

# A geometric XAI approach to protein pocket detection.

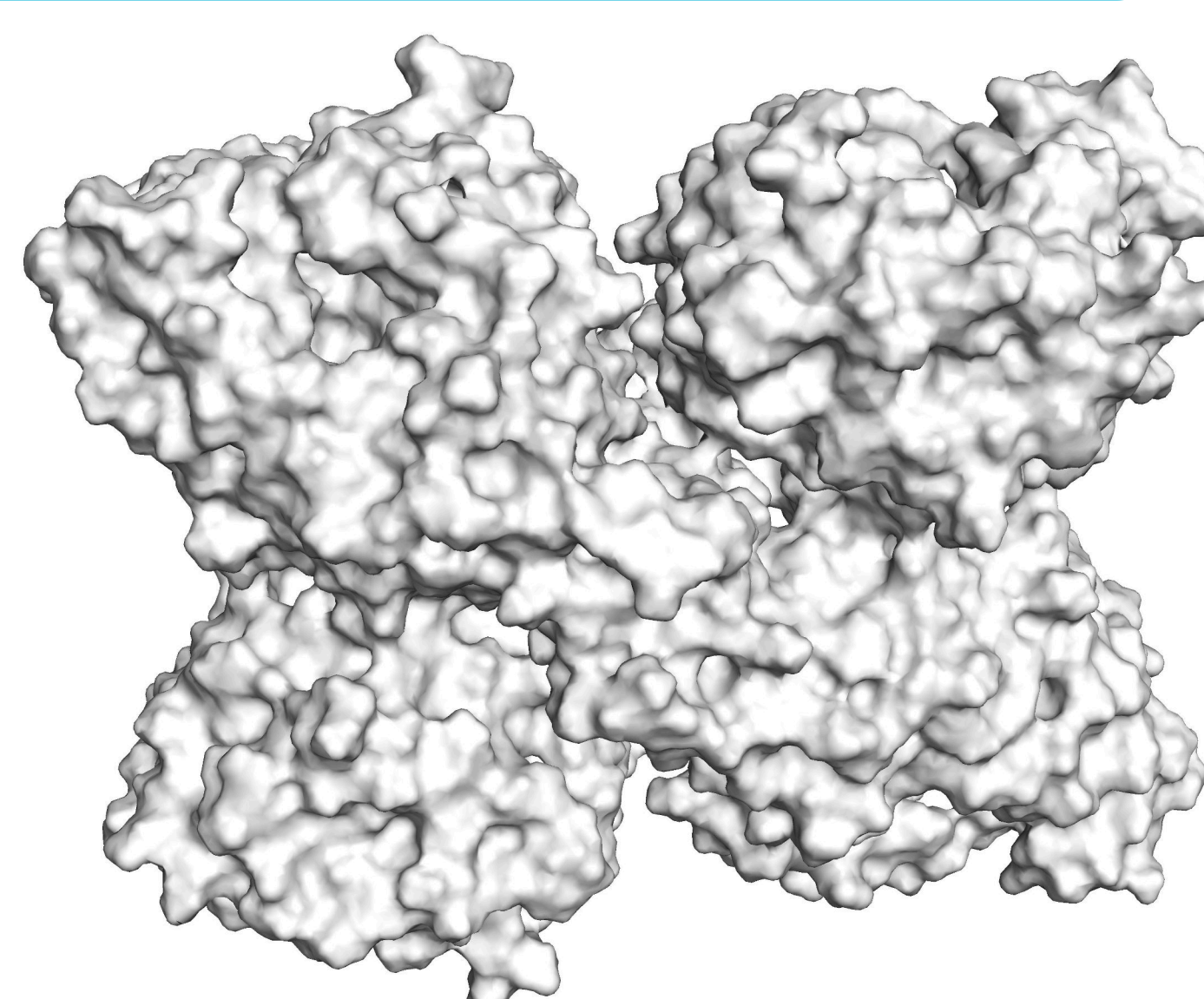


**Giovanni Bocchi** - Department of Environmental Science and Policy, University of Milan

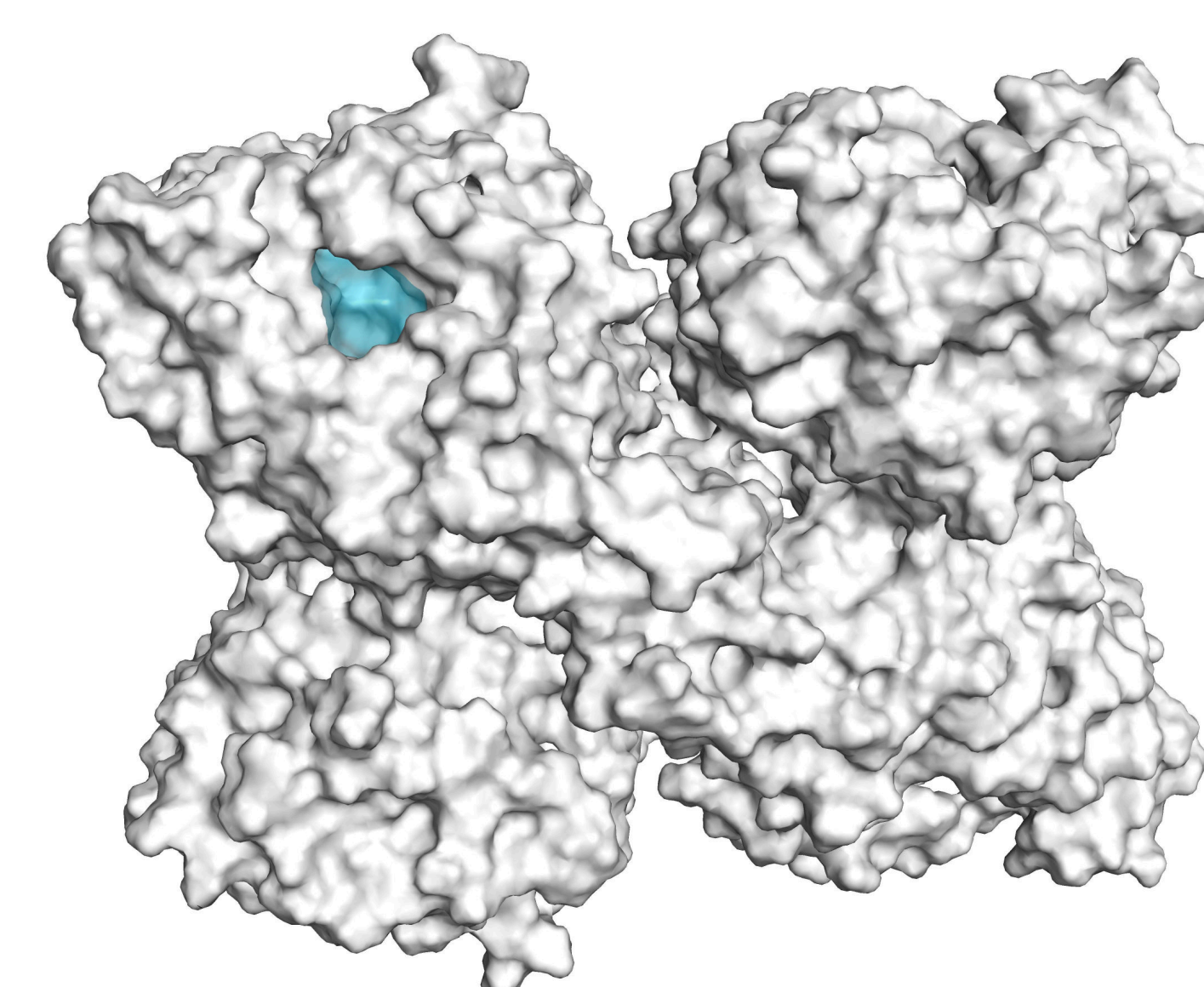
## The Problem

**Protein Pocket Detection** is a key problem in the context of Drug Discovery.

**Molecular Docking** screenings highly benefit restriction of the search (informed docking) to promising areas, reducing costs and increasing accuracy.



