Towards Open Science at RIKEN
オープンサイエンスに向けて

RIKEN Executive Director
国立研究開発法人理化学研究所
Dr. Shigeo Koyasu
小安重夫
Japan’s sole comprehensive research institute in the natural sciences

RIKEN's mission in the RIKEN Law (Purpose of the Institute : Article 3)

RIKEN aims to raise the standard of science and technology by comprehensively carrying out experiments, research and other operations related to science and technology (excluding those which solely concern the humanities).

理研法
科学技術に関する試験及び研究等の業務を総合的に行うことにより、科学技術の水準の向上を図ることを目的とする。
Cluster for Pioneering Research
Pioneering and creating new fields of science in order to sustain continuous innovation

Research Infrastructure Centers
Promotion of research and development, improvement, and public utilization of the world’s top-level research infrastructure

Strategic Research Centers
Promotion of strategic R&D to address national and social demands

Information R&D and Strategy Headquarters
Enhancement and implementation of digital research infrastructures for information and data science

Cluster for Science, Technology and Innovation Hub
Promotion of returning the benefits of research to society by strengthening partnerships with relevant organizations

RIKEN Innovation Co., Ltd.
Technology licensing
Start-up support
Joint research promotion
Membership-based co-creation

Chief Scientist Laboratories
Center for Computational Science
SPring-8 Center
BioResource Research Center

Program for Drug Discovery and Medical Technology Platforms
Baton Zone Program
Industrial Co-creation Program

Center for Advanced Intelligence Project
Interdisciplinary Theoretical and Mathematical Sciences Program
Center for Integrative Medical Sciences
Center for Biosystems Dynamics Research
Center for Brain Science
Center for Sustainable Resource Science
Center for Emergent Matter Science
Center for Quantum Computing
Center for Advanced Photonics
Nishina Center for Accelerator-Based Science

Infrastructure Research and Development Division
Advanced Data Science Project
Guardian Robot Project
Promotion of Open Access Journal

Proportion of Open Access Documents

学術論文のオープンアクセスの割合

年

% All Open Access Documents at RIKEN
% Gold Documents at RIKEN
% Green only Documents at RIKEN

Percentile of Open Access Documents to Published Documents


year 4
Towards Open Science

Processing of Data-Sharing, Open Data Construction Research Data Platform
研究データの公開および共有のための研究データ基盤構築

Promotion of Open Access Journal
学術論文のオープンアクセスの推進

Open Science
Raising the standard of science and technology
科学技術をより高い水準に

Research Integrity
公正な研究活動
Research results, Data used for analysis, and Analysis results are fully open.

国際連携に基づくプラットフォーム
FANTOM = Functional ANnoTation Of Mammalian genome

Global collaboration project led by RIKEN

Research results, Data used for analysis, and Analysis results are fully open.

理化学研究所の主導による国際共同研究プロジェクト

(Number of Hits for Fantom website)

<table>
<thead>
<tr>
<th>Year</th>
<th>Hits</th>
</tr>
</thead>
<tbody>
<tr>
<td>2010</td>
<td>1008432</td>
</tr>
<tr>
<td>2011</td>
<td>823657</td>
</tr>
<tr>
<td>2012</td>
<td>1328665</td>
</tr>
<tr>
<td>2013</td>
<td>1265565</td>
</tr>
<tr>
<td>2014</td>
<td>5219916</td>
</tr>
<tr>
<td>2015</td>
<td>8814263</td>
</tr>
<tr>
<td>2016</td>
<td>11858124</td>
</tr>
<tr>
<td>2017</td>
<td>14033060</td>
</tr>
<tr>
<td>2018</td>
<td>12592700</td>
</tr>
<tr>
<td>2019</td>
<td>12907220</td>
</tr>
</tbody>
</table>

←FANTOM5 Paper published
Platform based on Global collaboration

国際連携に基づくプラットフォーム

HUMAN CELL ATLAS

AREAS OF IMPACT

Where do we start?

Studying all the cells in the human body is an enormous endeavor—current estimates suggest that an average human being is made of at least 37.2 trillion cells. To take on this bold task, we are conducting preliminary pilot projects that will not only reveal interesting biology, but also inform us about efficient and effective sampling and analysis stra...
Open Access Database

FMO Database (FMODB)
The database of quantum mechanical data based on the FMO method
フラグメント分子軌道法（FMO法）によるオープンアクセス分子構造データベース

FMODB: The database of quantum mechanical data based on the FMO method
Last updated: 2022-02-03
All entries: 14924
Number of unique PDB entries: 2956

Information | ID Search | Keyword Search | Blast Search | Ligand Structure Search
--- | --- | --- | --- | ---
2020.4.17 COVID-19 | FMO data for COVID-19 related proteins have been released on Apr 17, 2020. here.

