



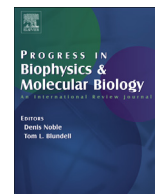
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Virtual article collection on infectious diseases

In honor of the 2020 Nobel Prize in Physiology or Medicine, Prof. Denis Noble penned an editorial titled “2020 – The year of the viruses” (Noble, 2020). The editorial also served to introduce our Progress in Biophysics and Molecular Biology Historic Articles and highlight Harvey Lodish’s 1968 review on RNA virus replication (Lodish, 1968). As we head to the start of our third year of the COVID-19 pandemic, it might perhaps be safe to say that these are the multiple years of the viruses. To this end, we have put together this virtual article collection on infectious diseases to highlight some of the work previously featured in our journal on this topic.

We had several recent special issues focusing on specific infectious disease topics, which feature reviews as well as original research articles. The May 2020 special issue focused on “Novel insights into TB research and drug discovery”. Mascolo et al. explored the role of cytochrome bd in TB infection and in the defense against antibacterials (Mascolo and Bald, 2020). Lee et al. reviewed cytochrome oxidases as possible targets for drug development for TB (Lee et al., 2020). Finally, Gila Kaplan provided a thorough review of tuberculosis control programs and the potential causes of the slow progress towards global TB control (Kaplan, 2020). The “Integration of scales: the dengue virus” special issue from May 2019 focused on how viruses interact over multiple length and time scales. Lim et al. reviewed the allostery of chymotrypsin-like proteases of a wide range of viruses including SARS, Dengue, and Zika (Lim et al., 2019). Sharma et al. reviewed single-molecule studies of flavivirus envelope dynamics; this included both experimental and computational approaches which can be applied to a wide range of viruses (Sharma et al., 2019). Ramesh et al. describe amide hydrogen deuterium exchange mass spectrometry (HDXMS) as a tool for observing viral macromolecular assembly dynamics (Ramesh et al., 2019).

Computational and modeling approaches have helped to further our understanding of infectious disease processes. Our journal featured several articles highlighting different computational approaches for understanding viral and microbial structure-function relationships. In our Special Issue on “Exploring mechanisms in biology: simulations and experiments come together,” Huber et al.’s 2017 review of multiscale molecular dynamics simulations to study of the structure and dynamics of viruses described the variety of techniques that can be used to model the multitude of interactions and structures associated with viral infections (Huber et al., 2017). From our Special Issue on “Experimental and Computational Model Interactions in Bio-Research: State of the Art”, Joshi et al. described new approaches to multiscale simulations that can be used to model and understand structural transitions important for a range of viruses including human papillomavirus (Joshi

et al., 2011). Montaseri et al.’s article in our “Quantitative Systems

Pharmacology (QSP): Methods and Tools” used a pharmacokinetic/pharmacodynamic model of oseltamivir to improve Influenza A treatment strategies (Montaseri et al., 2018).

Our ability to find new treatments or modify existing drugs to combat infectious diseases often hinges on understanding of the molecular structures that underlie how a virus or microbe interacts with host cells. Kabra et al. reviewed efflux pump activity, its role in antimicrobial resistance in several bacteria, fungi, viruses, and parasites, and how efflux pump inhibitors and anti-microbial peptides might be strategies to fight antimicrobial resistant superbugs (Kabra et al., 2019). Blundell et al. highlighted how protein disorder during protein-ligand interactions could lead to opportunities for new drug design targeting a wide range of pathogens (Blundell et al., 2020). Tiefenbrunn et al. utilized fragment-based drug discovery to find binding sites for proteins relevant to HIV as possible drug targets (Tiefenbrunn and Stout, 2014). More recently, in our “DNA-Replication and Repair, Structures” Special Issue, Brosey et al. used sequencing and evolutionary analyses combined with molecular structural analyses to find new compounds for possible SARS-CoV-2 antiviral therapies (Brosey et al., 2021).

As we see from the articles in this virtual collection, experimental and computational approaches in biophysics and molecular biology are keys to addressing ongoing and emerging infectious disease threats. Perhaps one of the few silver linings of this pandemic has been the renewed and sometimes quite public interest on the high impact that this field has on human health.

