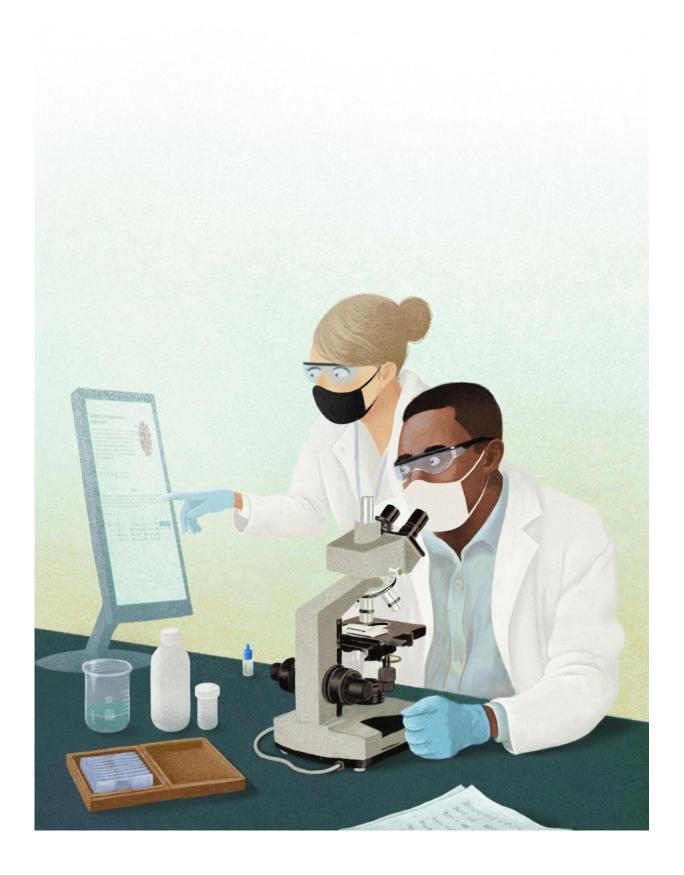


Scientists urge swift action to prepare for next pandemic

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An image created by Marcin Minor for the cover of the scientific journal IUCrJ to accompany a new article urging scientists to prepare now for the next pandemic. Credit: Marcin Minor

An international team of researchers led by a University of Virginia School of Medicine professor is warning that scientists must better prepare for the next pandemic—and has developed a plan to do just that.

Noting the avalanche of scientific data generated in response to COVID-19, UVA's Wladek Minor, Ph.D., and colleagues are calling for the creation of an advanced information system (AIS) to help scientists integrate, monitor and evaluate the vast amounts of data that will be produced as researchers reveal the molecular architecture of the next pathogen posing a big biological threat. This information on the shape, structure, and function of a pathogen is essential to the development of medications, vaccines and treatments. For example, the COVID-19 vaccines now available target the "spike" protein on the surface of the SARS-CoV-2 virus.

Their heavily cited online resource for COVID-19 (COVID-19.bioreproducibility.org/) demonstrates the usefulness of their approach and can be used as a foundation for the new research strategy, they say. The site includes carefully validated 3D structural models of numerous proteins related to the SARS-CoV-2 virus, including many potential drug targets.

"Structural models and other <u>experimental results</u> produced by various laboratories must follow a standard evaluation procedure to ensure that they are accurate and conform to accepted scientific standards," said Minor, Harrison Distinguished Professor of Molecular Physiology and Biological Physics at UVa. "Standardized validation is important for all



areas of biomedical sciences, especially for structural models, which are often used as a starting point in subsequent research, such as computer-guided drug docking studies and data mining. Even seemingly insignificant errors can lead such research astray."

Battling a Pandemic

One important role of AIS would be to identify structures that can be refined and improved, the researchers say. They were happy to note that inspection of the molecular blueprints produced for components of COVID-19 and deposited in the Protein Data Bank online database suggests that most were very good. Less than 1% needed significant reinterpretation and less than 10% could be optimized by moderate revisions.

Still, good buildings require good blueprints. The same is true with vaccines and disease treatments. It's critical, the researchers say, that the structural and other data for pathogens are as accurate as possible, and that scientists from various fields are speaking the same language when discussing and using them. The proposed AIS would help ensure conformity across disciplines.

"Almost 100,000 COVID-19-related papers have been published and over a thousand models of macromolecules encoded by SARS-CoV-2 have been experimentally determined in about a year. No single human can possibly digest this volume of information," Minor said. "We believe that the most promising solution to information overload and the lack of effective information retrieval is the creation of an advanced information system that is capable of harvesting results from all relevant resources and presenting the information in instructive ways that promote understanding and knowledge."

The researchers acknowledge that implementing their proposal would be



a major undertaking. Other resources that sought to offer similar benefits on a smaller scale have already come and gone. That's why it's so important, the scientists say, that we act now. "Creating an AIS will undoubtedly require the collaboration of many scientists who are experts in their respective fields, but it seems to be the only way to prepare biomedical science for the next pandemic," the researchers write in a new scientific paper outlining their proposal.

"In the history of humanity, the COVID-19 pandemic is relatively mild by comparison with the bubonic plague (Black Death) that killed a hundred times more people," the researchers conclude. "We might not be so lucky next time."

New Approach Outlined

The researchers—from UVA, the National Cancer Institute, Poland and Austria—have detailed their plan in an article in the scientific journal *IUCrJ*. The article is featured on the journal cover. The research team consists of Marek Grabowski, Joanna M. Macnar, Marcin Cymborowski, David R. Cooper, Ivan G. Shabalin, Miroslaw Gilski, Dariusz Brzezinski, Marcin Kowiel, Zbigniew Dauter, Bernhard Rupp, Alexander Wlodawer, Mariusz Jaskolski and Minor.

In their paper, the researchers gratefully acknowledged the financial support of the National Institutes of Health's National Institute of General Medical Sciences, grant R01-GM132595; the Polish National Agency for Academic Exchange, grant PN/BEK/2018/1/00058/U/00001; the Polish National Science Center, grant 2020/01/0/NZ1/00134; the Intramural Research Program of the NIH, National Cancer Institute, Center for Cancer Research; FWF (Austrian Science Foundation), grant P 32821; and the Polish National Science Centre, grant 2018/29/B/ST6/01989.



Minor and his longtime collaborator Zbyszek Otwinowski, Ph.D., of the University of Texas Southwestern Medical Center, were recently awarded the Tadeusz Sendzimir Applied Sciences Award by the Polish Institute of Arts and Sciences of America for their efforts to develop and promote software for biomedical applications in the structural biology field.

To keep up with the latest medical research news from UVA, subscribe to the Making of Medicine blog at <u>makingofmedicine.virginia.edu</u>.

More information: Marek Grabowski et al, Rapid response to emerging biomedical challenges and threats, *IUCrJ* (2021). <u>DOI:</u> 10.1107/S2052252521003018

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