Category

COVID-19(830)
- Papain like protease(141)
- Main protease(415)
- ADP ribose phosphatase(20)
- RNA dependent RNA polymerase(21)

News: FMO data for COVID-19 related proteins

Modified from the original by RCSB PDB

Search Sample
FMO Database (FMODB)

Contribution for Drug Design 創薬への貢献

The molecular interaction between the new coronavirus (SARS-CoV-2) protein and the therapeutic drug candidate compound is calculated by the "fragment molecular orbital method (FMO method)", and the data can be freely used by drug discovery researchers around the world.

新型コロナウイルス（SARS-CoV-2）タンパク質と治療薬候補化合物の分子間相互作用を「フラグメント分子軌道法（FMO法）」で計算し、そのデータを、世界中の創薬研究者が自由に利用できる「FMOデータベース（FMODB）」にて公開。

FMO data for COVID-19-related proteins
FMO計算による9種のタンパク質の代表構造

FMO-based interaction energy analysis of SARS-Cov-2 main protease and ligand complexes
メインプロテアーゼと治療薬候補化合物の相互作用解析
Predicted dynamic structures of the spike protein (S-protein) will be used to develop drugs for inhibiting the interaction between the S-protein and the receptor (ACE-2) on the host cell.

SARS-CoV-2 surface protein on the surface of SARS-CoV-2

SARS-CoV-2表面のスパイクタンパク質

Open source software:
Molecular dynamics and modeling software for bimolecular systems such as proteins, lipids, nucleic acids, glycans, and their complexes.
Exploring the molecular dynamics of the new coronavirus

新型コロナウイルス（SARS-CoV-2）メインプロテアーゼの分子動力学シミュレーションデータを公開

The raw data from the simulation has been published on Mendeley Data for use by researchers around the world.

世界の創薬研究者が自由に利用できるよう、RAW DATAをリポジトリMendeley Dataに2020年3月17日公開。

Mendeley Data is an open, free-to-use research data repository, which enables researchers to make their research data publicly available.
The Role and Responsibility in the Post-pandemic Era

Impact of COVID-19 pandemic on STI

COVID-19 pandemicが科学技術に与えた影響

• Changes in the environment surrounding global research activities
  Stagnation of International collaboration and Global brain circulation
  Activation of Discussion via remote at any time and place
  世界的な科学技術、研究活動を取り巻く環境の変化
  （特に、世界的な研究交流、国際頭脳循環の停滞）
• Impact on investment in STI and R&D due to economic stagnation
  経済活動の停滞、科学技術、研究開発に対する投資への影響

→ Accelerating Open Science

オープンサイエンスの推進

Social cohesion in With-/Post-COVID-19 pandemic era

COVID-19 pandemicの先にある社会との結束

• Expectations for Science, Technology and Innovation
  科学技術イノベーションへの期待

→ Prompt dissemination of
  “Accurate” and Comprehensible Information

“正確”でわかりやすい情報の迅速な普及
Two conspicuous retracted COVID-19 papers

The Lancet and The New England Journal of Medicine (NEJM) retracted two papers after a company declined to Provide the underlying data.

The LancetとThe New England Journal of Medicine (NEJM)に掲載された2報の論文は、企業がデータセットの提供やアクセスの要求に応じず、取下げることとなった。

**METHODS**
Using an observational database from 169 hospitals in Asia, Europe, and North America, we evaluated the relationship of cardiovascular disease and drug therapy with in-hospital death among hospitalized patients with Covid-19 who were admitted between December 20, 2019, and March 15, 2020, and were recorded in the Surgical Outcomes Collaborative registry as having either died in the hospital or survived to discharge as of March 28, 2020.

**RESULTS**
Of the 8910 patients with Covid-19 for whom discharge status was available at the time of the analysis, a total of 515 died in the hospital (5.8%) and 8395 survived to discharge. The factors found to be independently associated with an increased risk of in-hospital death were an age greater than 65 years (mortality of 10.0%, vs. 4.9% among those ≤65 years of age; odds ratio, 1.93; 95% confidence interval [CI], 1.60 to 2.41), coronary artery disease (10.2%, vs. 5.2% among those without disease; odds ratio, 2.70; 95% CI, 2.08 to 3.51), heart failure (15.3%, vs. 5.0% among those without heart failure; odds ratio, 2.48; 95% CI, 1.62 to 3.79), cardiac arrhythmia (11.5%, vs. 5.6% among those without arrhythmia; odds ratio, 1.39; 95% CI, 1.33 to 2.86), chronic obstructive pulmonary disease (14.2%, vs. 5.0% among those without disease; odds ratio, 2.96; 95% CI, 2.00 to 4.40), and current smoking (9.4%, vs. 5.6% among former smokers or nonsmokers; odds ratio, 1.79; 95% CI, 1.29 to 2.47). No increased risk of in-hospital death was found to be associated with the use of ACE inhibitors (2.1% vs. 6.1%; odds ratio, 0.33; 95% CI, 0.20 to 0.54) or the use of ARBs (6.8% vs. 5.7%; odds ratio, 1.23; 95% CI, 0.87 to 1.74).

