

Repurposing Drugs to Fight COVID-19

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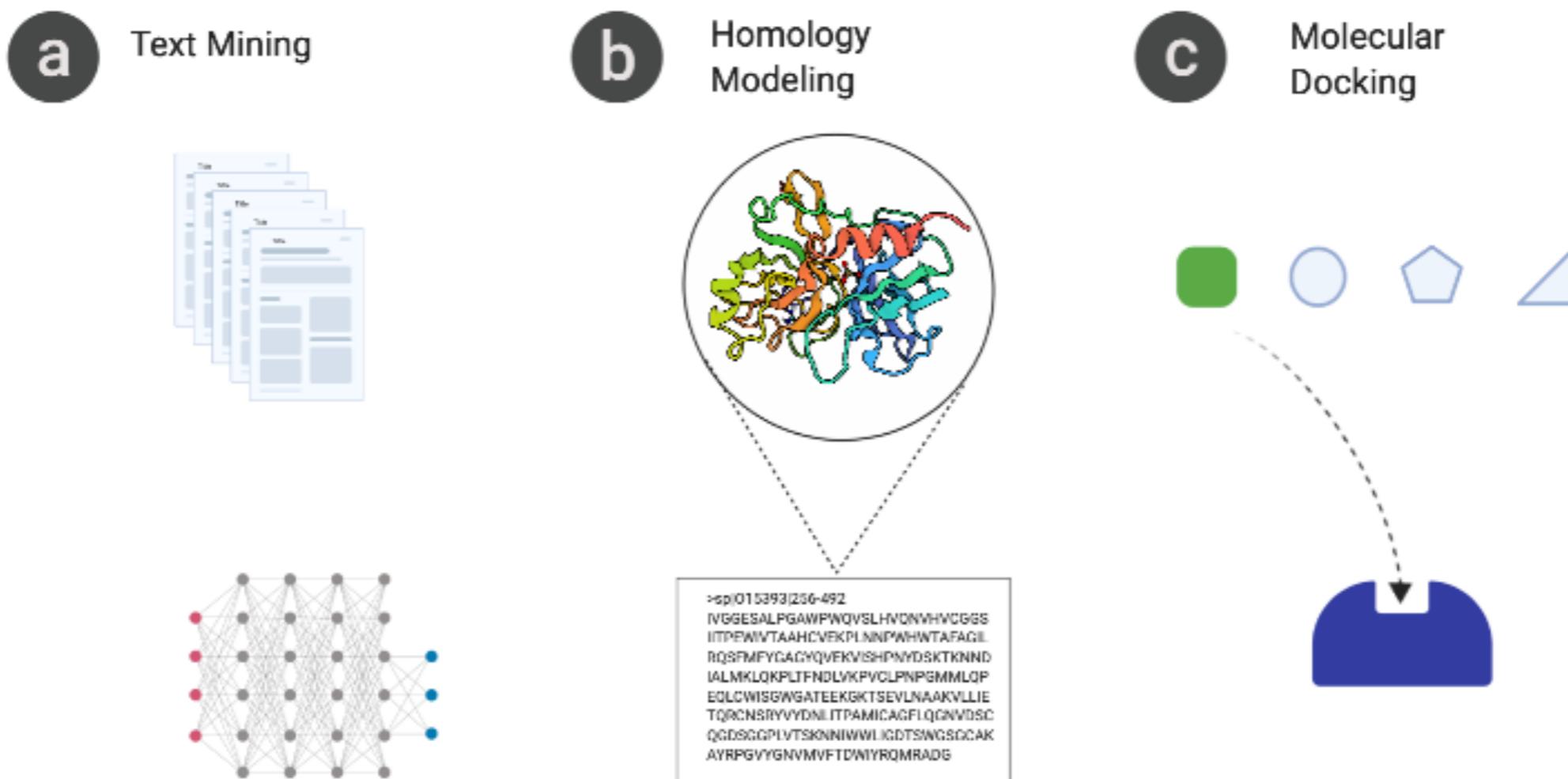
We need effective drugs to fight COVID-19.