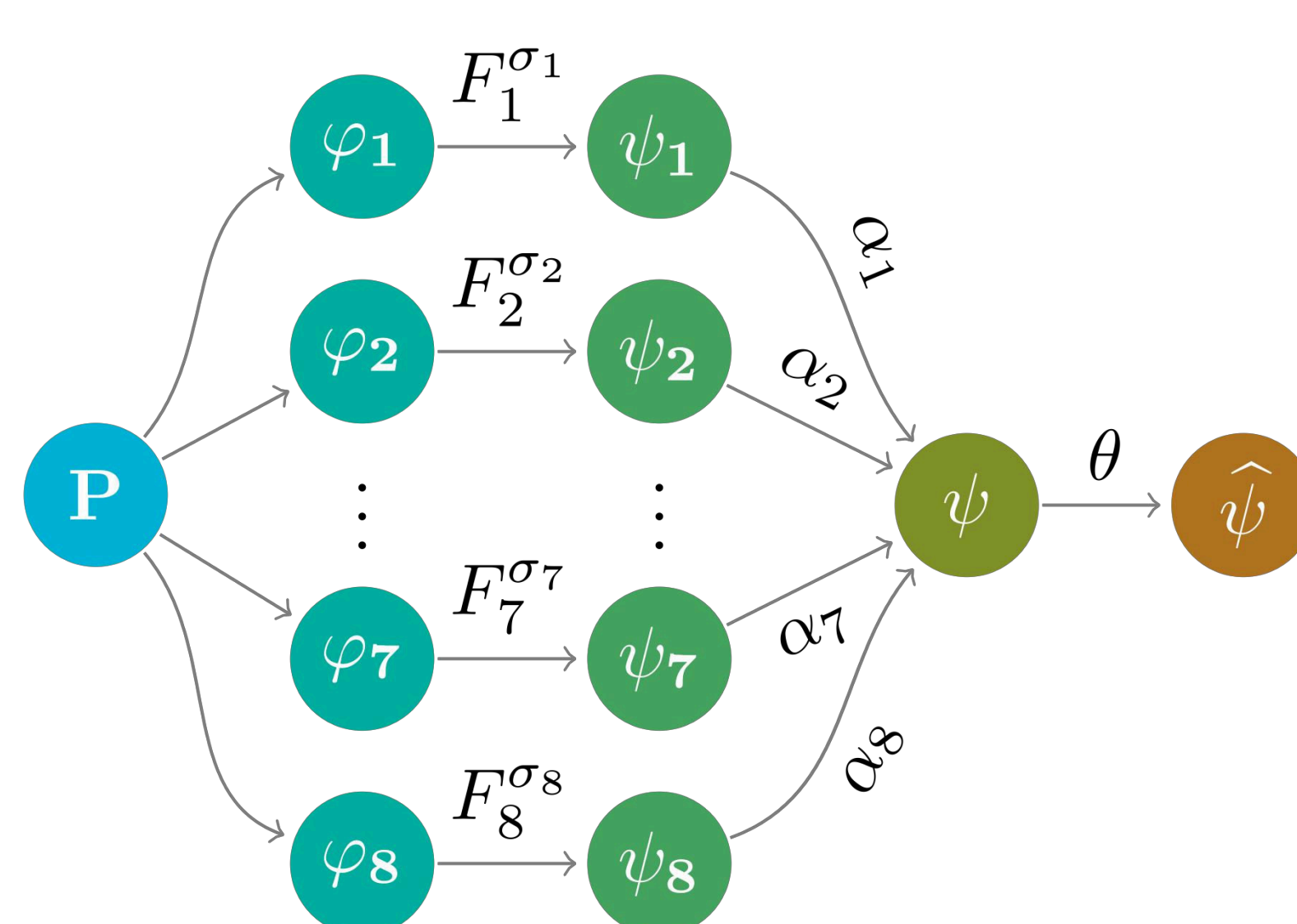
Blind Docking



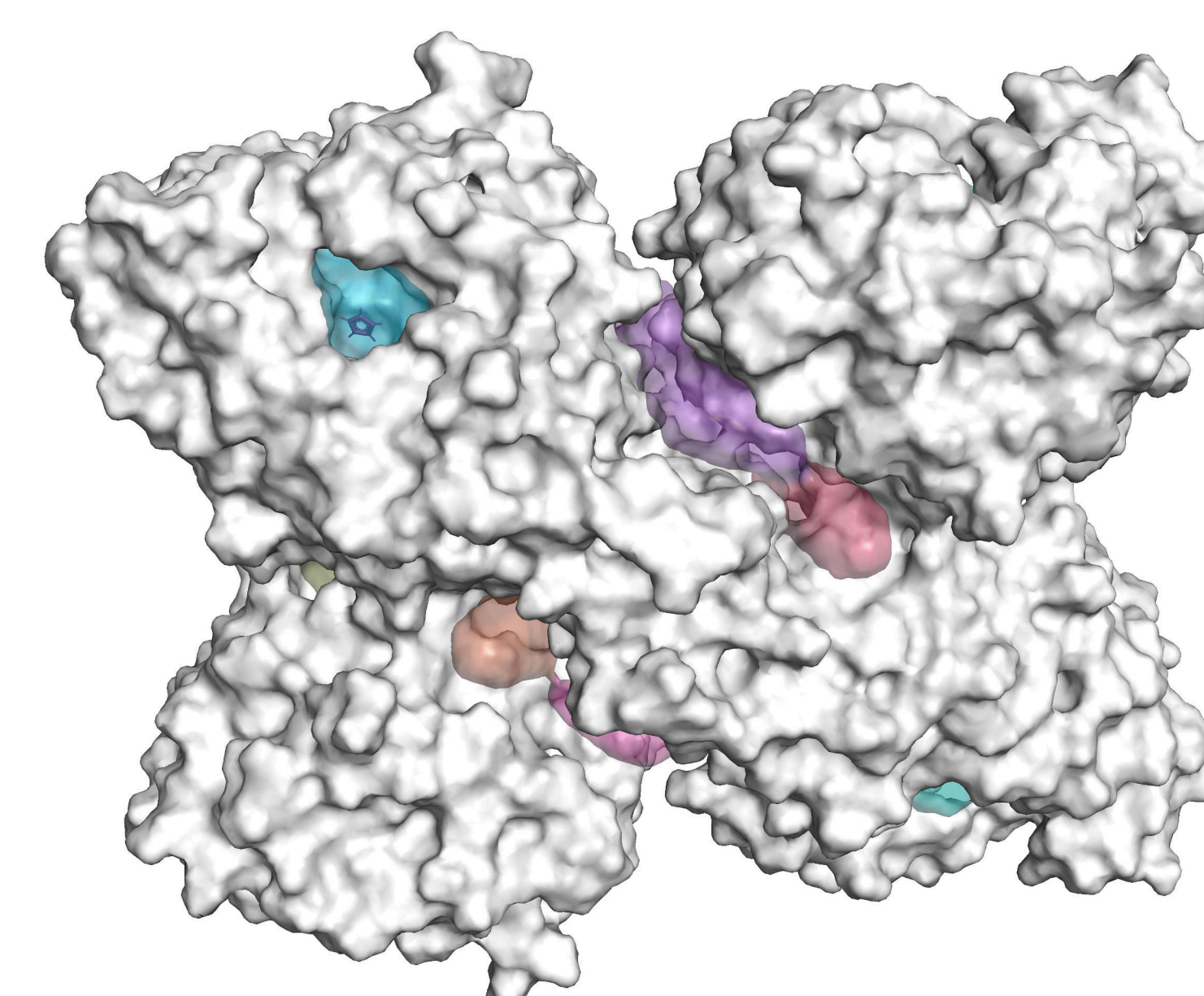
Informed Docking

