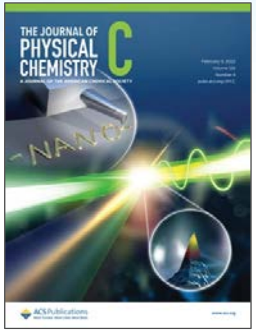

无机化学



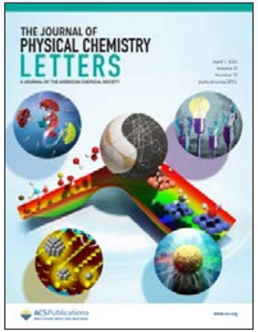

分析化学


物理化学 A


物理化学 B




物理化学 C

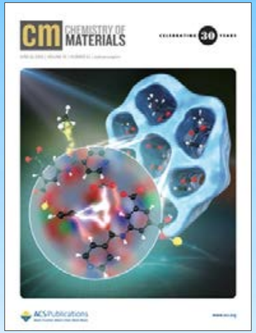



物理化学快报

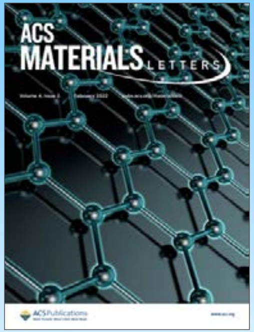

化工研究

# Materials Science & Engineering 材料科学与工程

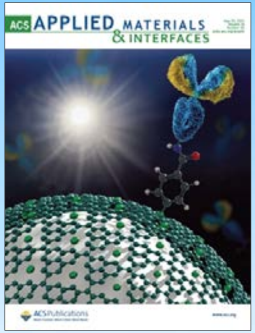
课程签到码




材料化学

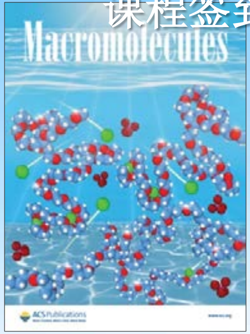



材料快报



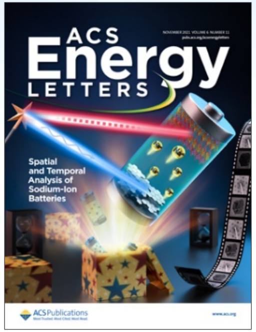

应用材料&界面


纳米材料



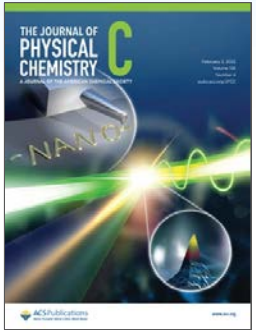

高分子材料


生物材料

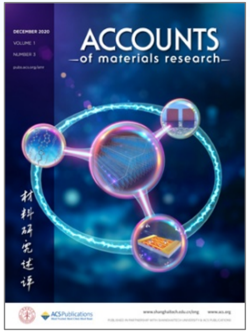



能源材料快报


催化科学




材料物理化学



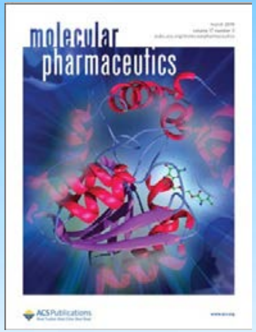

材料综述

# Pharmaceuticals 药物化学

课程签到码

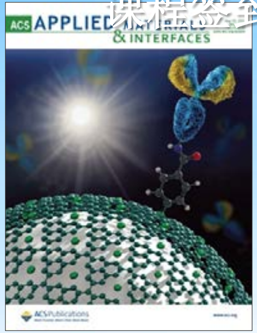

药物化学领域
的顶级期刊


药物化学快报




分子药剂学


药物制剂

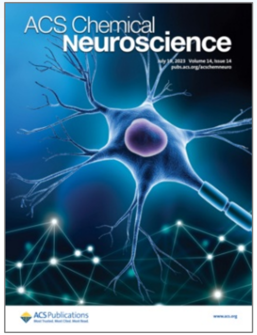



界面现象&应用


天然产物研究


毒理学


药学与转化科学




化学神经科学

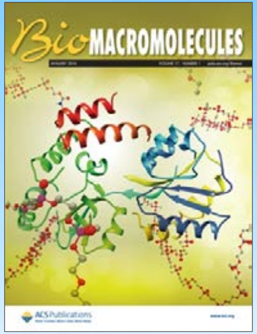

传染病研究

# Biotechnology 生物技术

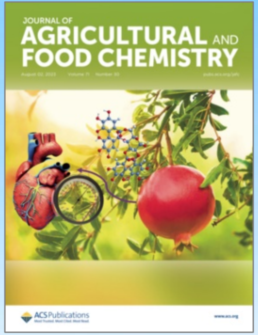
课程签到码


生物化学


生物共轭化学




生物大分子




农业&食品科学

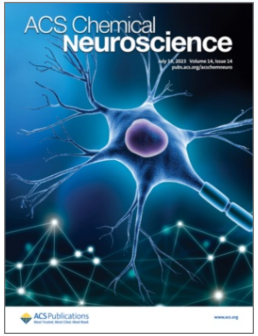

生物材料


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

课程签到码


**Environmental Science & Technology**

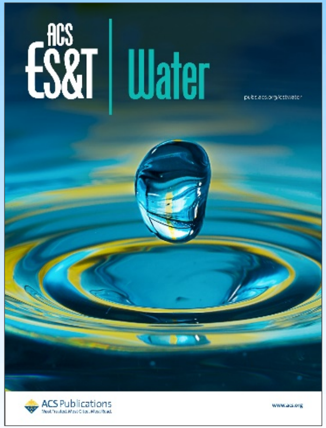
环境科学与技术


**Environmental Science & Technology Letters**

环境科学与技术快报

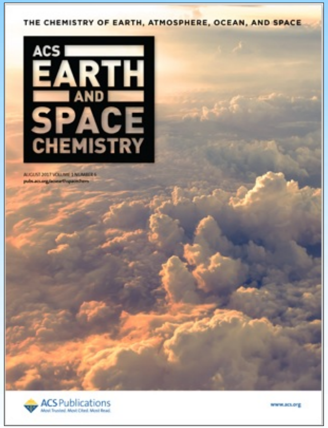

**ACS ES&T Engineering**

EST子刊: 环境工程




**ACS ES&T Water**

EST子刊: 水环境




**ACS Earth and Space Chemistry**

地球与空间化学

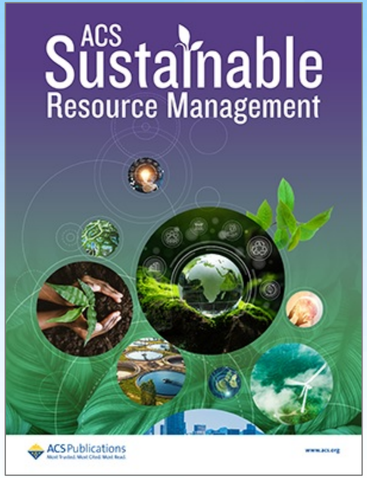
# ACS 新刊介绍  2024

课程签到码


*ACS ES&T Air*

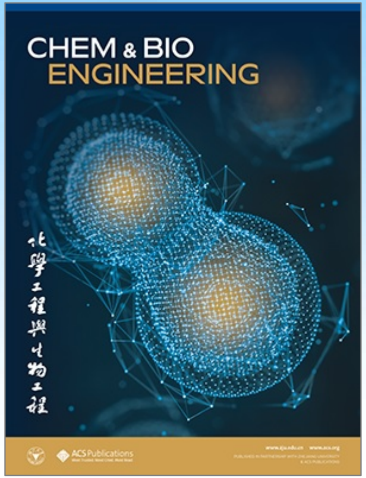
