

# Drug repurposing for COVID-19 using explainable machine learning and mechanistic models of signal transduction circuits related to SARS-CoV-2 infection with real world data validation

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Consejería de Salud  
y Consumo

Fundación  
Progreso y Salud



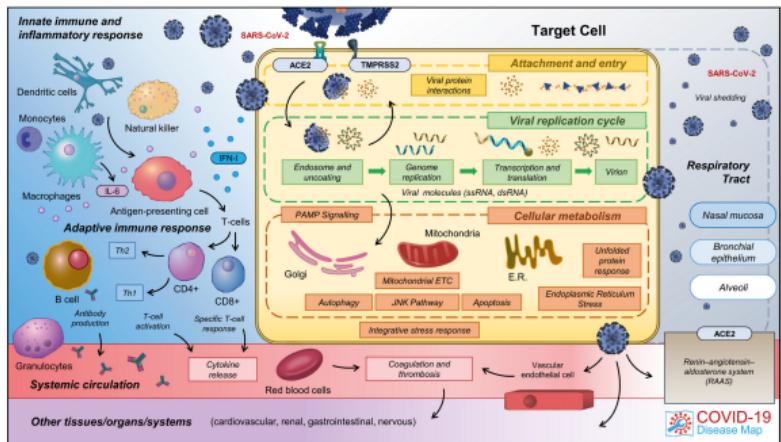
# Knowledge discovery

**Living Contradiction** is a fascinating, honest examination of that genuine contradiction faced by teachers in reconciling the effort made to encourage young people towards independent critical thinking, with the simultaneous sense of responsibility to instruct and insist on a particular behavior.

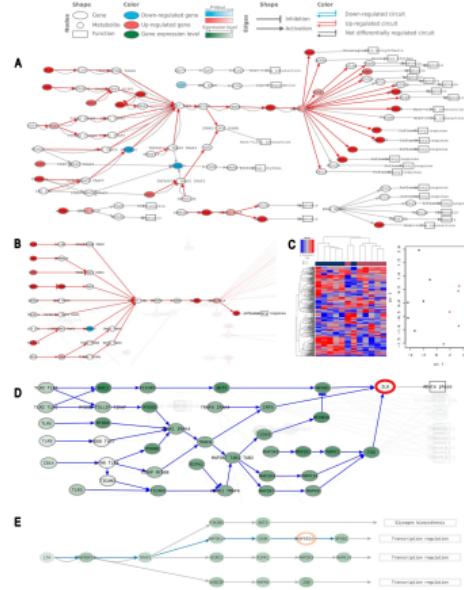
## Trustworthiness

The **WHY** is as important as the **WHAT**

# Building a COVID-19 Disease Map



COVID-19 Disease Map<sup>1</sup>

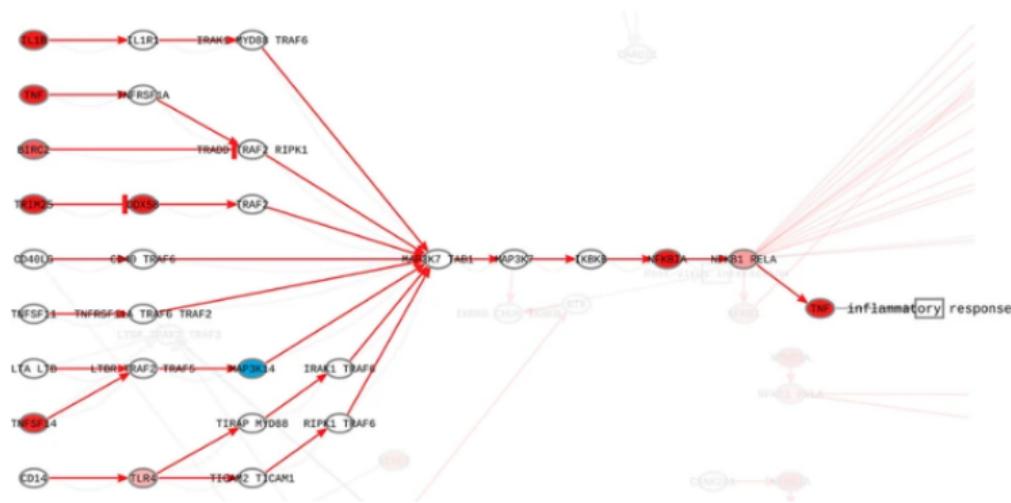


(Simplified) COVID-19 Disease Map<sup>2</sup>

<sup>1</sup> Marek Ostaszewski et al. (2021). "COVID19 Disease Map, a computational knowledge repository of virus–host interaction mechanisms." In: *Molecular systems biology* 17.10, e10387

