



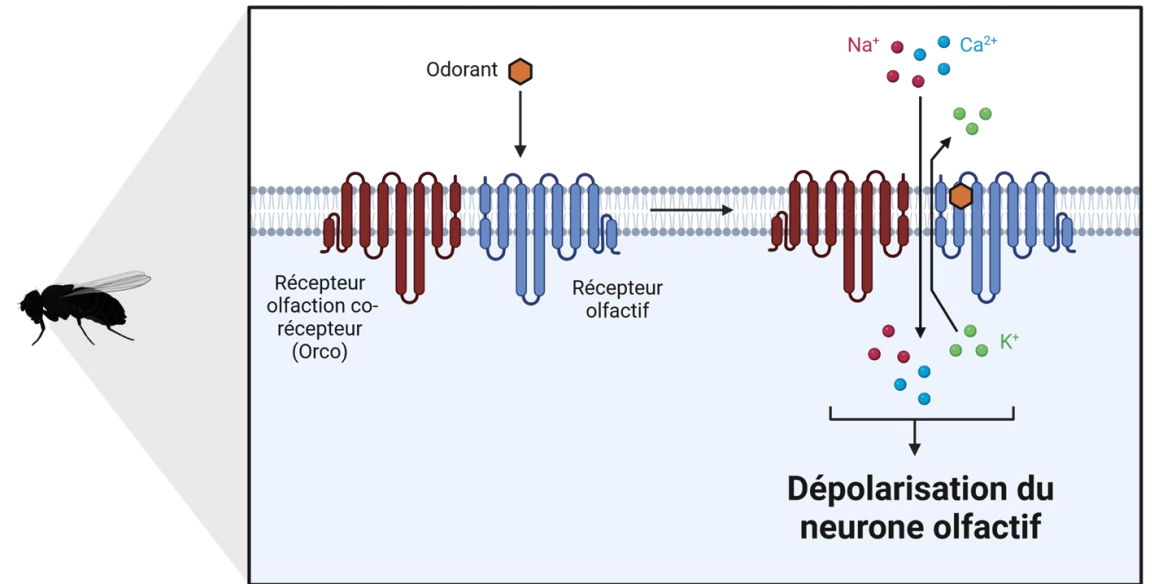
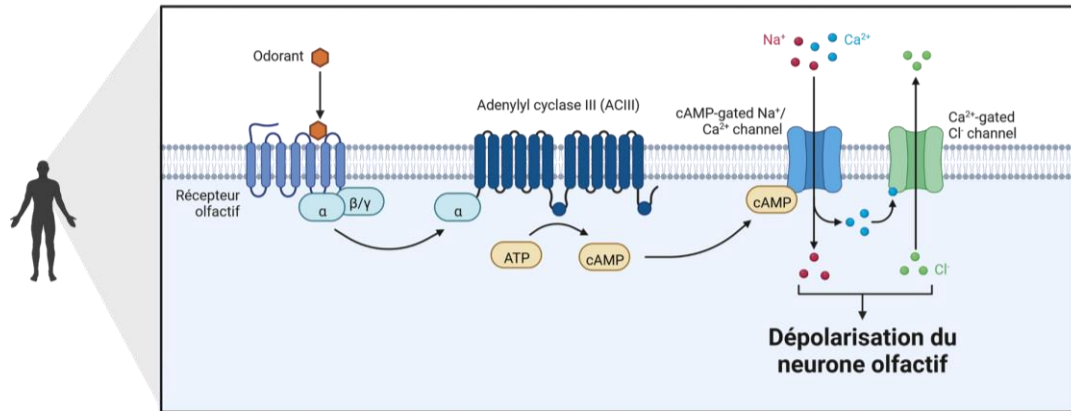
Numerical models decipher
odorant binding and receptor
activation at the molecular level