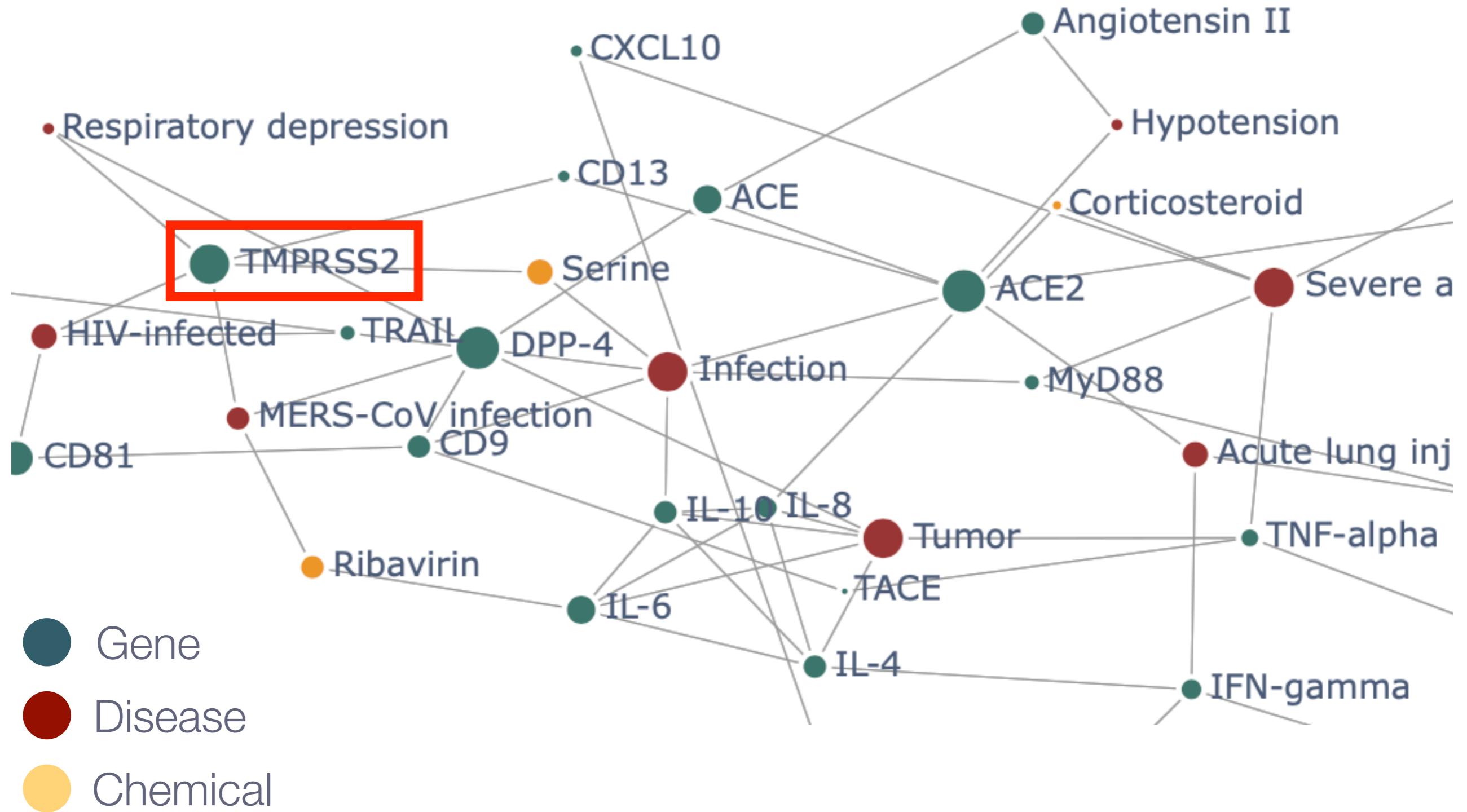
We need effective drugs to fight COVID-19.

The fastest way is to repurpose existing drugs.