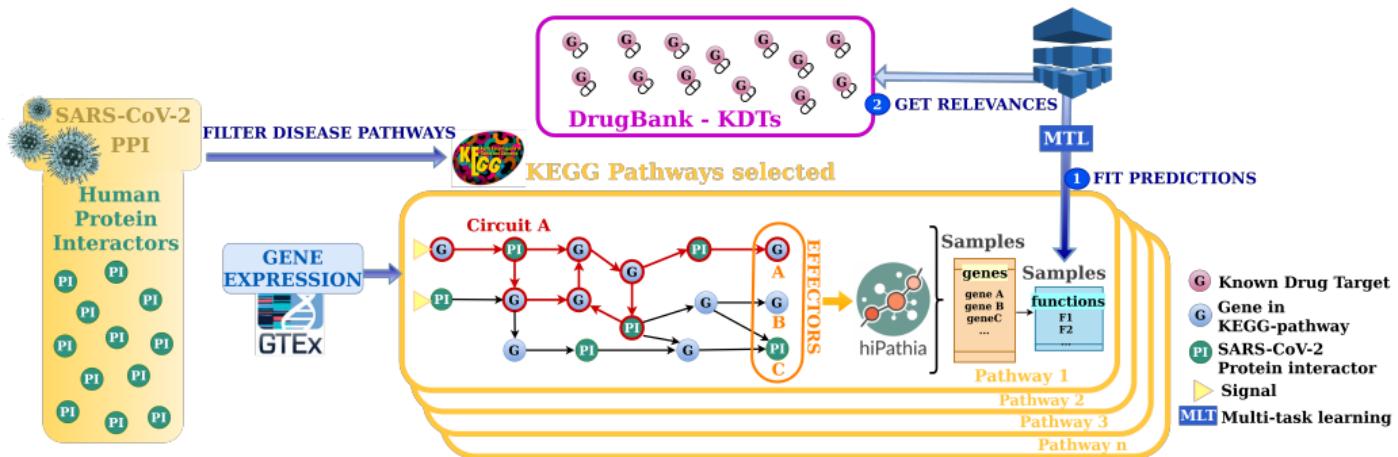
<sup>2</sup> Kinza Rian et al. (2021). "Mechanistic modeling of the SARS-CoV-2 disease map." In: *BioData Mining* 14.1, pp. 1–8

# Mechanistic modeling

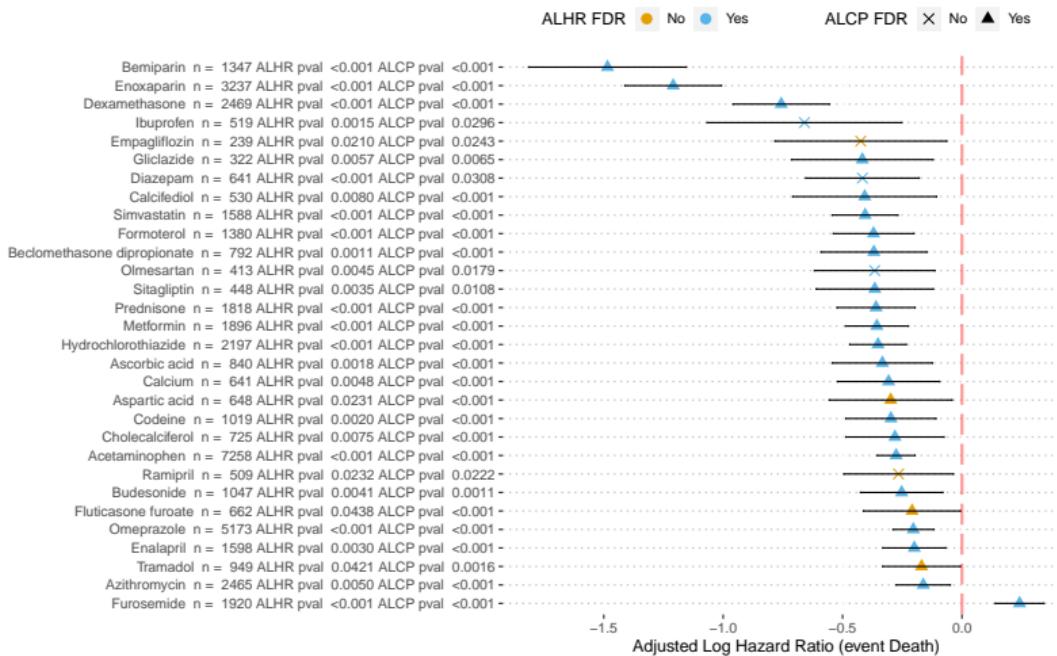


$$S_n = v_n \left( 1 - \prod_{s_a \in \mathcal{A}} (1 - s_a) \right) \prod_{s_i \in \mathcal{I}} (1 - s_i)$$