**Launched in 2024**

**EST子刊: 大气环境**




*ACS Sustainable Resource Management*

**Launched in 2024**




*Chem & Bio Engineering*

**Launched in 2024**

和浙江大学合作办刊

# Open Access Journals

美国化学会旗下的开放获取期刊总共有 15 种，分别具有不同的内容和定位。

课程签到码


*ACS Central Science*

**Launched in 2015**

IMPACT FACTOR

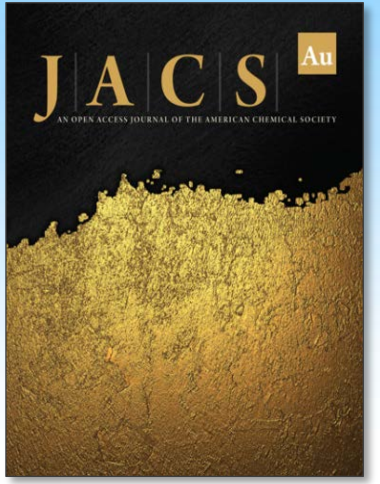
**18.2**


*ACS Omega*

**Launched in 2016**

IMPACT FACTOR

**4.1**




*JACS Au*

**Launched in 2020**

IMPACT FACTOR

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**ACS Central Science，ACS Omega，JACS Au 多学科化学期刊**

## ACS Au Journals 系列期刊

- ACS Bio & Med Chem Au
- ACS Engineering Au
- ACS Environmental Au
- ACS Materials Au
- ACS Measurement Science Au
- ACS Nanoscience Au
- ACS Organic & Inorganic Au
- ACS Physical Chemistry Au
- ACS Polymers Au


**ACS 与中国的高校及科研机构的合作期刊**

| | | |
|---|---|---|
| **Precision Chemistry** | 2023 | University of Science and Technology of China |
| **Chemical & Biomedical Imaging** | 2023 | Nanjing University |
| **Environment & Health** | 2023 | the Research Center for Eco-Environmental Sciences, CAS |

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- **ACS eBooks** 拥有超过 1,600 本专著，37,000个章节，正文章节都经过同行评审，每年大约新增 30 本新书。
- 由化学领域顶尖学者编写的专著，包括 40 多名诺贝尔奖获得者。
- ACS Symposiom Series (1974 - 至今)
- Advances in Chemistry (1949 - 1998)
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  ACS药化部门出品的制药行业年鉴

**37,000**
CHAPTERS

**1,600**
BOOKS

**41**
NOBEL LAUREATES

ACS IN
# FOCUS

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https://doi.org/10.1021/acsguide