**CONCLUSIONS**
This clinical context. (Funded by the William Harvey Distinguished Chair in Ad

Hydroxychloroquine or chloroquine with or without a macrolide for treatment of COVID-19: a multinational registry analysis

Mandeep R Mehra, Sapan S Desai, Frank Ruschitzka, Amit N Patel

Summary
Background Hydroxychloroquine or chloroquine, often in combination with a second-generation macrolide, are being widely used for treatment of COVID-19, despite no conclusive evidence of their benefit. Although generally safe when used for approved indications such as autoimmune disease or malaria, the safety and benefit of these treatment
drugs have been shown in laboratory conditions to have antiviral properties as well as immunomodulatory effects. However, the use of this class of drugs for COVID-19 is based on a small number of anecdotal experiences that have shown variable responses in uncontrolled observational analyses, and small, open-label, randomised trials that have largely been inconclusive. The combination of hydroxychloroquine with a second-generation macrolide, such as azithromycin or clarithromycin, has also been advocated,

This article was published on May 1, 2020, and updated on May 8, 2020, at NEJM.org.

This/uni0020article/uni0020has/uni0020been/uni0020retracted:/uni0020N/uni0020Engl/uni0020J/uni0020Med./uni0020DOI:/uni002010.1056/NEJMc2021225.

See corrected. The corrected version
In an examination of the most recent 200 academic articles published in 2020 that cite those papers, Science found that more than half-including many in leading journals-used the discredited papers to support scientific findings and failed to note the retractions.

これらの取下げ論文を引用した2020年に発表された200論文を精査した結果、有力誌を含むその半数以上が知見の裏付けとして引用、取下げについては示していないかった。

Refereed 15 JAN 2021 NEWS SCIENTIFIC COMMUNITY BY CHARLES PILLER

The absence of an effective treatment against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infection has led clinicians to redirect drugs that are known to be effective for other medical conditions to the treatment of COVID-19. Key among these repurposed therapeutic agents are the antimalarial drug chloroquine and its analogue hydroxychloroquine, which is used in the treatment of autoimmune diseases, such as systemic lupus erythematosus and rheumatoid arthritis. These drugs have been shown in laboratory conditions to have antiviral properties as well as immunomodulatory effects. However, the use of this class of drugs for COVID-19 is based on a small number of anecdotal experiences that have shown variable responses in uncontrolled observational analyses, and small, open-label, randomised trials that have largely been inconclusive.

The combination of hydroxychloroquine with a second-generation macrolide, such as azithromycin (or clarithromycin), has also been advocated,
Learning from a retraction

The publication and subsequent retraction\(^1\) in June, 2020, of the Article Hydroxychloroquine or chloroquine with or without a macrolide for treatment of COVID-19: a multinational registry analysis, based on an alleged dataset associated with Surgisphere, prompted us to examine The Lancet’s peer-review processes to identify ways of further reducing risks of research and publication misconduct. As a result of this review, with immediate effect, we have made changes to the declarations we seek from authors, the data sharing statements we require for published research papers, and the peer-review process for similar papers based on large datasets or real-world data.

Changes to the signed declarations by authors in the author declarations form will require that more than one author has directly accessed and verified the data reported in the manuscript. We will require that the authors who have accessed and verified underlying data are named in the contributors’ statement. For research Articles that are the result of an academic and commercial partnership, one of the authors named as having accessed and verified data must be from the academic team. In addition, all authors will be asked to sign the author statements form to confirm they had full access to the data reported in their Article, and accept responsibility for submitting the Article for publication.

Journals that adhere to guidance from the International Committee of Medical Journal Editors require a data-sharing statement for papers that report results of a clinical trial.\(^2\) Lancet journals will now require all research papers, irrespective of method, to include a data-sharing statement that details what data will be shared, whether additional documents will be shared (eg, the study protocol), when data will become available, and by what access criteria data will be shared. Investigators should be aware that editors will take data-sharing statements into account when making editorial decisions.

All Lancet journals will now introduce additional peer-review requirements for papers based on large, real-world datasets. Editors will ensure that at least one peer reviewer is knowledgeable about the details of the dataset being reported and can understand and comment on its strengths and limitations in relation to the research question being addressed. For studies that use very large datasets, editors will ensure that in addition to statistical peer review, a review from an expert in data science is obtained. Finally, we will explicitly ask reviewers if they have concerns about research integrity or publication ethics regarding the manuscript they are reviewing.

Throughout the COVID-19 pandemic the work of the research community in generating new knowledge has resulted in rapid advances in our understanding of severe acute respiratory syndrome coronavirus 2 and COVID-19. As trusted sources of information, the Lancet journals are committed to ensuring that our editorial processes continue to be as robust as possible.

The Editors of the Lancet Group

The Lancet, London EC2Y 5AS, UK