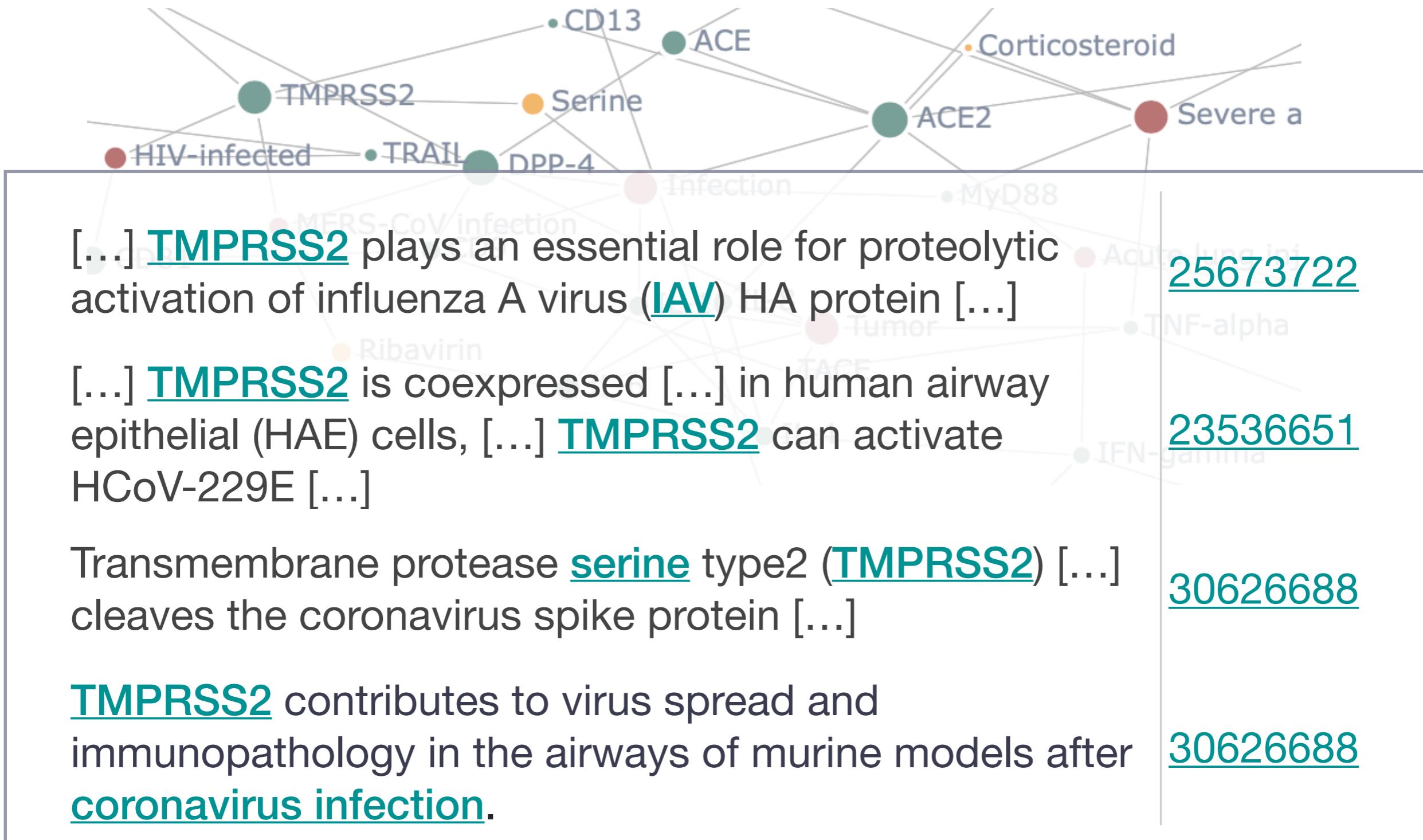
Repurposing Workflow