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- 适用于广泛的学科领域，蕴含生动的多媒体视频资源和科技论文写作的指导。
- **适用人群：本科生，研究生，教师。**

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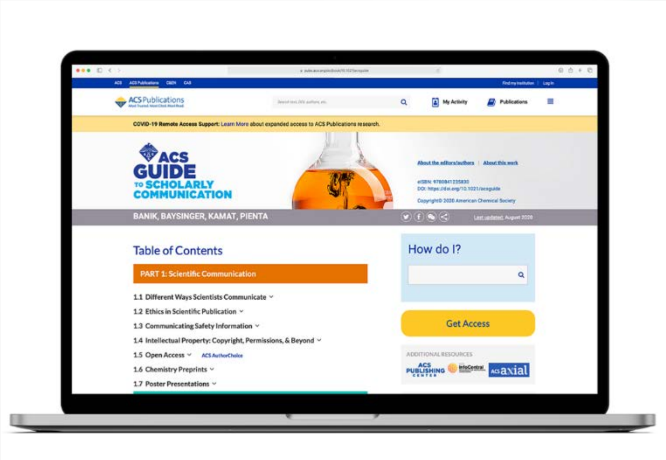

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https://pubs.acs.org/doi/book/10.1021/acsreagents

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- 提供符合本标准的化学品理化性质，详细的规格参数以及相应的测试方法，并且每年更新2次。
- 美国药典 USP 使用符合此标准的化学品用于药物测试。


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c&en
CHEMICAL & ENGINEERING NEWS

https://pubs.acs.org/journal/cgeabj

- **C&EN Global Enterprise** 是美国化学会旗下的知名杂志。
- 回溯年份自 2016 年起，每周出版一期。
- 关注化学所有领域的科技前沿动态，工业和商业信息以及政府和企业的新闻和政策等。


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# ACS 数据库平台主页 pubs.acs.org

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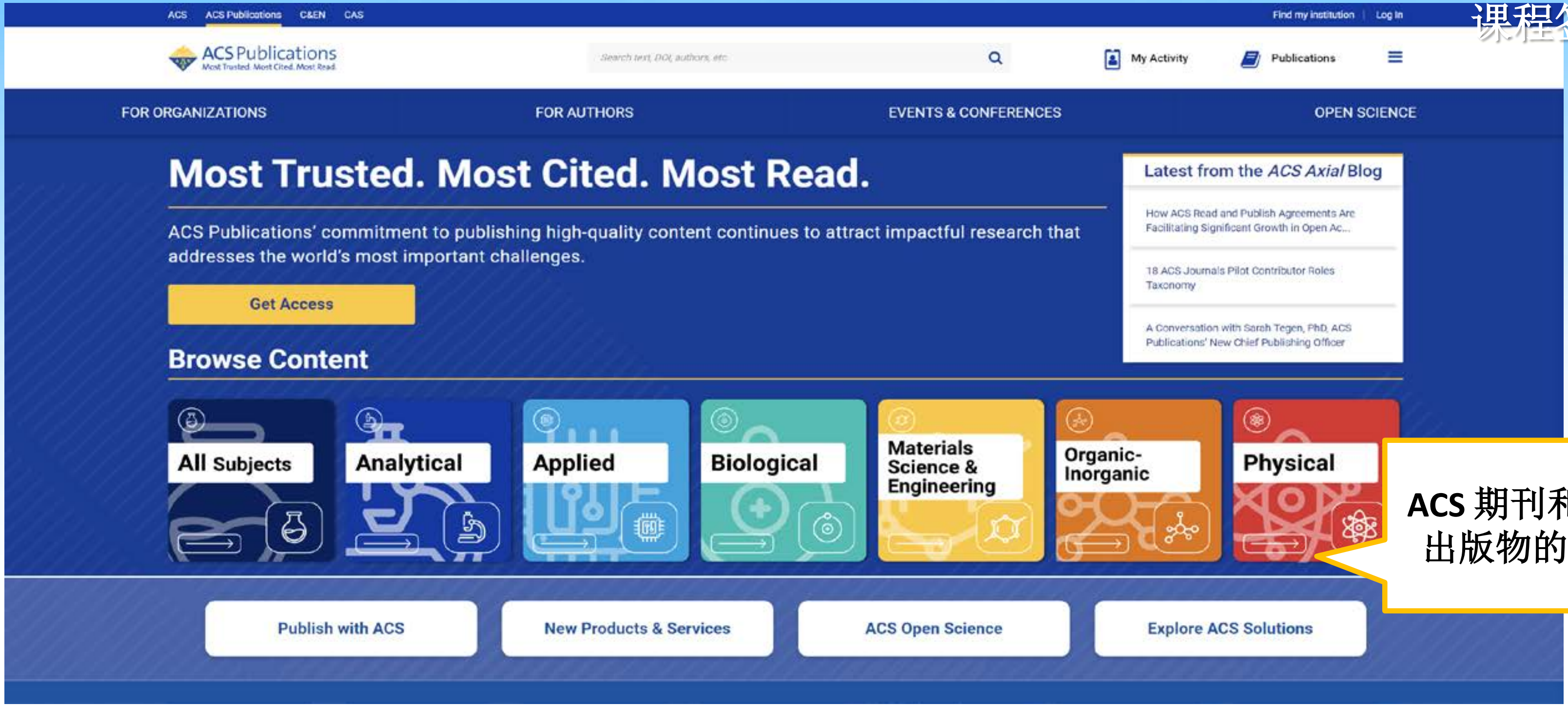