References

- Blundell, Tom L., Gupta, Munishwar N., Hasnain, Seyed E., 2020. Intrinsic disorder in proteins: Relevance to protein assemblies, drug design and host-pathogen interactions. *Prog. Biophys. Mol. Biol.* 156, 34–42. <https://doi.org/10.1016/j.pbiomolbio.2020.06.004>.
- Brosey, Chris A., Houl, Jerry H., Katsonis, Panagiotis, Balapiti-Modarage, Lakshitha P.F., Bommagani, Arvai, Andy, Moiani, Davide, Bacolla, Albino, Link, Todd, Warden, Leslie S., Lichtarge, Olivier, Jones, Darin E., Ahmed, Zamal, Tainer, John A., 2021. Targeting SARS-CoV-2 Nsp3 macrodomain structure with insights from human poly(ADP-ribose) glycohydrolase (PARG) structures with inhibitors. *Prog. Biophys. Mol. Biol.* 163, 171–186. <https://doi.org/10.1016/j.pbiomolbio.2021.02.002>.
- Huber, Roland G., Marzinek, Jan K., Holdbrook, Daniel A., Bond, Peter J., 2017. Multiscale molecular dynamics simulation approaches to the structure and dynamics of viruses. *Prog. Biophys. Mol. Biol.* 128, 121–132. <https://doi.org/10.1016/j.pbiomolbio.2016.09.010>.
- Joshi, Harshad, Singharoy, Abhishek, Sereda, Yuriy V., Chelvaraja, Srinath C., Ortoleva, Peter J., 2011. Multiscale simulation of microbe structure and dynamics. *Prog. Biophys. Mol. Biol.* 107, 200–217. <https://doi.org/10.1016/j.pbiomolbio.2011.07.006>.

- Kabra, Ritika, Chauhan, Nutan, Kumar, Anurag, Ingale, Prajakta, Singh, Shailza, 2019. Efflux pumps and antimicrobial resistance: Paradoxical components in systems genomics. *Prog. Biophys. Mol. Biol.* 141, 15–24. <https://doi.org/10.1016/j.pbiomolbio.2018.07.008>.
- Kaplan, Gilla, 2020. *Prog. Biophys. Mol. Biol.* 152, 6–9. <https://doi.org/10.1016/j.pbiomolbio.2019.10.001>.
- Lee, Bei Shi, Sviriaeva, Ekaterina, Pethe, Kevin, 2020. Targeting the cytochrome oxidases for drug development in mycobacteria. *Prog. Biophys. Mol. Biol.* 152, 45–54. <https://doi.org/10.1016/j.pbiomolbio.2020.02.001>.
- Lim, Liangzhong, Gupta, Garvita, Roy, Amrita, Kang, Jian, Srivastava, Shagun, Shi, Jiahai, Song, Jianxing, 2019. Structurally- and dynamically-driven allostery of the chymotrypsin-like proteases of SARS, Dengue and Zika viruses. *Prog. Biophys. Mol. Biol.* 143, 52–66. <https://doi.org/10.1016/j.pbiomolbio.2018.08.009>.
- Lodish, Harvey F., 1968. The replication of RNA-containing bacteriophages. *Prog. Biophys. Mol. Biol.* 18, 285–312. [https://doi.org/10.1016/0079-6107\(68\)90027-8](https://doi.org/10.1016/0079-6107(68)90027-8).
- Mascolo, Ludovica, Bald, Dirk, 2020. Cytochrome bd in *Mycobacterium tuberculosis*: A respiratory chain protein involved in the defense against antibacterials. *Prog. Biophys. Mol. Biol.* 152, 55–63. <https://doi.org/10.1016/j.pbiomolbio.2019.11.002>.
- Montaseri, Ghazal, Boianelli, Alessandro, Hernandez-Vargas, Esteban A., Meyer-Hermann, Michael, 2018. PK/PD-based adaptive tailoring of oseltamivir doses to treat within-host influenza viral infections. *Prog. Biophys. Mol. Biol.* 139, 31–42. <https://doi.org/10.1016/j.pbiomolbio.2018.07.007>.
- Noble, Denis, 2020. Editorial: 2020 – The year of viruses. *Prog. Biophys. Mol. Biol.* 158, 1–3. <https://doi.org/10.1016/j.pbiomolbio.2020.10.004>.
- Ramesh, Ranita, Lim, Xin Xiang, Raghuvamsi, Palur Venkata, Wu, Chao, Wong, Sek Man, Anand, Ganesh Srinivasan, 2019. Uncovering metastability and disassembly hotspots in whole viral particles. *Prog. Biophys. Mol. Biol.* 143, 5–12. <https://doi.org/10.1016/j.pbiomolbio.2018.12.006>.
- Sharma, Kamal Kant, Marzinek, Jan K., Tantirimudalige, Sarala Neomi, Bond, Peter J., Wohland, Thorsten, 2019. Single-molecule studies of flavivirus envelope dynamics: Experiment and computation. *Prog. Biophys. Mol. Biol.* 143, 38–51. <https://doi.org/10.1016/j.pbiomolbio.2018.09.001>.
- Tiefenbrunn, Theresa, Stout, C. David, 2014. Towards novel therapeutics for HIV through fragment-based screening and drug design. *Prog. Biophys. Mol. Biol.* 116, 124–140. <https://doi.org/10.1016/j.pbiomolbio.2014.09.009>.

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