



НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ
УНИВЕРСИТЕТ

Библиотека

ACS PUBLICATIONS

Издания ведущего научного общества American
Chemical Society в области химических наук

Москва, 2021



ACS PUBLICATIONS

- Компания American Chemical Society издает авторитетные журналы по химии и смежным наукам: органической химии, неорганической химии, физической химии, медицинской химии, аналитической химии, биохимии, молекулярной биологии, прикладной химии и химической технологии.
- Авторитетность журналов подтверждается включением большинства из них в Web of Science и высокими значениями импакт-факторов в Journal Citation Reports.

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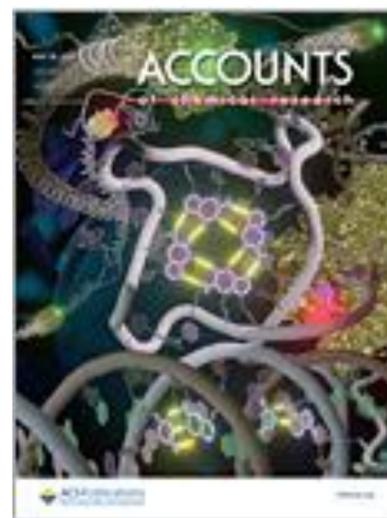


Chemical Reviews

IF 52.760

2019 JCR Ranking*: 1/171 Chemistry,
Multidisciplinary Category

Годы охвата: от 1996 до 2021 гг.



**Accounts of Chemical
Research**

IF 20.834

2019 JCR Ranking*: 7/177 Chemistry,
Multidisciplinary Category

Годы охвата: от 1996 до 2021 гг.



Analytical Chemistry

IF 6.785

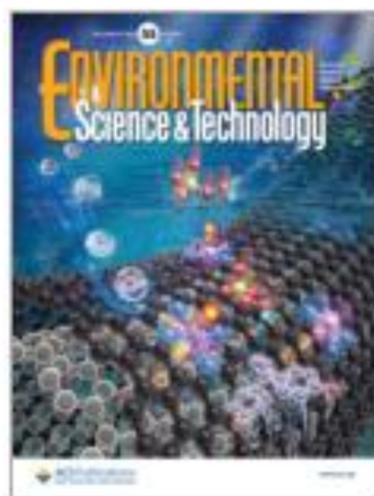
2019 JCR Ranking*: 7/86 Chemistry,
Analytical Category

Годы охвата: от 1996 до 2021 гг.

* по данным Journal Citation Report (JCR-19) от Clarivate Analytics.

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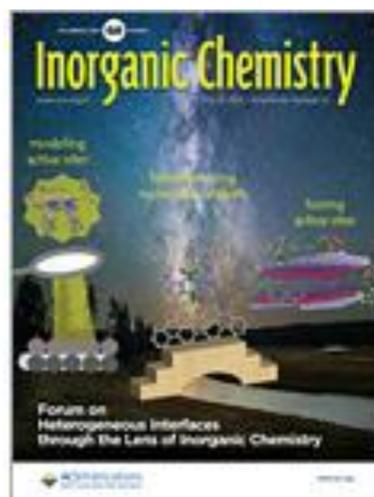


Environmental Science & Technology

IF 7.864

2019 JCR Ranking: 15/265 Environmental Sciences Category

Годы охвата: от 1996 до 2021 гг.

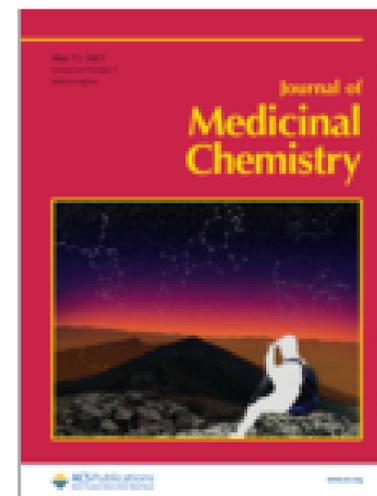


Inorganic Chemistry

IF 4.825

2019 JCR Ranking: 4/45 Chemistry, Inorganic & Nuclear Category

Годы охвата: от 1996 до 2021 гг.

