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Miro's PhD work was interdisciplinary. He performed extensive simulations MD in silico to make a substantial contribution to our understanding of CF pathogenesis. Chapters 4 and 5 of his PhD thesis have been peer reviewed and published in *IScience* and *The American Journal of Respiratory Cell and Molecular Biology* respectively. While chapter 6 is in preparation for submission to *Frontiers in Pediatrics*.

- (Chapter 4) Wong, Sharon L.^, Nikhil T. Awatade^, **Miro A. Astore**^, Katelin M. Allan, Michael J. Carnell, Iveta Slapetova, Po-chia Chen, et al. "Molecular Dynamics and Functional Characterization of I37R-CFTR Lasso Mutation Provide Insights into Channel Gating Activity." *IScience* 25, no. 1 (January 2022): 103710. https://doi.org/10.1016/j.isci.2021.103710.

- (Chapter 5) Wong, Sharon L.^, Nikhil T. Awatade^, **Miro A. Astore**^, Katelin M. Allan, Michael J. Carnell, Iveta Slapetova, Po-Chia Chen, et al. "Molecular Dynamics and Theratyping in Airway and Gut Organoids Reveal R352Q-CFTR Conductance Defect." American Journal of Respiratory Cell and Molecular Biology, April 2022. https://doi.org/10.1165/rcmb.2021-0337OC.

- (Chapter 6) Katelin M. Allan, **Miro A. Astore**, Laura Fawcett, Po-Chia Chen, Renate Griffith, Adam Jaffe, Serdar Kuyucak, Shafagh Waters. "Unique S945L-CFTR defect restored by CFTR modulator co-therapy in vitro correlates with in vivo biomarkers post-therapy" (In preparation for submission to *Frontiers in Pediatrics*)

^ These authors contributed equally to this work.

For the in silico components, Po-chia Chen, Jeffry Setiadi, Renate Griffith and Serdar Kuyucak assisted Miro with the design and interpretation of his results and all authors on these publications assisted him with preparing the manuscripts for publication. Detailed descriptions of each author's contribution can be found in each publication.

As corresponding author on these publications, I give Miro permission to include content from these manuscripts in his PhD thesis.

I concur with A. Prof Serdar Kuyucak that Miro independently designed and executed the in silico components of each of these studies. This computational modelling contributed to our understanding of rare Cystic Fibrosis mutations and the function of the CFTR protein overall.

Kind regards,

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