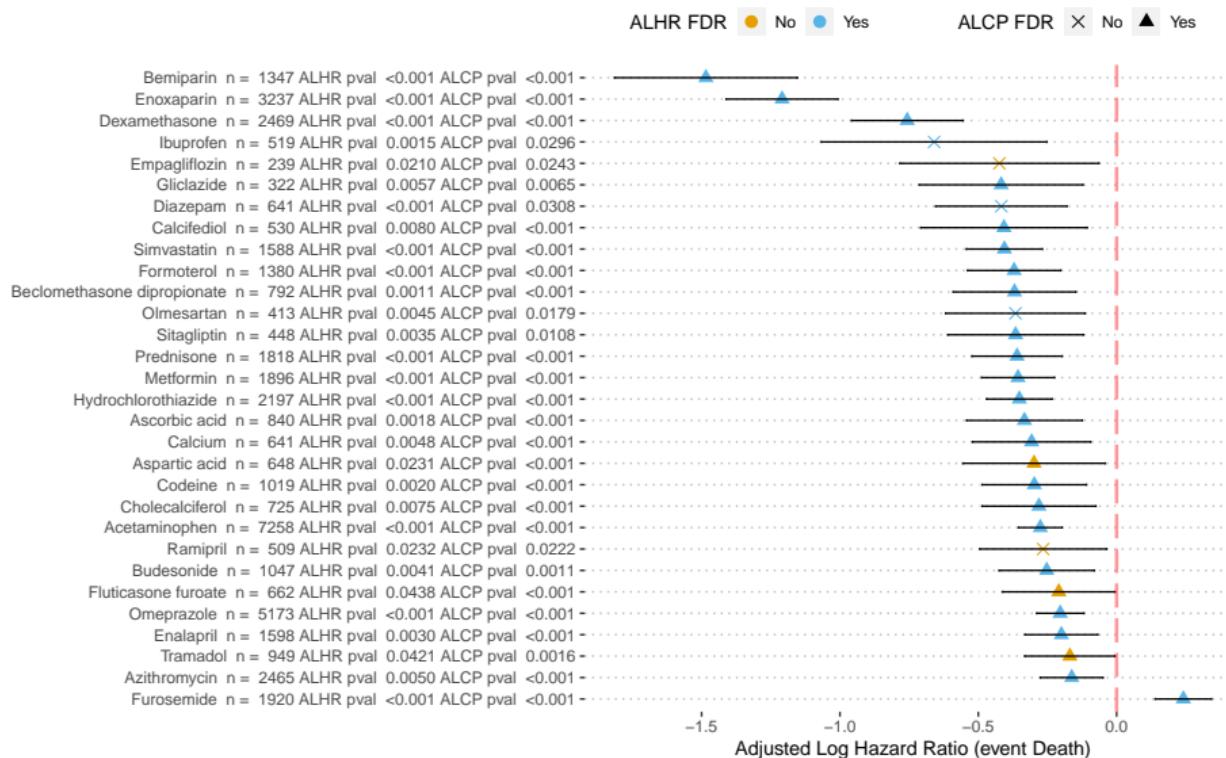
# Drug repurposing schema



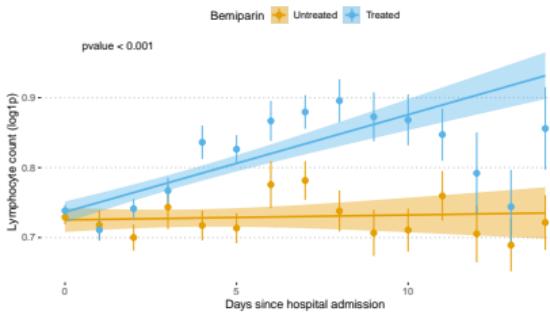
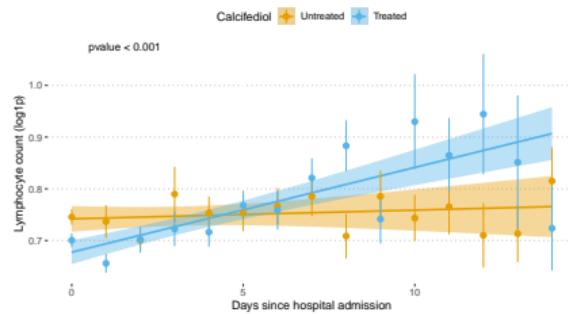
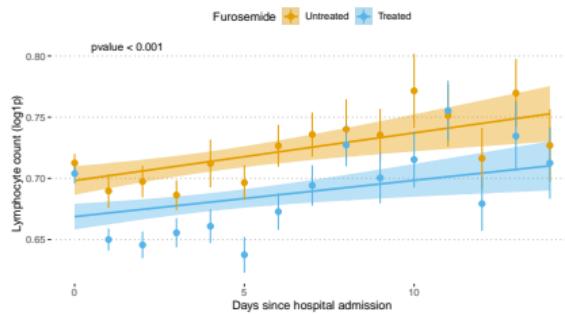
# Covariate-Adjusted LHR by Treatment



# Covariate-Adjusted LHR by Treatment



# Covariate-Adjusted Lymphocyte trend



# Thank You!

Personal funding. Contact: carlos.loucera@juntadeandalucia.es



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