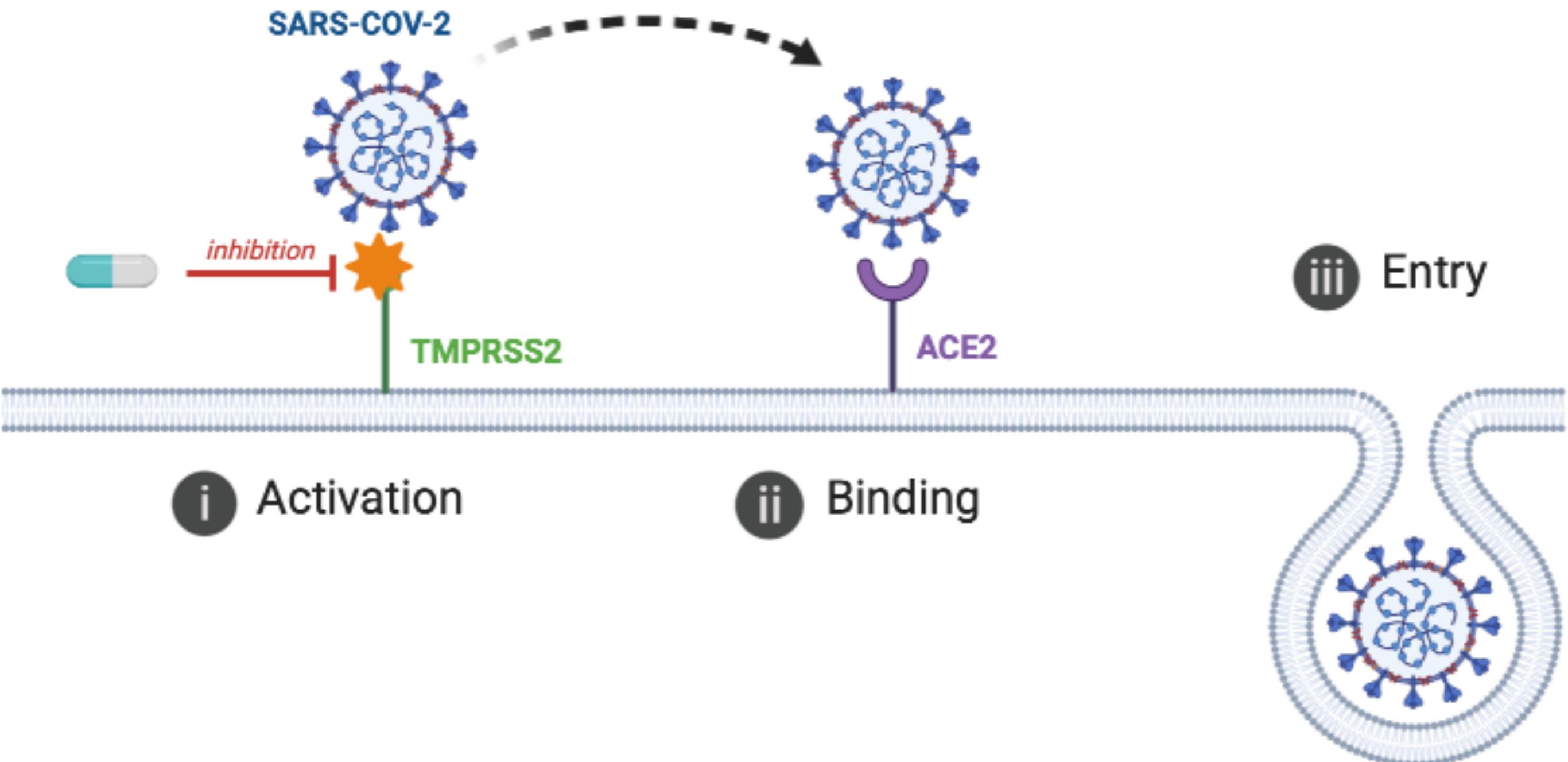
We mined the literature for therapeutic targets