## GENEOnet

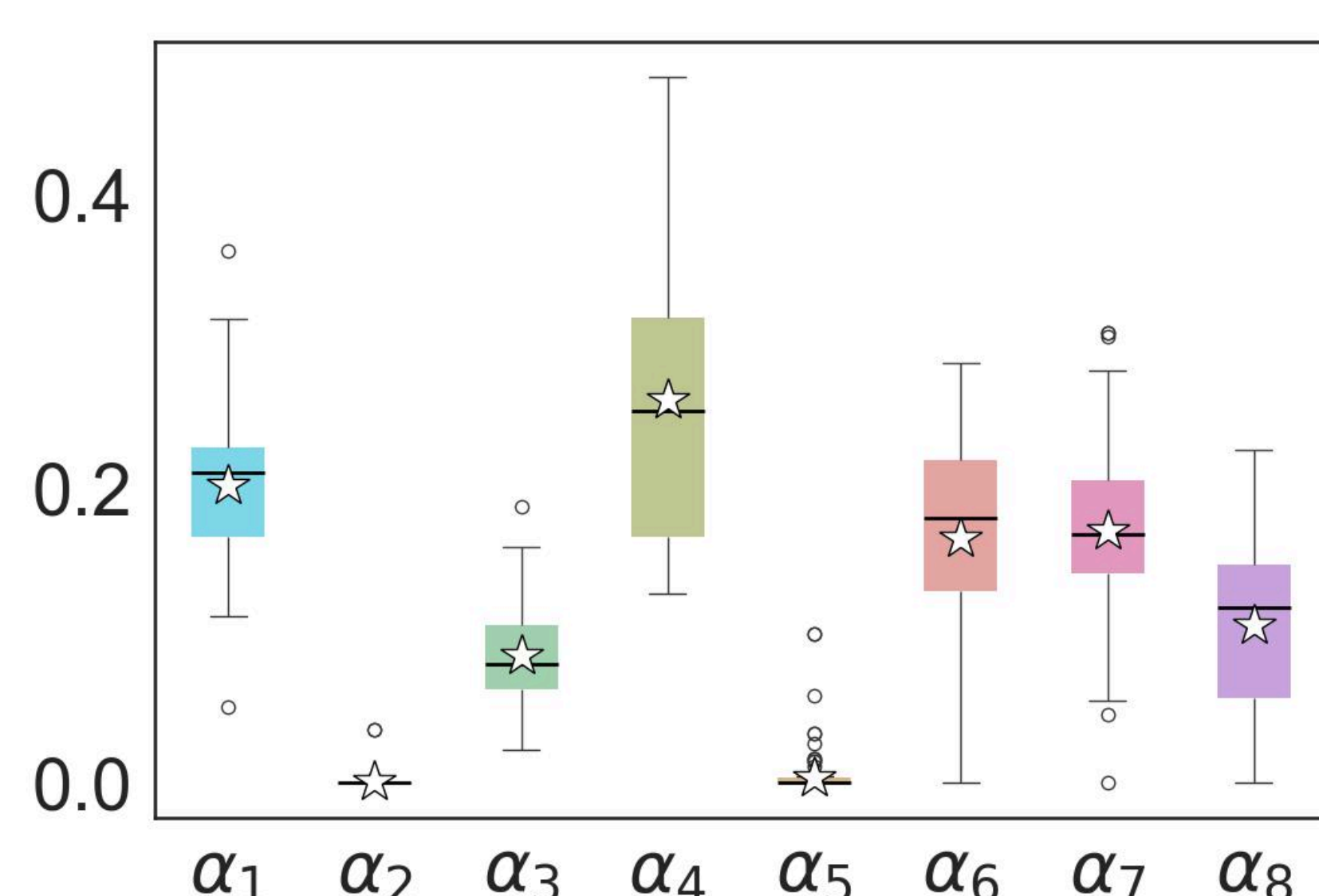
**GENEOnet** is a shallow network of GENEOnets dependent on only 17 trainable parameters. This, combined with equivariance and the need of less training examples make the model explainable and less expensive.