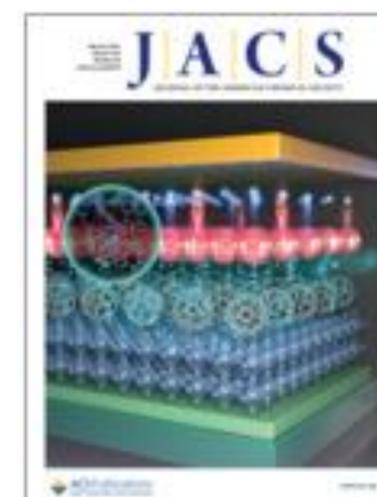


Journal of Medicinal Chemistry

IF 6.205

2019 JCR Ranking: 3/61 Chemistry, Medicinal Category

Годы охвата: от 1996 до 2021 гг.



Journal of the American Chemical Society

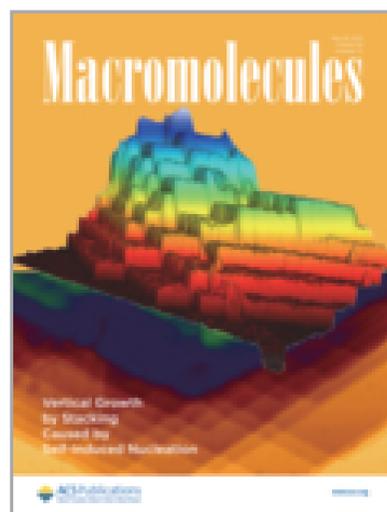
IF 14.612

2019 JCR Ranking: 13/177 Chemistry, Multidisciplinary Category

Годы охвата: от 1996 до 2021 гг.

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Macromolecules

IF 5.918

2019 JCR Ranking: 7/89 Polymer Science Category

Годы охвата: от 1996 до 2021 гг.

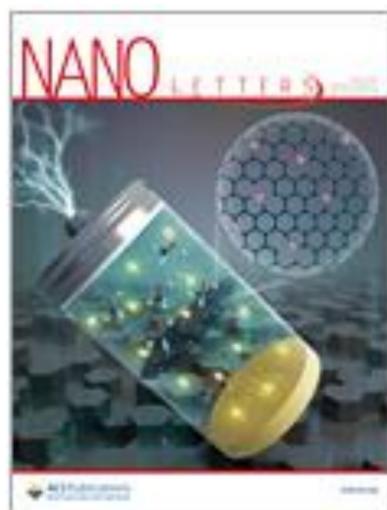


Organic letters

IF 6.091

2019 JCR Ranking: 4/57 Chemistry, Organic Category

Годы охвата: от 1996 до 2021 гг.

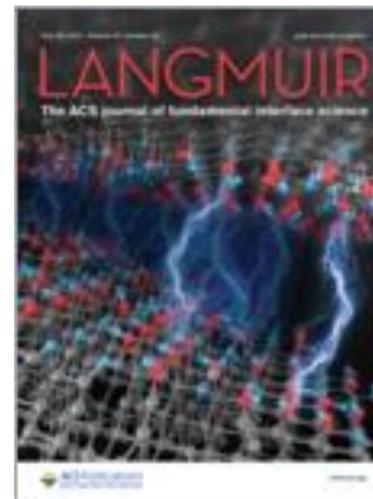


Nano Letters

IF 11.238

2019 JCR Ranking: 18/159 Chemistry, Physical Category

Годы охвата: от 1996 до 2021 гг.



Langmuir

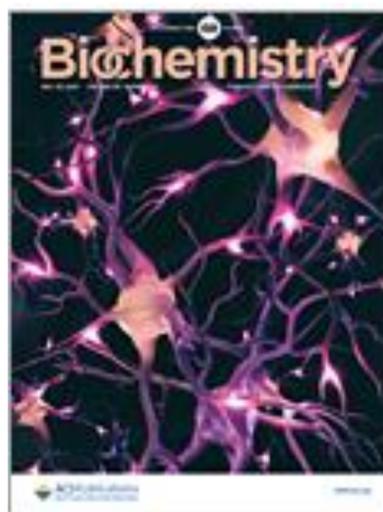
IF 3.557

2019 JCR Ranking: 107/314 Materials Science, Multidisciplinary Category

Годы охвата: от 1996 до 2021 гг.