ACS 期刊和所有出版物的入口

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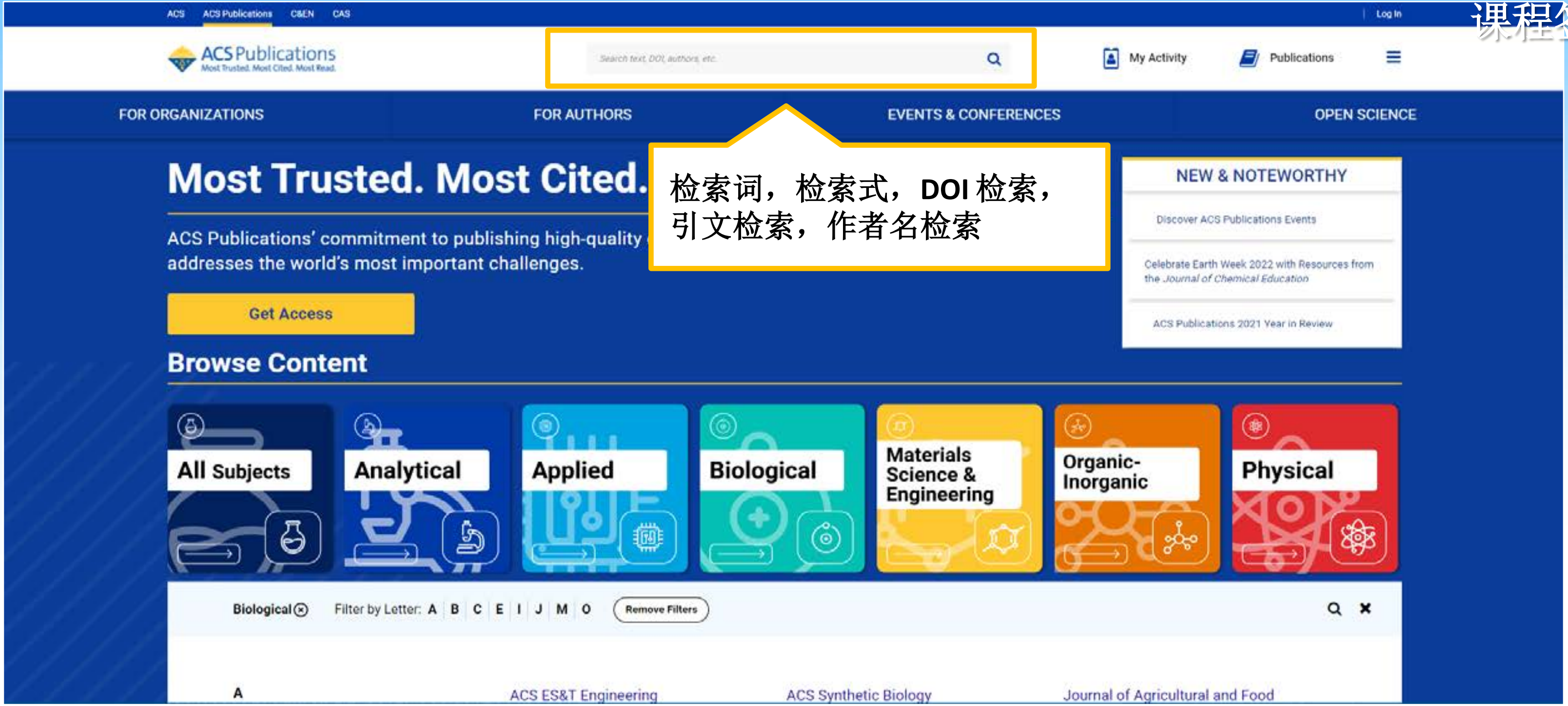


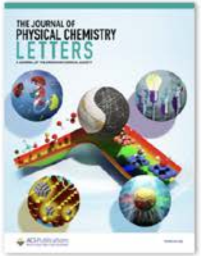

检索词，检索式，DOI 检索，
引文检索，作者名检索

# ACS Editors’ Choice 编辑良择

课程签到码

## ACS Editors' Choice

*Based on recommendations from the scientific editors of ACS Journals. See all articles.*



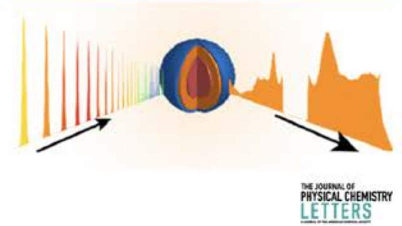

**Fluctuations in the Photoluminescence Excitation Spectra of Individual Semiconductor Nanocrystals**

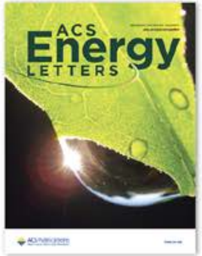
Robert C. Keitel, Raphael Brechbühler, Ario Cocina, Felipe V. Antolinez, Stefan A. Meyer, Sander J. W. Vonk, Henar Rojo, Freddy T. Rabouw, and David J. Norris*