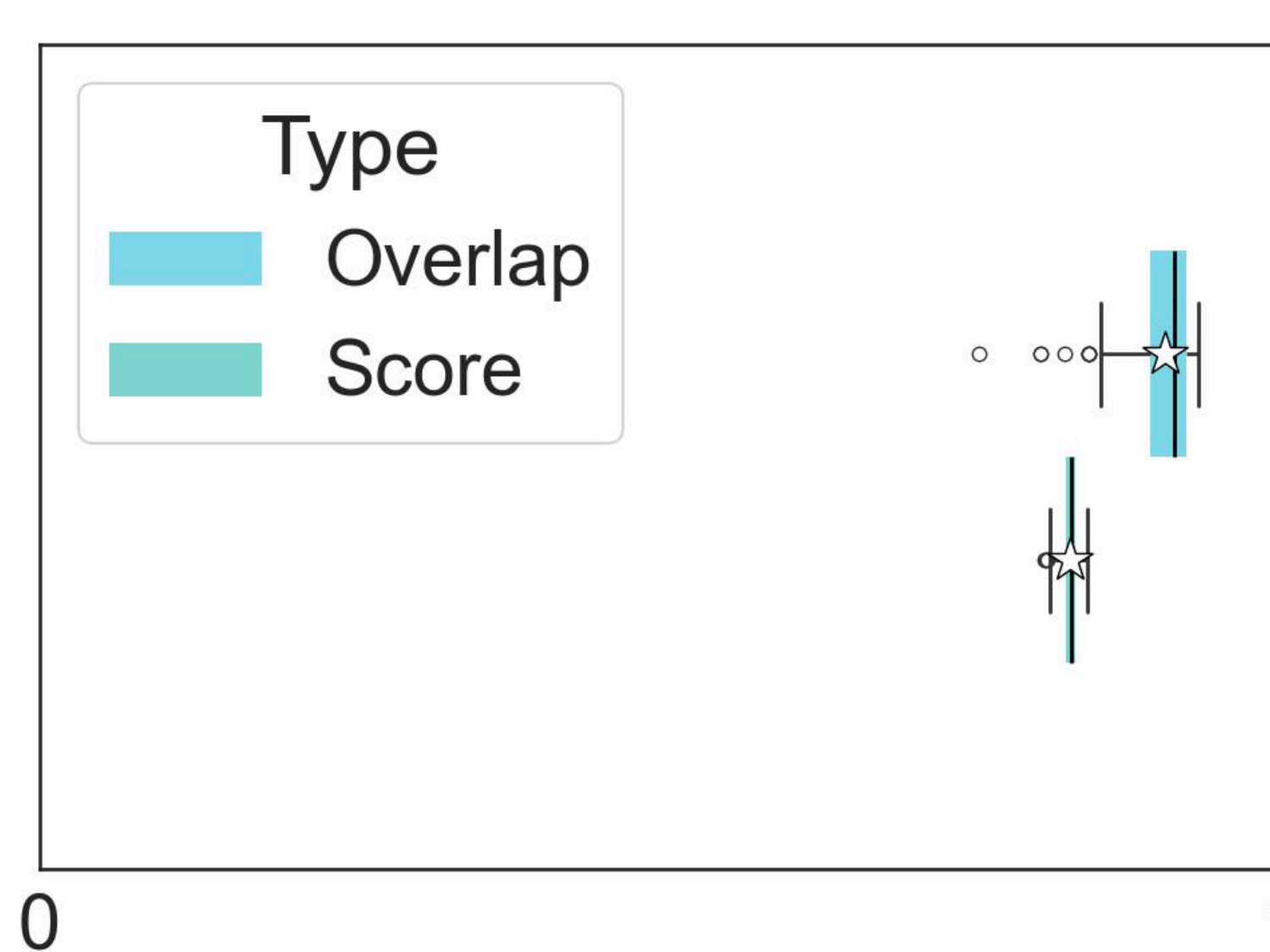
## Prediction



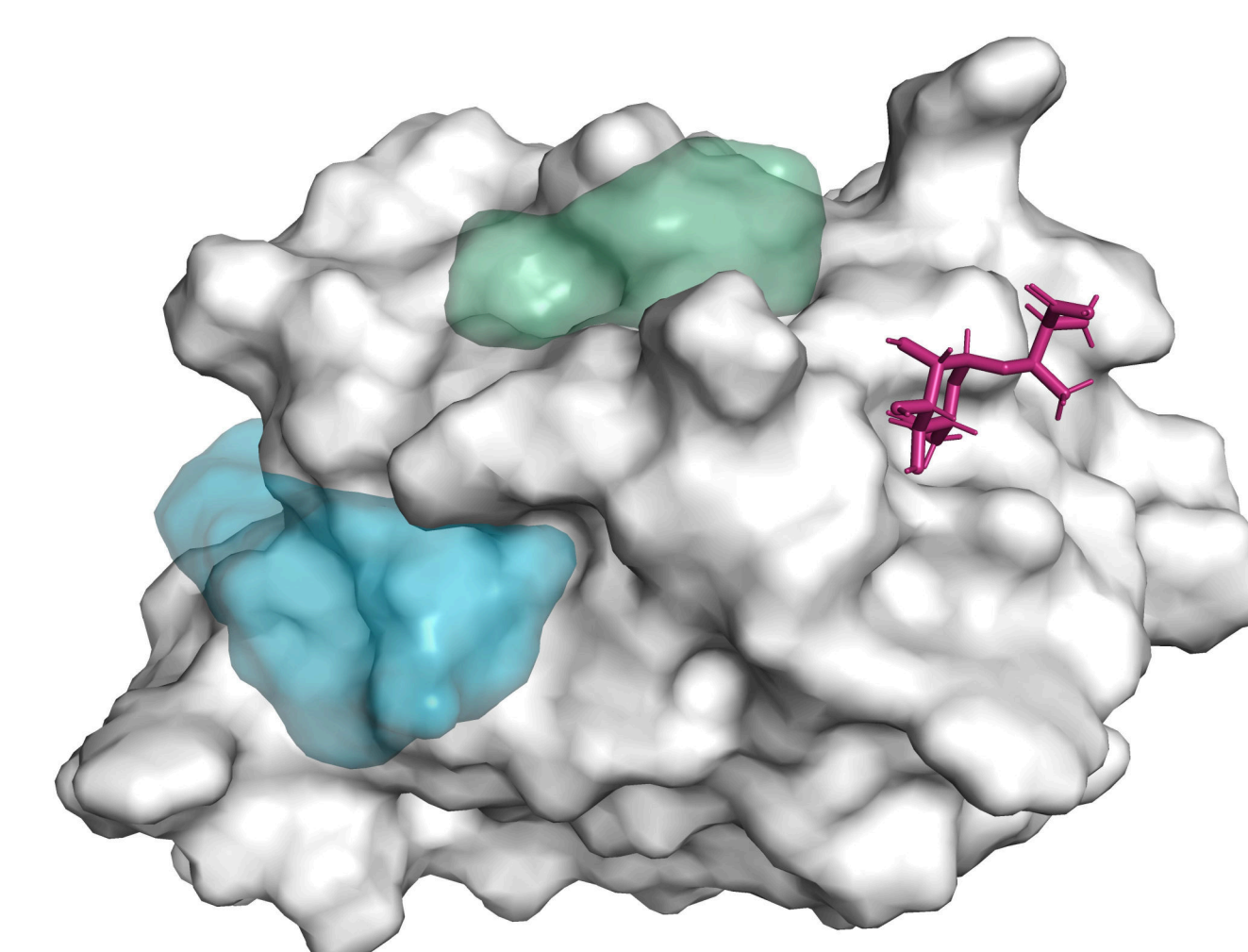
## Analysis



**Sensitivity Analysis** of parameters with respect to variations of the training set.



**Random Perturbation Analysis** to test model robustness to variations in the protein conformation.