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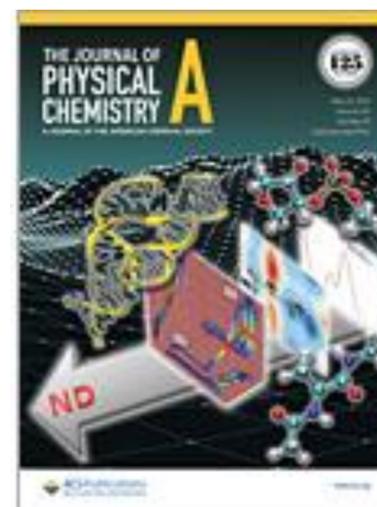


Biochemistry

IF 2.865

2019 JCR Ranking: 169/297 Biochemistry & Molecular Biology Category

Годы охвата: от 1996 до 2021 гг.



The Journal of Physical Chemistry A

IF 2.600

2019 JCR Ranking: 15/37 Physics, Atomic, Molecular & Chemical Category

Годы охвата: от 1996 до 2021 гг.

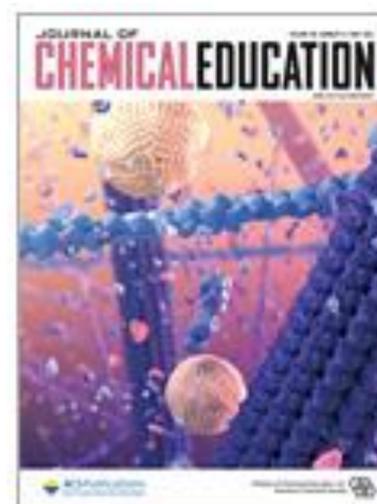


The Journal of Organic Chemistry

IF 4.335

2019 JCR Ranking: 9/57 Chemistry, Organic Category

Годы охвата: от 1996 до 2021 гг.



Journal of Chemical Education

IF 1.385

2019 JCR Ranking: 26/42 Education, Scientific Disciplines Category

Годы охвата: от 1996 до 2021 гг.

ACS PUBLICATIONS

Главная страница

The screenshot shows the ACS Publications website homepage. At the top, there is a navigation bar with 'ACS Publications', 'C&EN', and 'CAS' links, and a 'Log In' link. The main header features the ACS Publications logo and the tagline 'Most Trusted. Most Cited. Most Read.' Below this is a search bar with the text 'Search publications / articles / authors / dois / keywords / etc' and a magnifying glass icon. A prominent button reads 'Access COVID-19 research here'. Statistics are displayed: '1,300,000 Research Articles', '100,000 News Stories', '35,000 Book Chapters', and '1,000 References & Standards'. The 'Browse Publications' section is active, showing a grid of journal covers including 'ACCOUNTS', 'AGRICULTURAL SCIENCE & TECHNOLOGY', 'APPLIED BIO MATERIALS', 'APPLIED ELECTRONIC MATERIALS', 'APPLIED ENERGY MATERIALS', 'APPLIED MATERIALS INTERFACES', 'APPLIED NANO MATERIALS', 'APPLIED POLYMER MATERIALS', 'ACS BIO & MED CHEM', 'ACS Biomaterials SCIENCE & ENGINEERING', 'ACS Catalysis', 'ACS central science', 'ACS chemical biology', 'ACS CHEMICAL HEALTH & SAFETY', 'ACS Chemical Neuroscience', 'ACS EARTH AND SPACE CHEMISTRY', and 'ACS Energy LETTERS'. The interface includes view options for 'Grid View', 'List View', and 'Browse by Subject'.

ACS PUBLICATIONS

Страница журнала

Выпуски журнала

Актуальное

Информация о журнале

The screenshot shows the ACS Publications website for the journal Chemical Reviews. At the top, there is a navigation bar with 'ACS Publications', 'C&EN', and 'CAS'. A search bar and 'My Activity' and 'Publications' links are also present. The main header features the 'CHEMICAL REVIEWS' logo, 'Related Journals' dropdown, and 'Submit Manuscript', 'Subscriber Info', and 'Get e-Alerts' buttons. Below the header, there are tabs for 'ASAP Articles', 'Current Issue', and 'Authors'. The 'Current Issue' tab is active, displaying a carousel of articles. The first article is 'Thermostability, Tunability, and Tenacity of RNA as Rubbery Anionic Polymeric Materials in Nanotechnology and ...' by Daniel W. Binzel et al., dated May 26, 2021. The second article is 'Oxide-Zeolite-Based Composite Catalyst Concept That Enables Syngas Chemistry beyond Fischer-Tropsch Synthesis' by Xiulian Pan et al., dated May 25, 2021. The third article is 'Nonequilibrium Processes in Polymer Membrane Formation: Theory and Experiment' by Marcus Müller et al., dated May 25, 2021. The fourth article is 'Microfluidics for Drug Development From Synthesis to Evaluation' by Yuxiao Liu et al., dated May 22, 2021. Below the carousel is a 'Featured Content' section with three items: 'Thematic Issues', 'Latest Thematic Issue: Transporters, Porins, and Efflux Pumps' (dated May 12, 2021), and 'Beyond Li-Ion Battery Chemistry'.