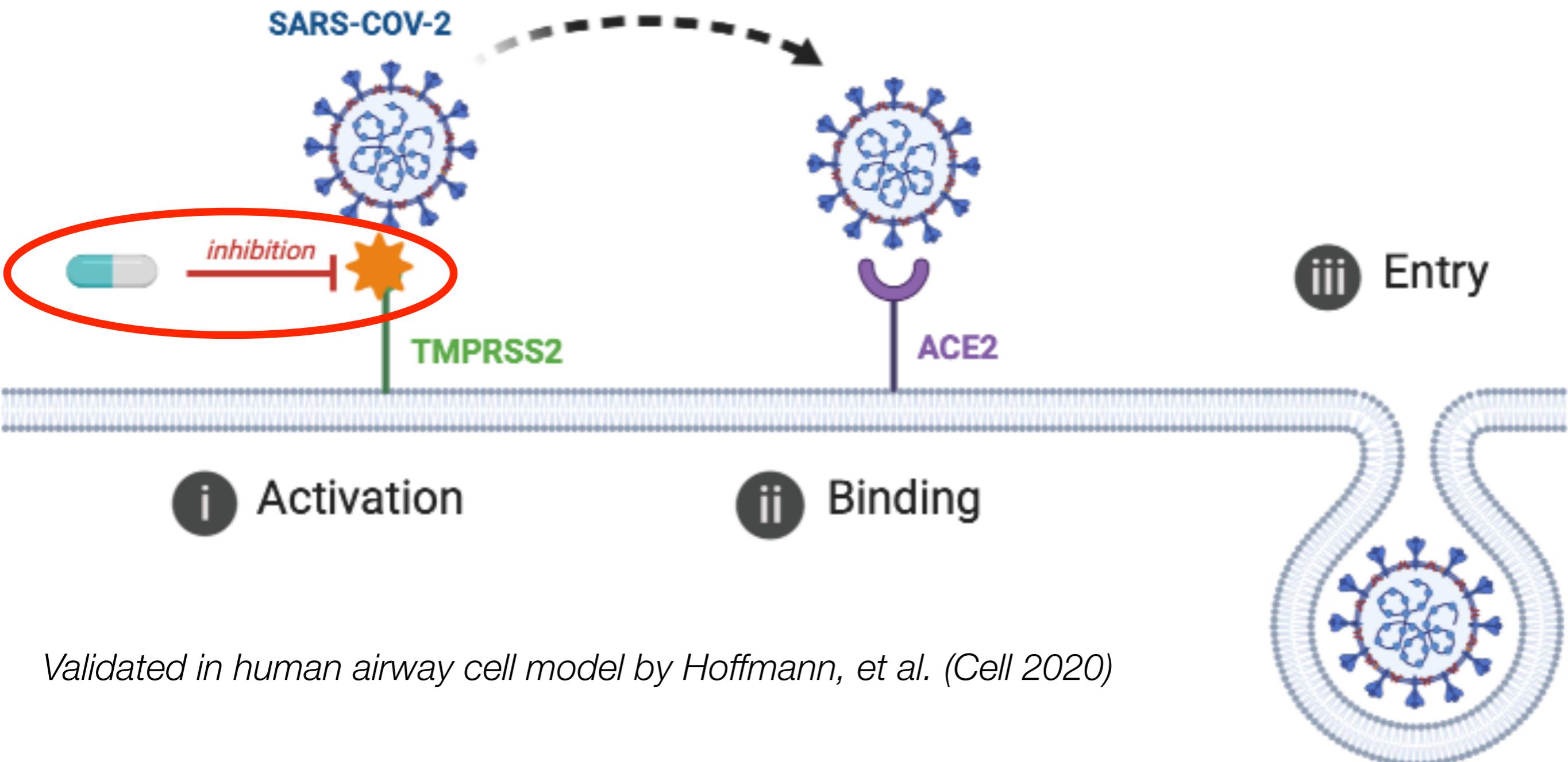
...and identified TMPRSS2 as a candidate