*J. Phys. Chem. Lett.* (Article) Open Access Editors' Choice

**ACS Editors' Choice Date:** April 29, 2024

**Cite This:** *J. Phys. Chem. Lett.* 2024, 15, XXX, 4844–4850



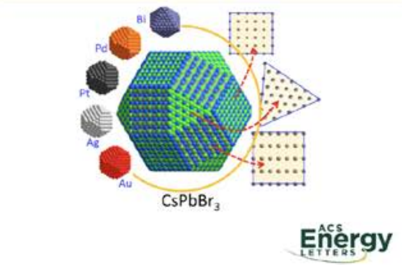

**Design Strategies for Epitaxial Metal(0)–Halide Perovskite Nanocrystal Heterostructures**

Narayan Pradhan*

*ACS Energy Lett.* (Article) Free to Read Editors' Choice

**ACS Editors' Choice Date:** April 28, 2024

**Cite This:** *ACS Energy Lett.* 2024, 9, XXX, 2378–2386

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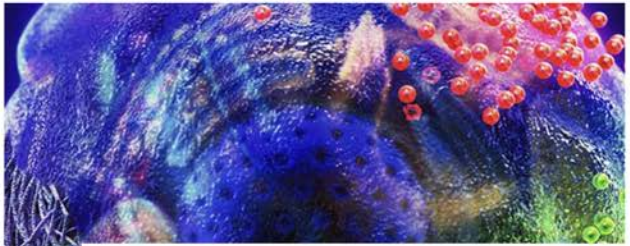
**ACS GUIDE TO SCHOLARLY COMMUNICATION**

This comprehensive guide provides the academic and publishing communities with the instruction and advice they need to master the art of scholarly communication.



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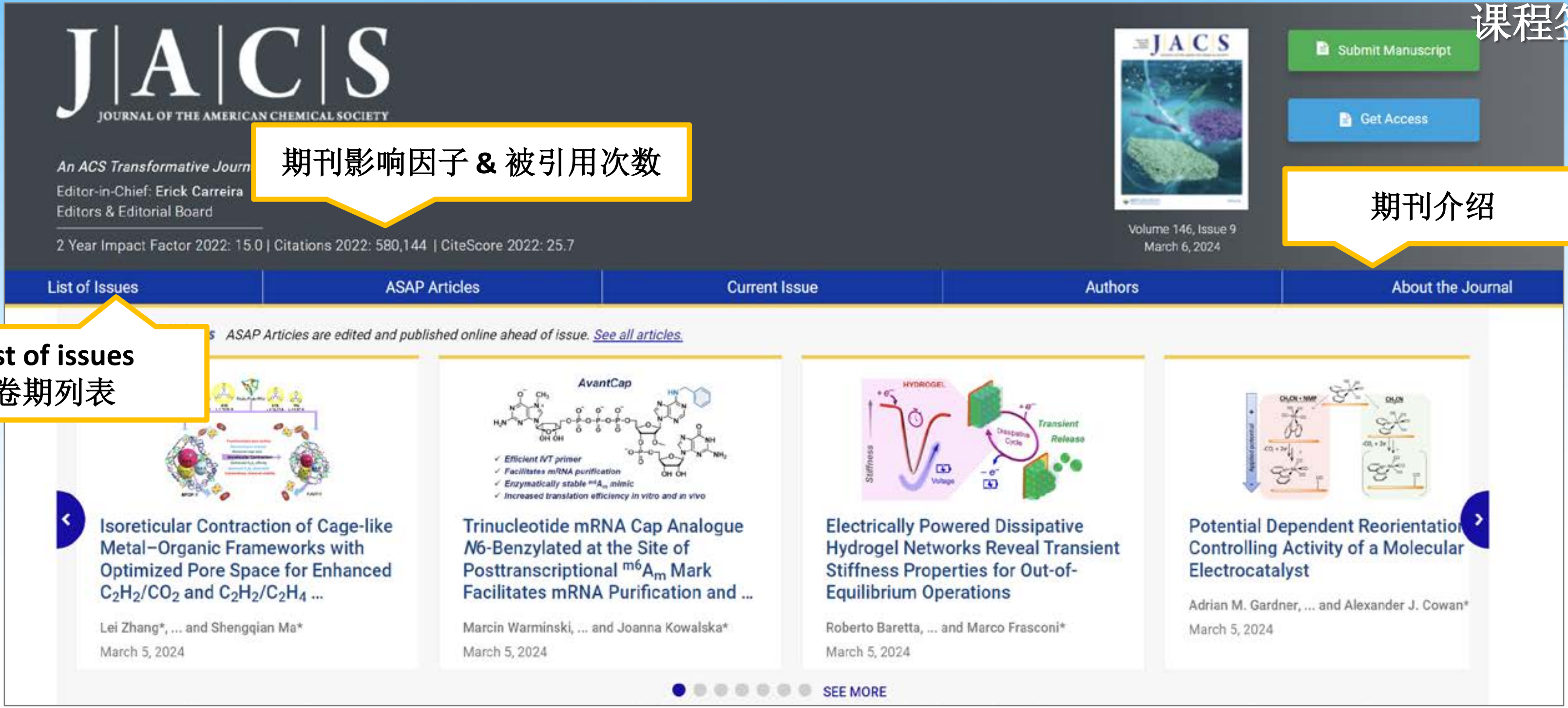