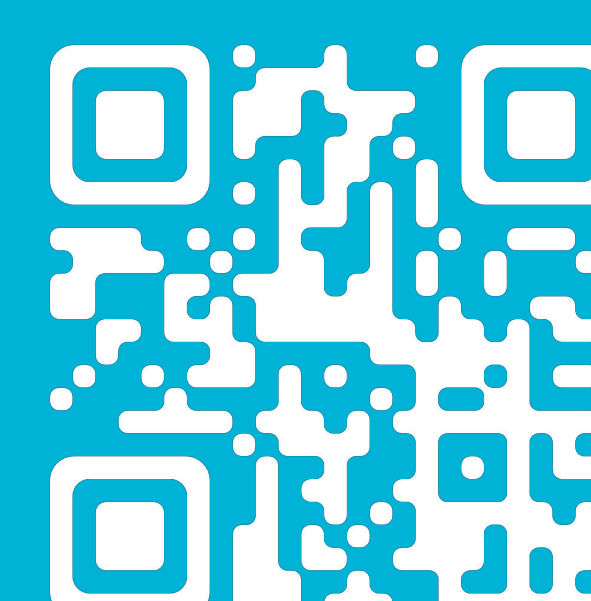
**Failure Analysis** to understand the possible reasons for not recognizing a pocket.

### Joint work with

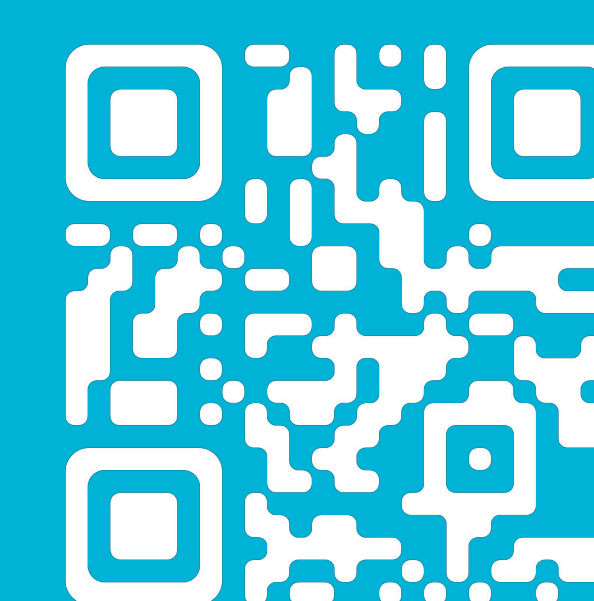
A. Micheletti, P. Frosini,  
A. Pedretti, G. Palermo,  