This sidebar provides detailed information about the journal. It includes the journal title 'CHEMICAL REVIEWS', the Editor-in-Chief 'Sharon Hammes-Schiffer', and a link to 'About the Journal'. Under the 'About the Journal' section, it lists the Editor-in-Chief, the Editorial Board, and ISSN numbers (Print Edition: 0009-2665, Web Edition: 1520-6890). It also provides the 2019 Impact Factor (52.758) and Total Citations (200,014). The 'Journal Scope' section describes the journal as one of the most highly regarded and highest-ranked in chemistry, covering general topics in organic, inorganic, physical, analytical, theoretical, and biological chemistry. It also mentions that the journal has published thematic issues since 1985.

ACS PUBLICATIONS

Выпуск журнала

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REVIEWS

Quantum Chemistry Calculations for Metabolomics

Focus Review

Ricardo M. Borges, Sean M. Colby, Susanta Das, Arthur S. Edison, Oliver Fiehn, Tobias Kind, Jesi Lee, Amy T. Merrill, Kenneth M. Merz Jr., Thomas O. Metz, Jamie R. Nunez, Dean J. Tantillo, Lee-Ping Wang, Shunyang Wang, and Ryan S. Renslow*

Chemical Reviews 2021, 121, 10, 5633-5670 (Review)

Publication Date (Web): May 12, 2021

[Abstract](#) [Full text](#) [PDF](#)

ABSTRACT

A primary goal of metabolomics studies is to fully characterize the small-molecule composition of complex biological and environmental samples. However, despite advances in analytical technologies over the past two decades, the majority of small molecules in complex samples are not readily identifiable due to the immense structural and chemical diversity present within the metabolome. Current gold-standard identification methods rely on reference libraries built using authentic chemical materials ("standards"), which are not available for most molecules. Computational quantum chemistry methods, which can be used to calculate chemical properties that are then measured by analytical platforms, offer an alternative route for building reference libraries, i.e., in silico libraries for "standards-free" identification. In this review, we cover the major roadblocks currently facing metabolomics and discuss applications where quantum chemistry calculations offer a solution. Several successful examples for molecular magnetic resonance spectroscopy, ion mobility spectrometry, infrared spectroscopy, and mass spectrometry methods are reviewed. Finally, we consider current best

Информация о статье

ACS PUBLICATIONS

Страница публикации

Сведения о статье (название, авторы, номер выпуска, doi)

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Quantum Chemistry Calculations for Metabolomics

Focus Review

Ricardo M. Borges, Sean M. Colby, Susanta Das, Arthur S. Edison, Oliver Fiehn, Tobias Kind, Jesi Lee, Amy T. Merrill, Kenneth M. Merz Jr., Thomas O. Metz, Jamie R. Nunez, Dean J. Tantillo, Lee-Ping Wang, Shunyang Wang, and Ryan S. Renslow*

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PDF (8 MB)

SUBJECTS: Metabolomics, Metabolism, Molecules, Quantum mechanics, Nuclear magnetic resonance spectroscopy

Abstract

A primary goal of metabolomics studies is to fully characterize the small-molecule composition of complex biological and environmental samples. However, despite advances in analytical technologies over the past two decades, the majority of small molecules in complex samples are not readily identifiable due to the immense structural and chemical diversity present within the metabolome. Current gold-standard identification methods rely on reference libraries built using authentic chemical materials (“standards”), which are not available for most molecules. Computational quantum chemistry methods, which can be used to calculate chemical properties that are then measured by analytical platforms, offer an alternative route for building reference libraries, *i.e.*, *in silico* libraries for “standards-free” identification. In this review, we cover the major roadblocks currently facing metabolomics and discuss applications where quantum chemistry calculations offer a solution. Several successful examples for nuclear magnetic resonance spectroscopy, ion mobility spectrometry, infrared spectroscopy, and mass spectrometry methods are reviewed. Finally, we consider current best practices, sources of error, and provide an outlook for quantum chemistry calculations in metabolomics studies. We expect this review will inspire researchers in the field of small-molecule identification to accelerate adoption of *in silico* methods for generation of reference libraries and to add quantum chemistry calculations as another tool at their disposal to characterize complex samples.