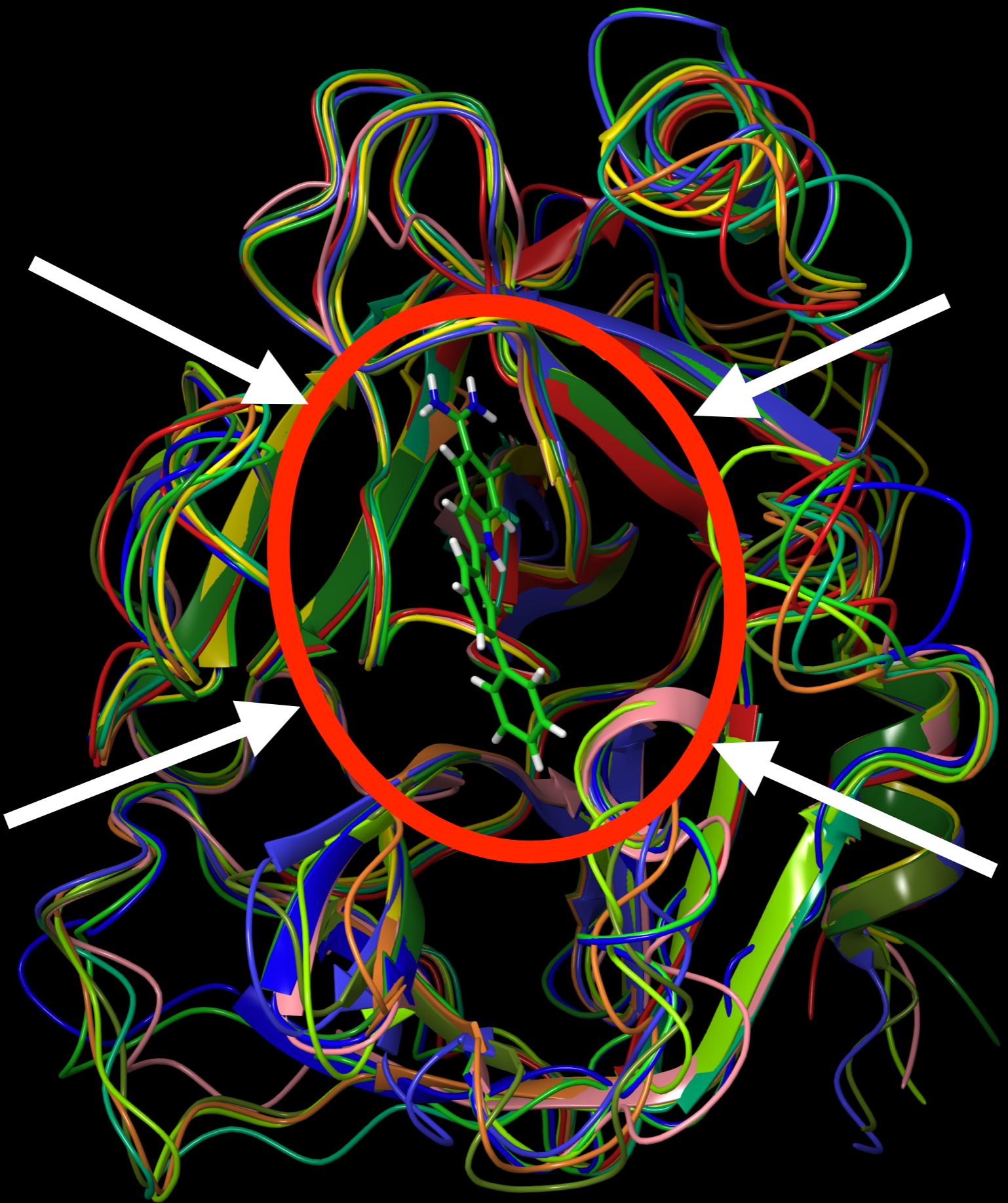
Proposed Mechanism of Action

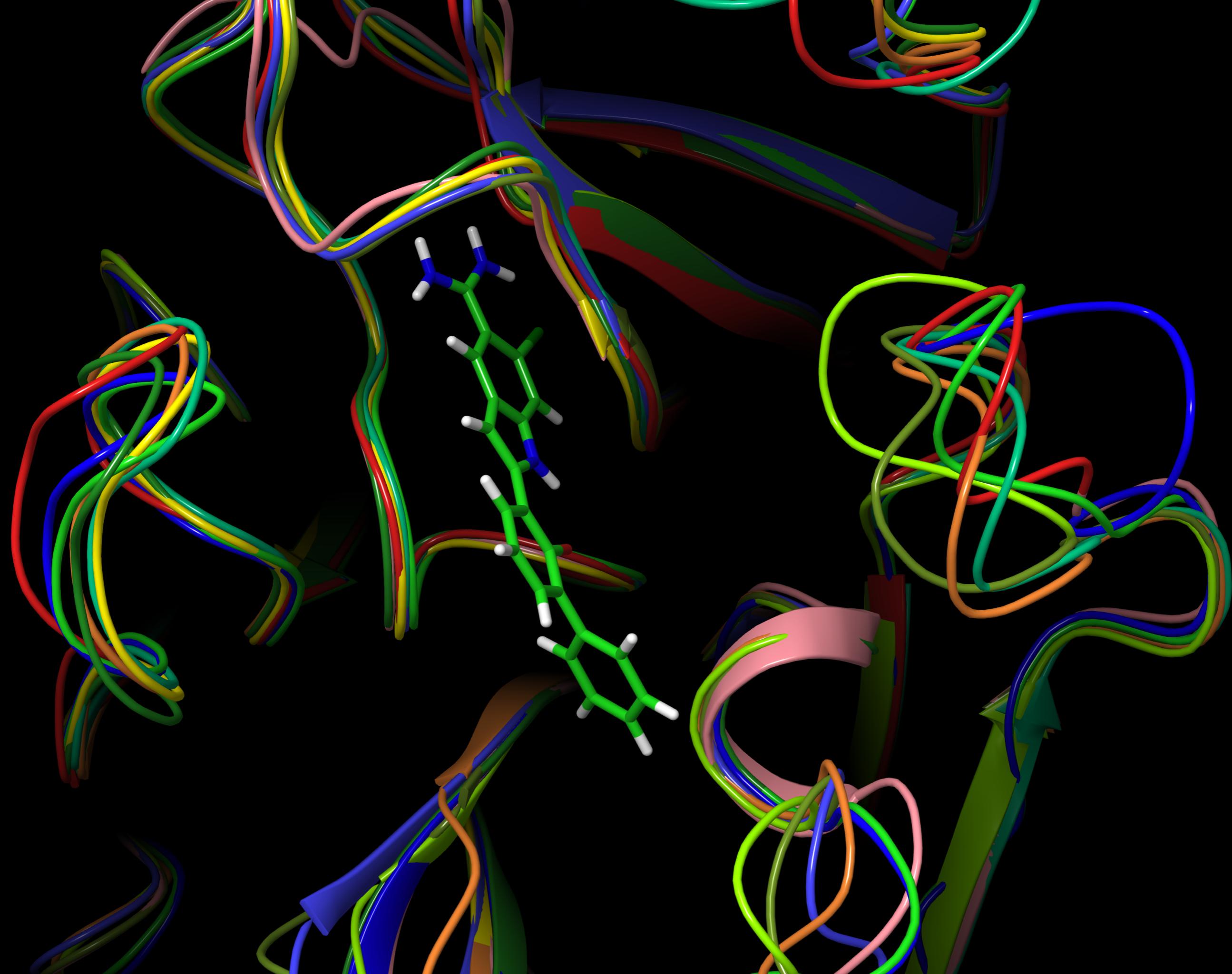


