

Biophysicists' outstanding response to Covid-19

As we faced our challenges during 2020 and beyond, there is no doubt that some positive outcomes have also come our way. For example, the unprecedented collaboration among scientists and the dedication of many to COVID-19 related research has been a strong testimony to the importance of science and to the crucial role we can play in our world.

Indeed, a fundamental understanding of the complex viral apparatus, from the protein exterior to the RNA viral genome; a more accurate understanding of the role of face coverings in disease prevention and spread; and a more precise description of the many factors that influence such disease spread are all invaluable. Biophysicists have been at the forefront of these multidisciplinary efforts, with research on the basic biophysical elements of the viral machinery, drug and vaccine design, infection analysis, face covering assessment, and more.

The response to our two special issues of COVID-19 related studies, of which this is the first, has been overwhelming. Many Biophysical Society members sent us their premier work, and helped us review the other papers with rigor and speed that we strive for in *Biophysical Journal*.

In coordination with the special Biophysical Society Symposium on Covid-19, held in October 2020, we invited original article contributions from scientists working to advance our understanding of all aspects of the Covid-19 disease and the SARS-CoV-2 virus, on multiple scales, levels, and points of view using novel experimental, mathematical, statistical, and computational approaches.

In this issue, you will taste some of these excellent works that were submitted from the summer of 2020 through the end of the year, with more to come in a future issue. Three of the articles are accompanied by New and Notable articles that highlight the uniqueness of the approach and impact of the study. The three original studies analyze the flexibility of the ACE2 receptor using molecular dynamics simulations (R. Amaro and team (1), commentary by G. Colombo

(2)); describe a multiscale coarse-grained model of the SARS-CoV-2 virion (G. Voth and coworkers (3), commentary by J. Straub (4)); and present a graph-theoretical approach for identifying structure-altering mutations in the viral frameshifting element, whose pseudoknot structure is thought to be key in the RNA transcript frameshifting that is essential to viral protein production (T. Schlick et al. (5), commentary by S.-J. Chen (6)).

Other classic structure-dynamics-function works describe studies related to the notorious spike protein and its ACE2 receptor, NSP13 helicase proteins, S protein, and the SARS-CoV-2 fusion peptide (A. Schug collaborators (7), X. Frank Zhang and coworkers (8), T. Kapoor and collaborators (9), M. Klein and group (10), Y. Sugita and team (11), A. Mulholland and co-workers (12), and G. Khelashvili and team (13).

Studies of mask decontamination, why masks lower the severity of the disease, and thermal inactivation of the virus are also part of our issue (T. Huber and colleagues (14), A. Bax and colleagues (15), S. Seifer and researchers (16).

Finally, J. Richardson and colleagues discuss how to improve SARS-CoV-2 structures from a structural accuracy point of view (17).

Significantly, both protein and RNA biophysicists have their hands full of projects and ideas, and the swiftly-changing virus and pandemic status—with viral variants and vaccination campaigns changing the infection parameters—offer new lines of investigation. We look forward to the continued innovation of our community members and to a return to in-face meetings where we can discuss these discoveries.

Tamar Schlick,^{1,*} Eric J. Sundberg,² Susan J. Schroeder,³ and M. Madan Babu⁴

¹New York University, New York, New York;

²Emory University, Atlanta, Georgia;

³University of Oklahoma, Norman, Oklahoma and

⁴St Jude Children's Research Hospital, Memphis, Tennessee

Submitted February 17, 2021, and accepted for publication February 17, 2021.

*Correspondence: schlick@nyu.edu

Editor: Elizabeth Rhoades.

<https://doi.org/10.1016/j.bpj.2021.02.020>

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REFERENCES

1. Barros, E. P., L. Casalino, ..., R. E. Amaro. 2021. The flexibility of ACE2 in the context of SARS-CoV-2 infection. *Biophys. J.* 120:1072–1084.



2. Serapian, S. A., and G. Colombo. 2021. Bow to the enemy: How flexibility of host protein receptors can favor SARS-CoV-2. *Biophys. J.* 120:977–979.
3. Yu, A., A. J. Pak, ..., G. A. Voth. 2021. A multiscale coarse-grained model of the SARS-CoV-2 virion. *Biophys. J.* 120:1097–1104.
4. Straub, J. E. 2021. New and notable: A multiscale coarse-grained model of the SARS-CoV-2 virion. *Biophys. J.* 120:975–976.
5. Schlick, T., Q. Zhu, ..., S. Yan. 2021. Structure-altering mutations of the SARS-CoV-2 frame shifting RNA element. *Biophys. J.* 120:1040–1053.
6. Chen, S. J. 2021. Graph, pseudoknot, and SARS-CoV-2 genomic RNA: A biophysical synthesis. *Biophys. J.* 120:980–982.
7. Peter, E. K., and A. Schug. 2021. The inhibitory effect of a coronavirus spike protein fragment with ACE2. *Biophys. J.* 120:1001–1010.
8. Cao, W., C. Dong, ..., X. F. Zhang. 2021. Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction. *Biophys. J.* 120:1011–1019.
9. Mickolajczyk, K. J., P. M. M. Shelton, ..., T. M. Kapoor. 2021. Force-dependent stimulation of RNA unwinding by SARS-CoV-2 nsp13 helicase. *Biophys. J.* 120:1020–1030.
10. Klein, M. L., A. Romero, ..., H. J. Gabius. 2021. From examining the relationship between (corona)viral adhesins and galectins to glyco-perspectives. *Biophys. J.* 120:1031–1039.
11. Mori, T., J. Jung, ..., Y. Sugita. 2021. Elucidation of interactions regulating conformational stability and dynamics of SARS-CoV-2 S-protein. *Biophys. J.* 120:1060–1071.
12. Oliveira, A. S. F., A. A. Ibarra, ..., A. J. Mulholland. 2021. A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. *Biophys. J.* 120:983–993.
13. Khelashvili, G., A. Plante, ..., H. Weinstein. 2021. Ca^{2+} -dependent mechanism of membrane insertion and destabilization by the SARS-CoV-2 fusion peptide. *Biophys. J.* 120:1105–1119.
14. Huber, T., O. Goldman, ..., T. P. Sakmar. 2021. Principles and practice for SARS-CoV-2 decontamination of N95 masks with UV-C. *Biophys. J.* Published online March 4, 2021. <https://doi.org/10.1016/j.bpj.2021.02.039>.
15. Courtney, J. M., and A. Bax. 2021. Hydrating the respiratory tract: an alternative explanation why masks lower severity of COVID-19. *Biophys. J.* 120:994–1000.
16. Seifer, S., and M. Elbaum. 2021. Thermal inactivation scaling applied for SARS-CoV-2. *Biophys. J.* 120:1054–1059.
17. Croll, T. I., C. J. Williams, ..., J. S. Richardson. 2021. Improving SARS-CoV-2 structures: peer review by early coordinate release. *Biophys. J.* 120:1085–1096.