UNIVERSITÉ
CÔTE D'AZUR
ChEmoSim

Dr. Jérémie Topin

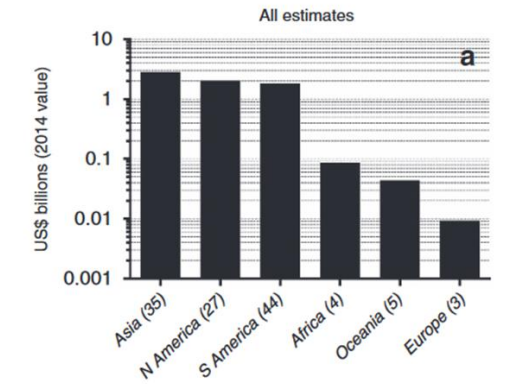
Nature created two olfaction systems



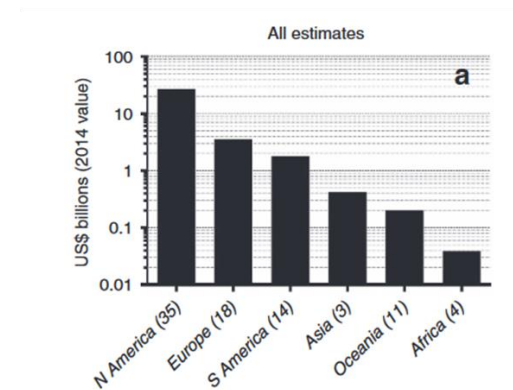
Massive yet grossly underestimated global costs of invasive insects



Dr. J. Pacalon



Goods and services costs associated with invasive insects

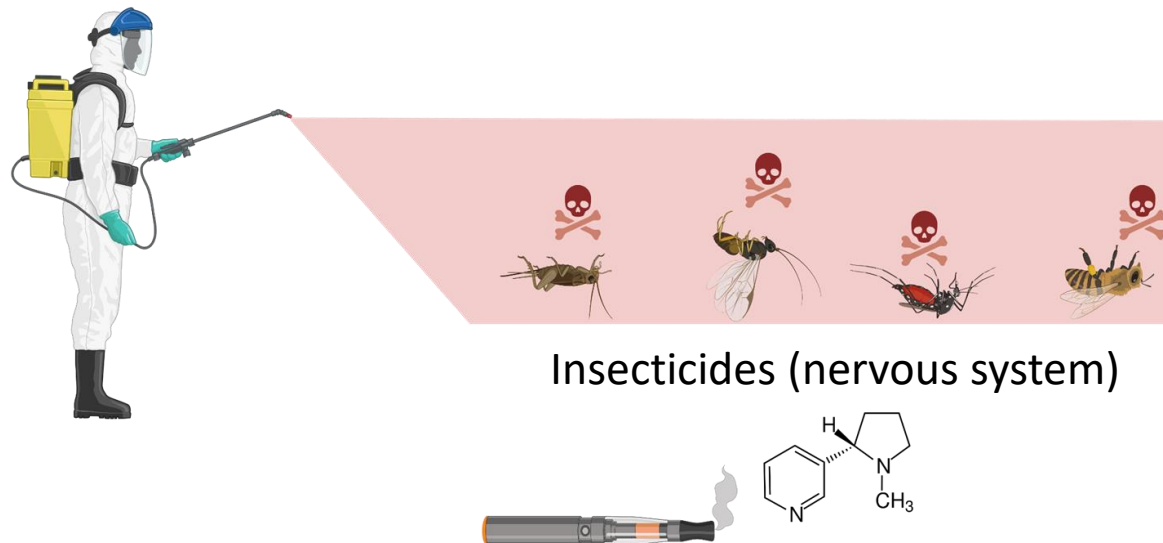


Human health costs associated with invasive insect

Targeting Insect Olfaction



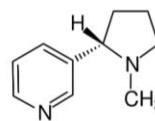
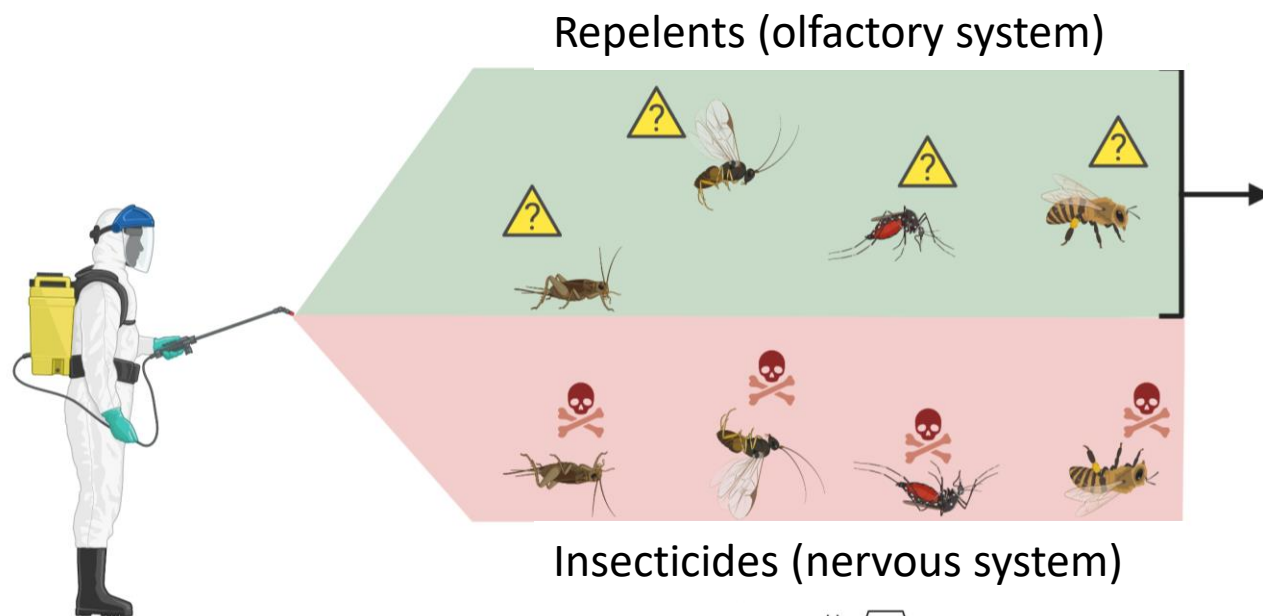
Dr. J. Pacalon



