DeepInhibition: IC50 prediction through ligand-receptor pairs interactions

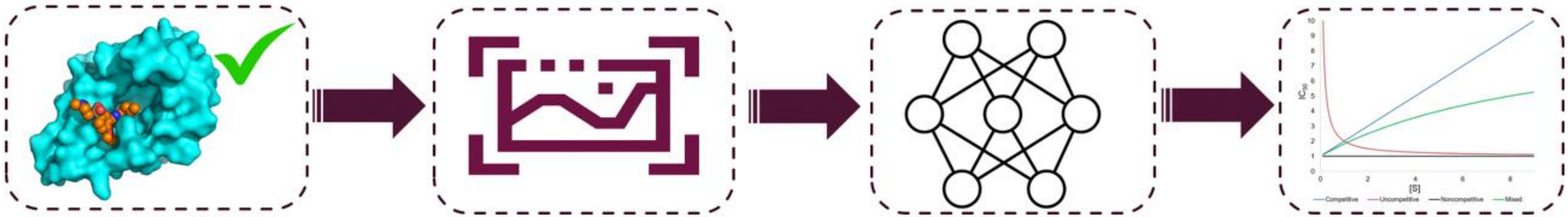
PI: Dr Theodora Katsila

European High Performance Computing Joint Undertaking

- A joint initiative between the EU, European countries & private partners to develop a World Class Supercomputing Ecosystem in Europe.
- Accompanied by a budget of €7 billion for the 2021-2027 period.

Our Research Challenge: Computational models in drug development & repurposing have largely evolved in the last decades. Yet, the prediction of IC50 values is a task with insufficient solutions.

Our Research Answer: We propose an assay- and dose- free, deep-learning framework which would determine protein inhibition metrics according to ligand-protein structural characteristics.



Ligand-protein interactions → Image processing → Neural networks → IC50 values

Our Impact:

- Datasets on 7,500 drugs (approved, experimental & in clinical trials)
- Datasets on structurally determined human proteins (drug targets) sharing structural info with ligands
- Datasets on proteome & variome spaces
- A better-informed, faster, cheaper, drug repurposing pipeline