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**Reversible Spatiotemporal Control of Induced Protein Degradation by Bistable PhotoPROTACs**

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出版信息

Cite this: *ACS Cent. Sci.* 2019, 5, 10, 1682–1690
Publication Date: September 17, 2019
https://doi.org/10.1021/acscentsci.9b00713


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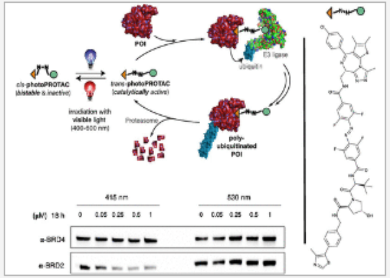
, Molecular structure, Peptides and proteins

Abstract
摘要

## Abstract

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*-$F_4$-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*-$F_4$-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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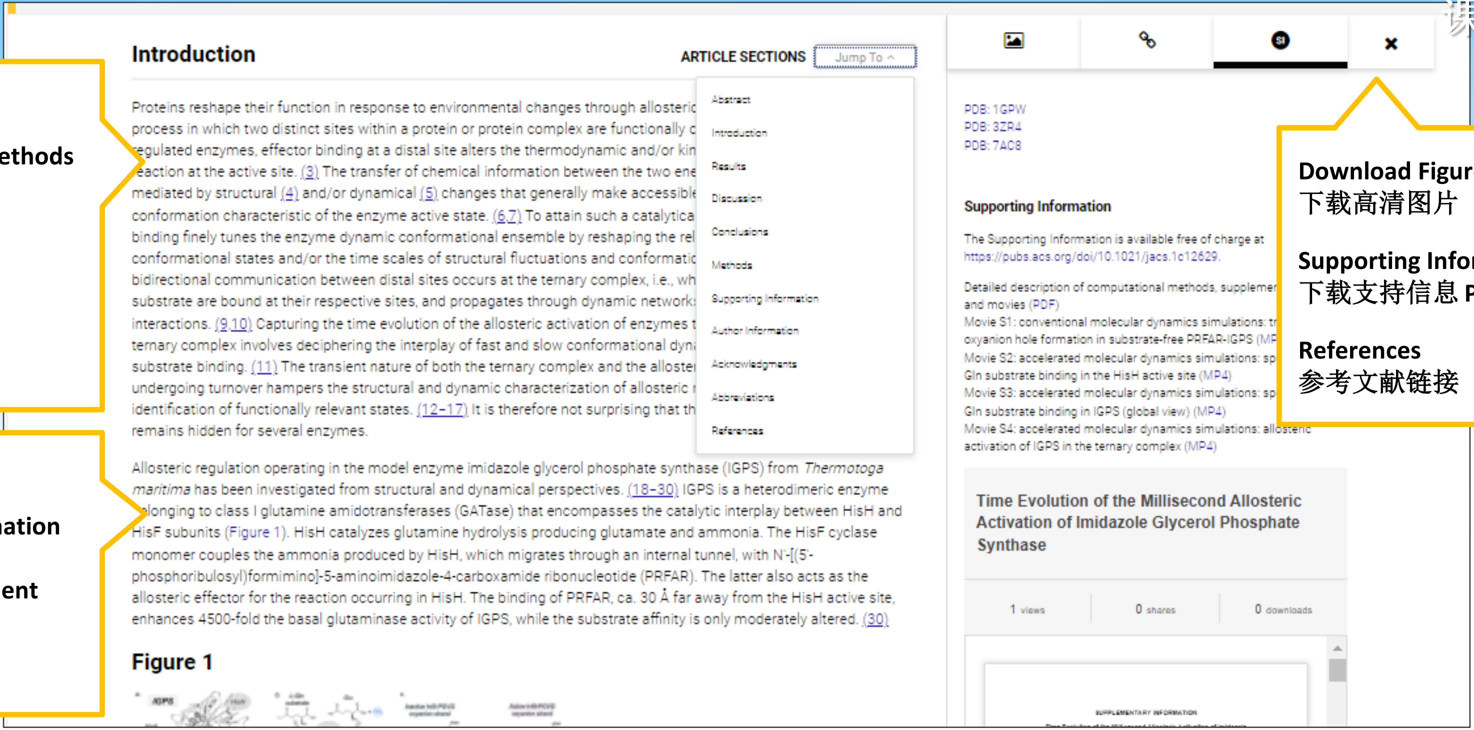

## Introduction

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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 c
regulated enzymes, effector binding at a distal site alters the thermodynamic and/or kin
reaction at the active site. (3) The transfer of chemical information between the two ene
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 catalytica
binding finely tunes the enzyme dynamic conformational ensemble by reshaping the rel
conformational states and/or the time scales of structural fluctuations and conformatic
bidirectional communication between distal sites occurs at the ternary complex, i.e., wh
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 t
ternary complex involves deciphering the interplay of fast and slow conformational dyna
substrate binding. (11) The transient nature of both the ternary complex and the alloster
undergoing turnover hampers the structural and dynamic characterization of allosteric r
identification of functionally relevant states. (12−17) It is therefore not surprising that th
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′-phosphoribulosyl)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**