D. Gadioli, C. Gratteri, F. Lunghini,  
A.R. Beccari, A. Fava and C. Talarico

### More Questions ?

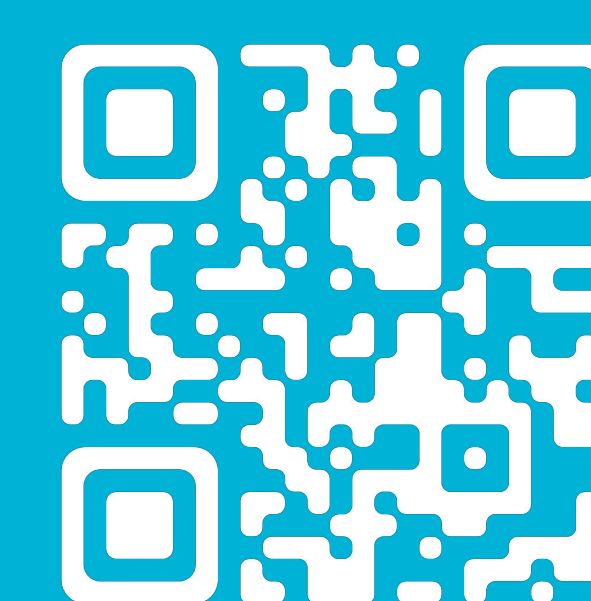
Reach me at  
giovanni.bocchi1@unimi.it  
www.linkedin.com/in/giovanni-bocchi-01998b197



Try it



GENEOnet



GENEOnets