MS fragmentation
 NMR spectra
 IR spectra
 Collision Cross Section

1. Introduction

1.1. Growth and Impact of the Omics

Current basic and applied research of living systems occurs amid several rapidly evolving scientific paradigms, omics (*e.g.*, genomics, transcriptomics, proteomics, and metabolomics),^(1–7) systems biology,^(8–10) and synthetic biology,^(11–13) that influence the researcher to look broadly at the holistic system or organism under study. Propelled by key developments of the Information Age, these scientific paradigms encourage scientists to aim for the comprehensive characterization and quantification of the relevant functional units of a cell,

ARTICLE SECTIONS | Jump To

Figures | References

References

This article references 542 other publications.

1. Aebersold, R.; Mann, M. Mass spectrometry-based proteomics. *Nature* **2003**, *422*, 198–207, DOI: 10.1038/nature01511 [Crossref], [PubMed], [CAS], [Google Scholar]

2. Gianj, A. M.; Gallo, G. R.; Gianfranceschi, L.; Formenti, G. Long walk to genomics.

Publication History

- Received 24 August 2020
- Published online 12 May 2021
- Published in issue 26 May 2021

История публикации

Ключевые слова

Похожие статьи

ACS PUBLICATIONS

Простой поиск

Фильтры поискового запроса

The screenshot shows the ACS Publications search results page for the query "Clinical Biomarker". The search bar at the top contains the query. Below the search bar, there are options to refine the search, per page settings (20, 50, 100), and a sort order dropdown set to "RELEVANCE". The results are displayed in a list format, with the first two articles highlighted. The first article is "Microarray-Formatted Clinical Biomarker Assay Development Using Peptide Aptamers to Anterior Gradient-2" by Euan Murray et al., published in *Biochemistry* in 2007. The second article is "Comprehensive and Scalable Highly Automated MS-Based Proteomic Workflow for Clinical Biomarker Discovery in Human Plasma" by Loïc Dayon et al., published in *Journal of Proteome Research* in 2014. The page also features a sidebar with various filters such as Content Group Type, Content Type, Article Type, Publication Date, Contributor, Publication, and Topics.

Поисковый запрос

Результаты запроса

Информация о найденных статьях

ACS PUBLICATIONS

Расширенный поиск

Составление поискового запроса

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Anywhere +

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Сохранение поискового запроса

Ограничение результатов поиска годами публикации

ACS PUBLICATIONS

Поиск по цитатам

The screenshot displays the ACS Publications search interface. At the top, there is a search bar with the text "Clinical Biomarker" and a search icon. Below the search bar, there is a section for "OR SEARCH CITATIONS" with a dropdown menu set to "Accounts of Chemical Research", a search icon, and the number "54". To the right of this section, there is another search bar with the number "1631" and a search icon. Below the search bar, there is a "Journals" dropdown menu. The menu is open, showing a list of journals. The first journal, "Accounts of Chemical Research", is highlighted in blue. The list of journals includes: Accounts of Chemical Research, Accounts of Materials Research, ACS Agricultural Science & Technology, ACS Applied Bio Materials, ACS Applied Electronic Materials, ACS Applied Energy Materials, ACS Applied Materials & Interfaces, ACS Applied Nano Materials, ACS Applied Polymer Materials, ACS Bio & Med Chem Au, ACS Biomaterials Science & Engineering, ACS Catalysis, ACS Central Science, ACS Chemical Biology, ACS Chemical Health & Safety, ACS Chemical Neuroscience, ACS Combinatorial Science, ACS Earth and Space Chemistry, and ACS Energy Letters. Two red dashed arrows point to the interface: one from the left pointing to the search bar area, and one from the right pointing to the journal dropdown menu.

Ввод данных публикации

Выбор журнала, выпадающее меню

ACS PUBLICATIONS

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Название журнала

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Уведомление о новых выпусках

Периодичность

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Saved Searches

Saved Search Name	Frequency	Saved on	Last run on	User actions	User actions
Clinical Biomarker	Never	May 27, 2021	May 27, 2021	RUN	DELETE

Save this search

Name:

Alert me to new results:
 Never Daily Weekly Monthly

Поисковые запросы My account > Saved Searches



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