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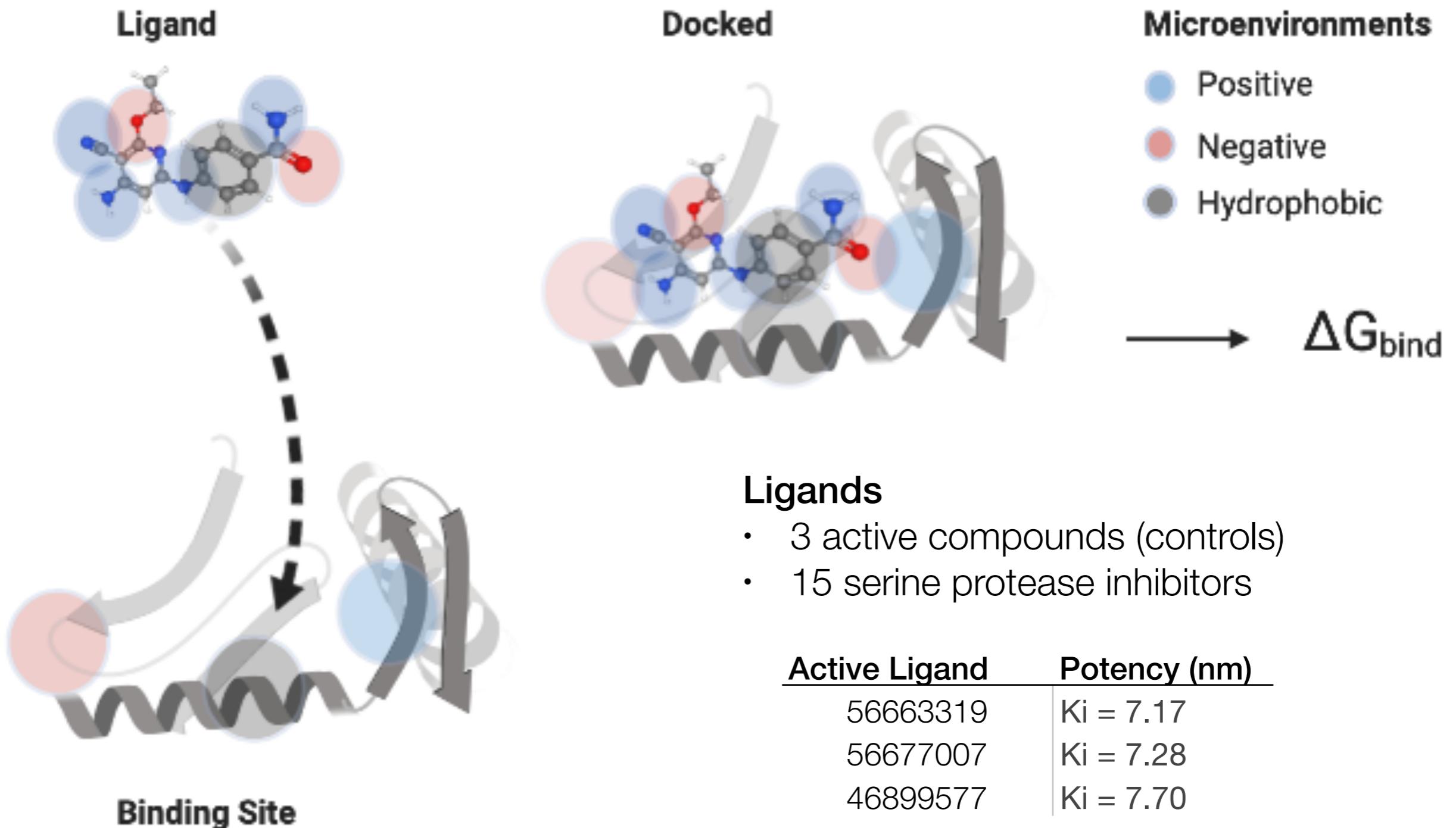