PDB: 1GPW
PDB: 3ZR4
PDB: 7AC8

**Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/jacs.1c12629.

Detailed description of computational methods, supplemen
and movies (PDF)
Movie S1: conventional molecular dynamics simulations: tr
oxyanion hole formation in substrate-free PRFAR-IGPS (MP
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)

Time Evolution of the Millisecond Allosteric Activation of Imidazole Glycerol Phosphate Synthase

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**Supporting Information**
文章的支持信息描述研究工作的完整实验细节，实现可重复性。

Reversible Spatiotemporal Control of Induced Protein Degradation by Bistable PhotoPROTACs

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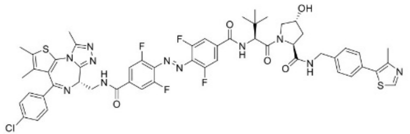
Content



**Content**
化合物，表格，实验等应以在文章中的提及顺序呈现，对应稿件中使用的编号系统。

活性化合物命名, 编号
结构式
合成步骤

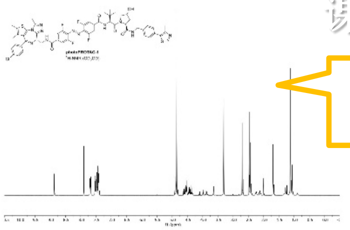
**(2S,4R)-1-((S)-2-(4-((E)-(4-((((S)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl)methyl)carbamoyl)-2,6-difluorophenyl)diazenyl)-3,5-difluorobenzamido)-3,3-dimethylbutanoyl)-4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide (photoPROTAC-1)**



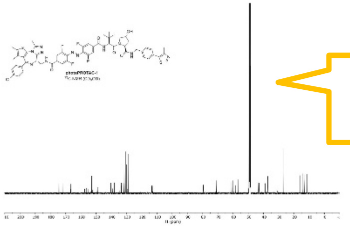
JQ-1 amine **18** (10.5 mg, 28.0 µmol, 1.00 equiv) and acid **S4** (21.4 mg, 28.0 µmol, 1.00 equiv) were dissolved in anhydrous DMF (0.28 ml, 0.1 M). DIPEA (12 µl, 85 µmol, 3.00 equiv) and HATU (11.3 mg, 30.0 µmol, 1.05 equiv) were added to the reaction mixture at room temperature. After 2 hours, the reaction mixture was quenched by addition of sat. aq. $NaHCO_3$ 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% $H_2O$) to afford **photoPROTAC-1** as an orange oil (16.0 mg, 14.0 µmol, 51%).

活性化合物表征分析
Rf, NMR, IR, ESI-HRMS

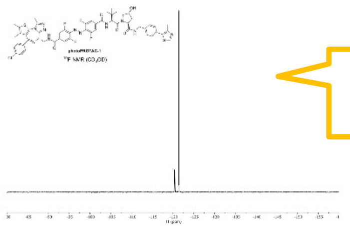
**Rf** = 0.36 (85% EtOAc/10% iPrOH/5% $H_2O$).
**$^1$H NMR** (500 MHz, $CD_3OD$) δ = 8.87 (s, 1H), 7.70 (dd, J = 5.1, 1.6 Hz, 2H), 7.67 (dd, J = 5.1, 1.6 Hz, 2H), 7.52 (d, J = 8.5 Hz, 2H), 7.48 (d, J = 8.5 Hz, 2H), 7.44 – 7.40 (m, 4H), 4.91 (s, 1H), 4.65 – 4.50 (m, 4H), …3 (dd, J = 13.6, 7.0 Hz, 2H), 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, 1H), 1.13 (s, 9H).
**$^{13}$C NMR** (126 MHz, $CD_3OD$) 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, $CD_3OD$) δ = -121.4, -121.5.
**IR**: 3322, 2925. 28855, 1665, 1533, 1427, 1343, 1243, 1090, 1047, 967, 843.
**ESI-HRMS**: calcd. for $C_{56}H_{51}ClF_4N_{11}O_5S_2$ $[M+H]^+$ 1108.3135, found 1108.3144.