Targeting Insect Olfaction

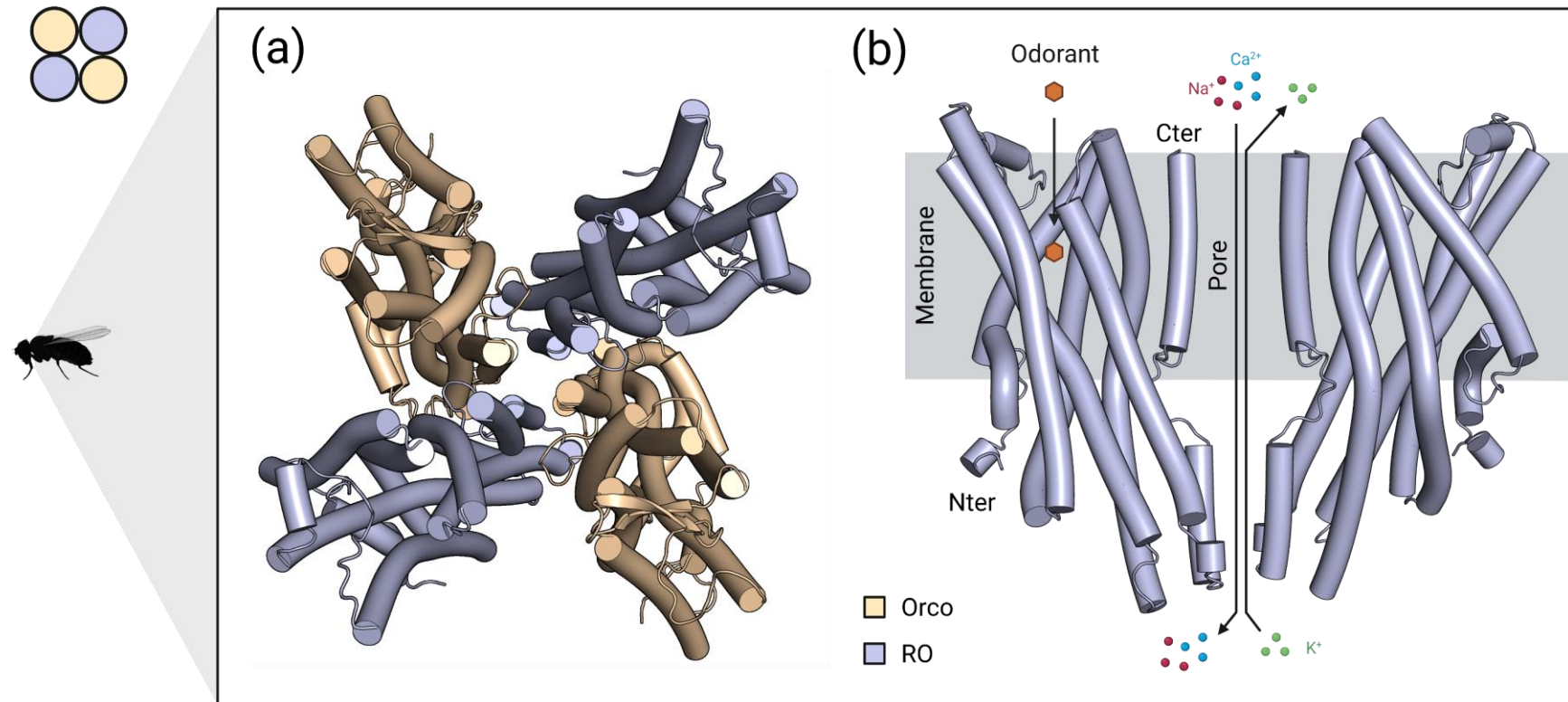


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