In Silico Evaluation of Paxlovid's Pharmacometrics for SARS-CoV-2: a Multiscale Approach

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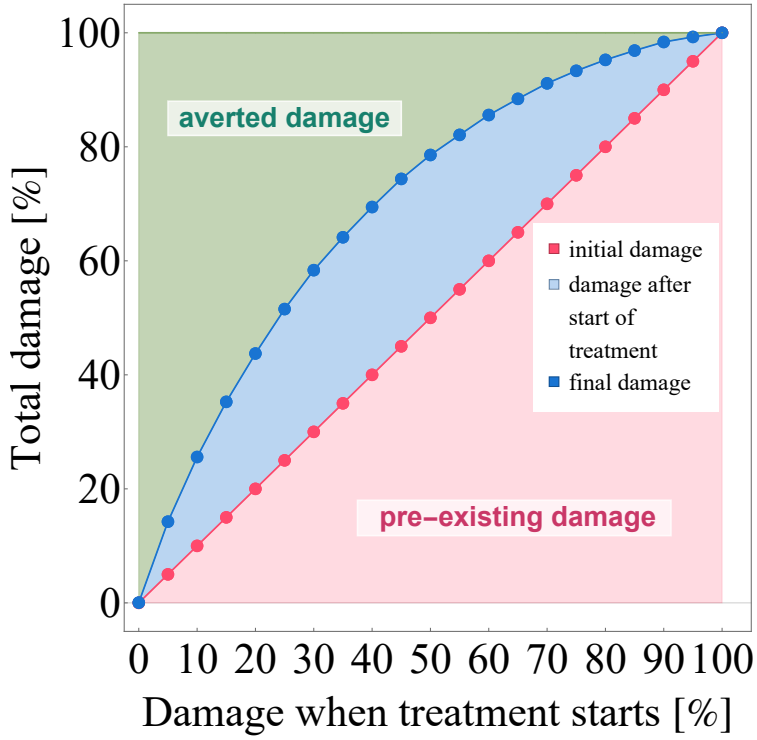
Paxlovid is a promising, orally bioavailable novel drug for SARS–CoV–2 with excellent safety profiles. Our main goal here is to explore the pharmacometric features of this new antiviral. To provide a detailed assessment of Paxlovid, we propose a hybrid multiscale mathematical approach. We demonstrate that the results of the present *in silico* evaluation match the clinical expectations remarkably well: on the one hand, our computations successfully replicate the outcome of an actual *in vitro* experiment; on the other hand we verify both the sufficiency and the necessity of Paxlovid's two main components (nirmatrelvir and ritonavir) for a simplified *in vivo* case. Moreover, in the simulated context of our computational framework we visualize the importance of early interventions, and identify the time window where a unit–length delay causes the highest level of tissue damage. Finally, the results' sensitivity to the diffusion coefficient of the virus is explored in details. *Joint work with Ferenc Bartha, Sadegh Marzban, Renji Han and Gergely Röst.*



[1] F. Bartha et al., In silico evaluation of Paxlovid's pharmacometrics for SARS-CoV-2: a multiscale approach, *Viruses* **14(5), 1103** (2022); https://doi.org/10.3390/v14051103