$^1$H-NMR



$^{13}$C-NMR



$^{19}$F-NMR

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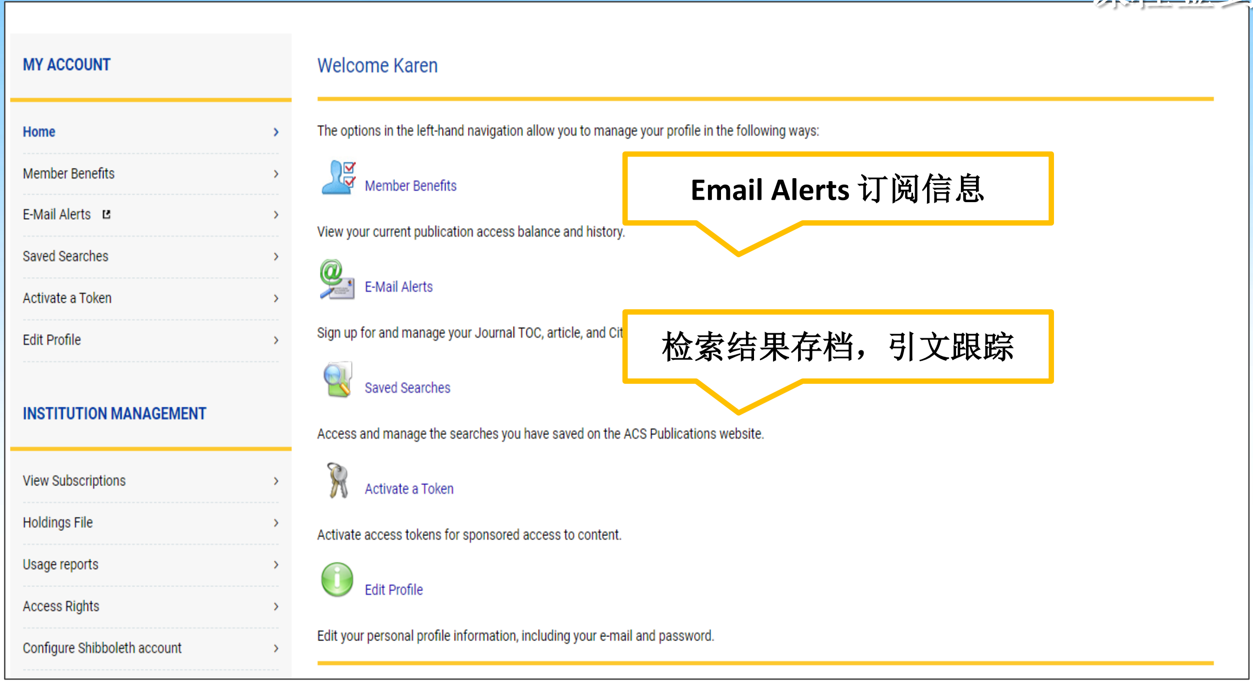

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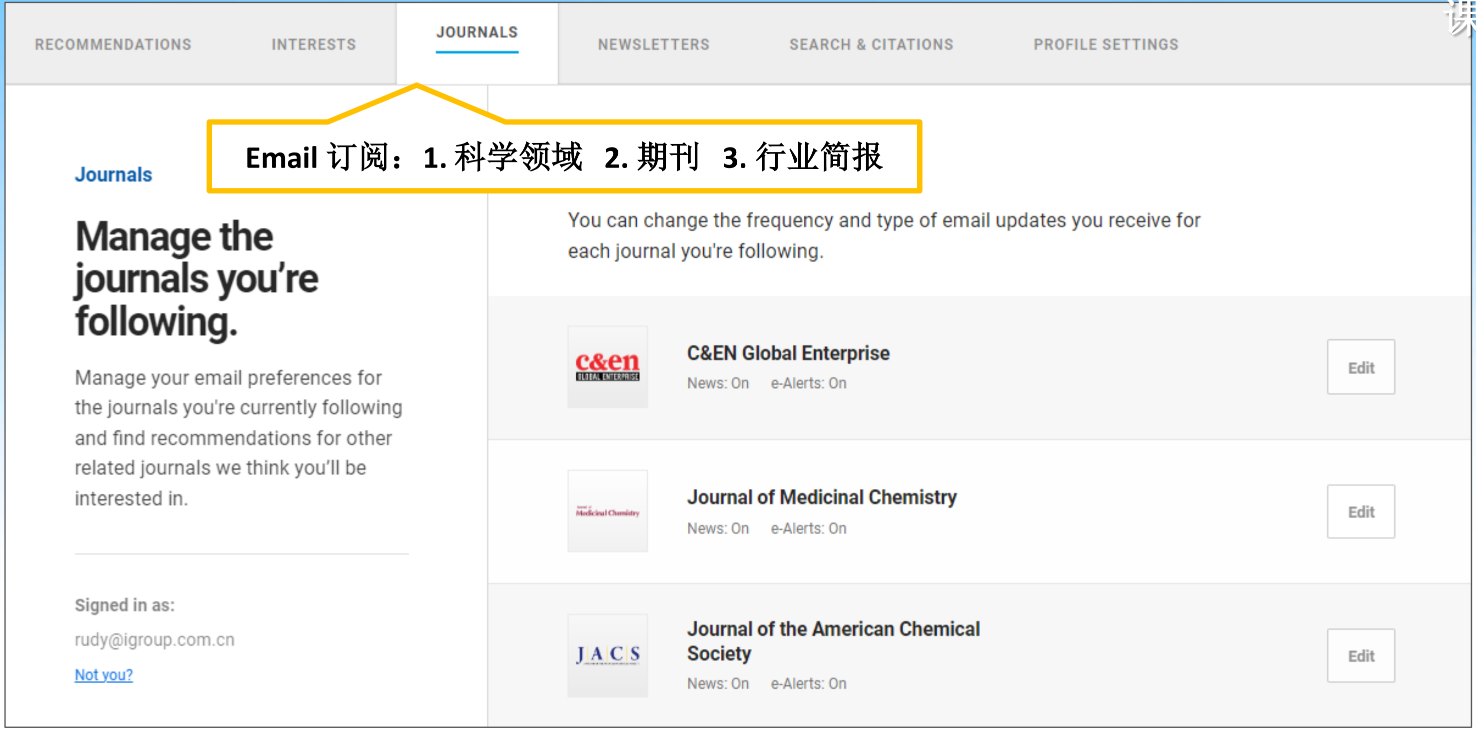

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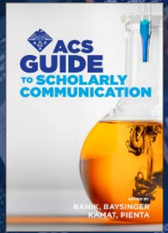


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