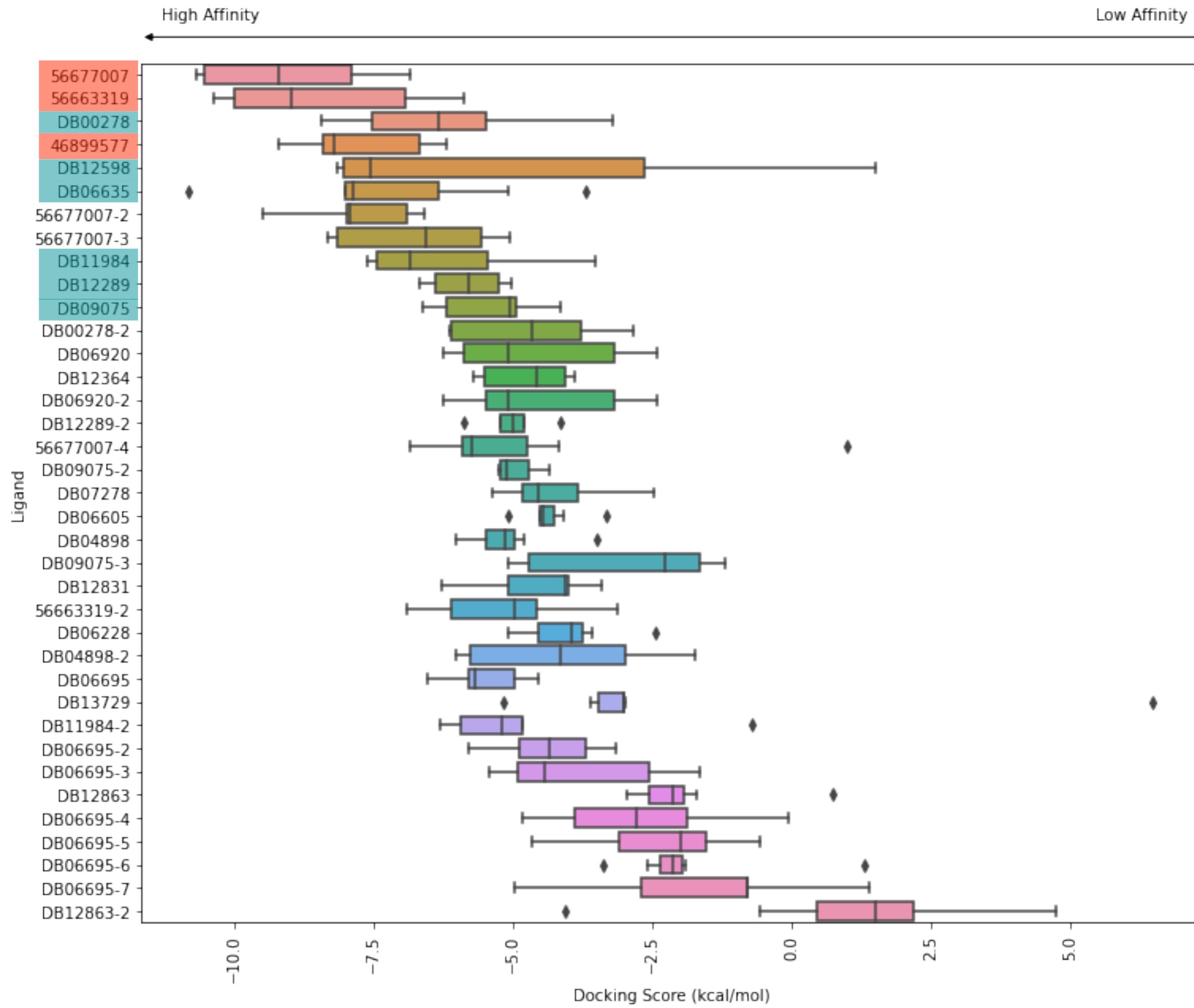






Docking simulations can predict binding





Top Scoring Compounds

Identifier	Status	Indication¹	Side Effects²	Min Score	Avg Score
DB06635	Experimental	Thrombosis	Catheter site hematoma Gastrointestinal hemorrhage Vascular pseudoaneurysm	-10.81	-7.29
DB00278	Marketed	Thrombosis Heparin induced thrombocytopenia	Increased INR Prolonged aPTT Hemorrhage	-8.45	-6.29
DB12598	Marketed	Disseminative blood vessel coagulation	Platelet count decreased Abnormal hepatic function	-8.14	-5.08
DB11984	Experimental	Thrombosis Venous thromboembolism	Angina Pectoris Epistaxis Hematauria	-7.60	-6.26
DB12289	Experimental	Thrombosis Venous thromboembolism	Bleeding events	-6.67	-5.83
DB09075	Marketed	Thromboemolsim Deep vein thrombosis	Gastrointestinal hemorrhage Epistaxis Rash	-6.62	-5.43

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Future Directions

Experimental Validation



Acknowledgements

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Thank You

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