Christophe Moreau

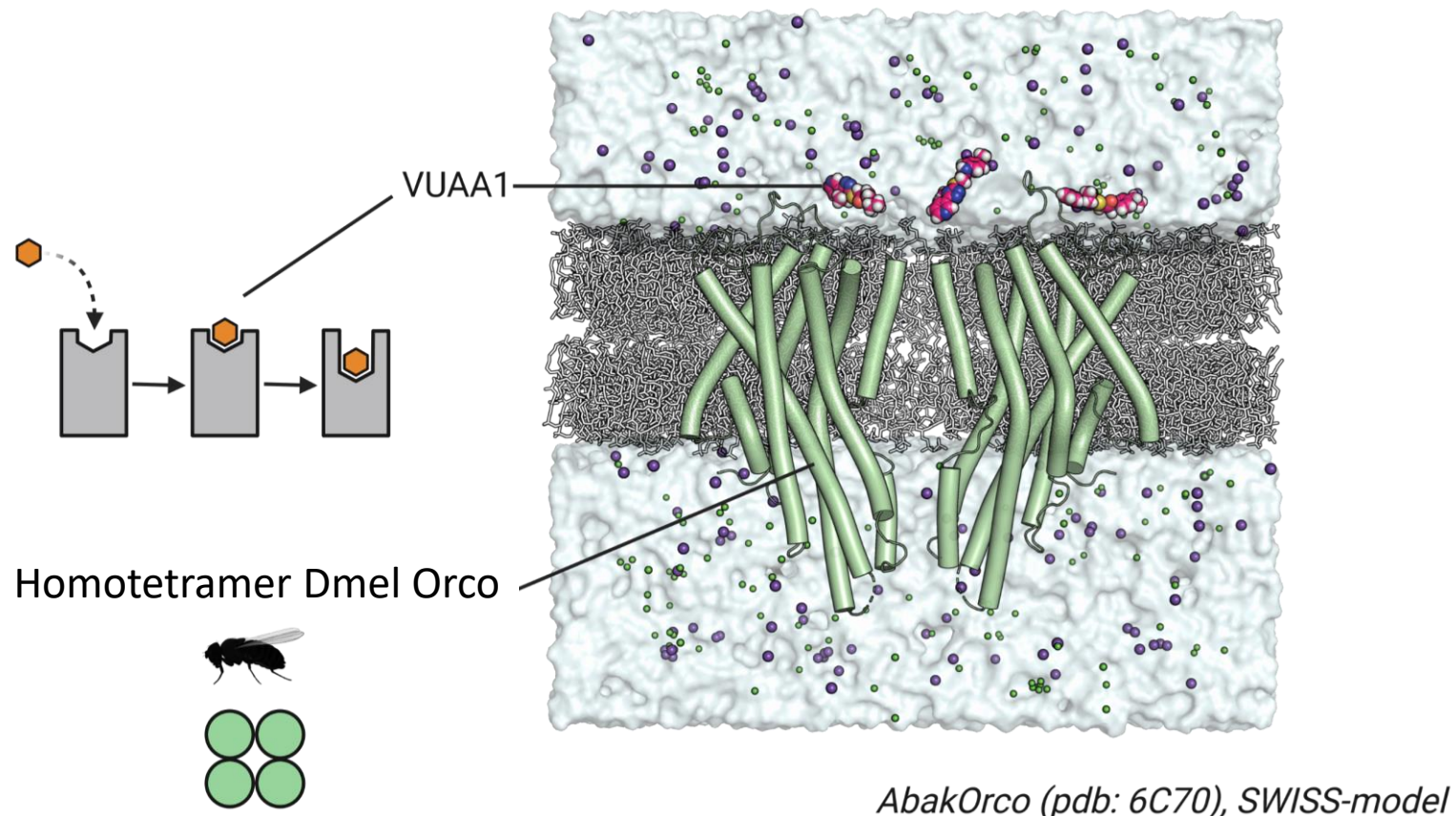
Quaternary structure of Insect OR



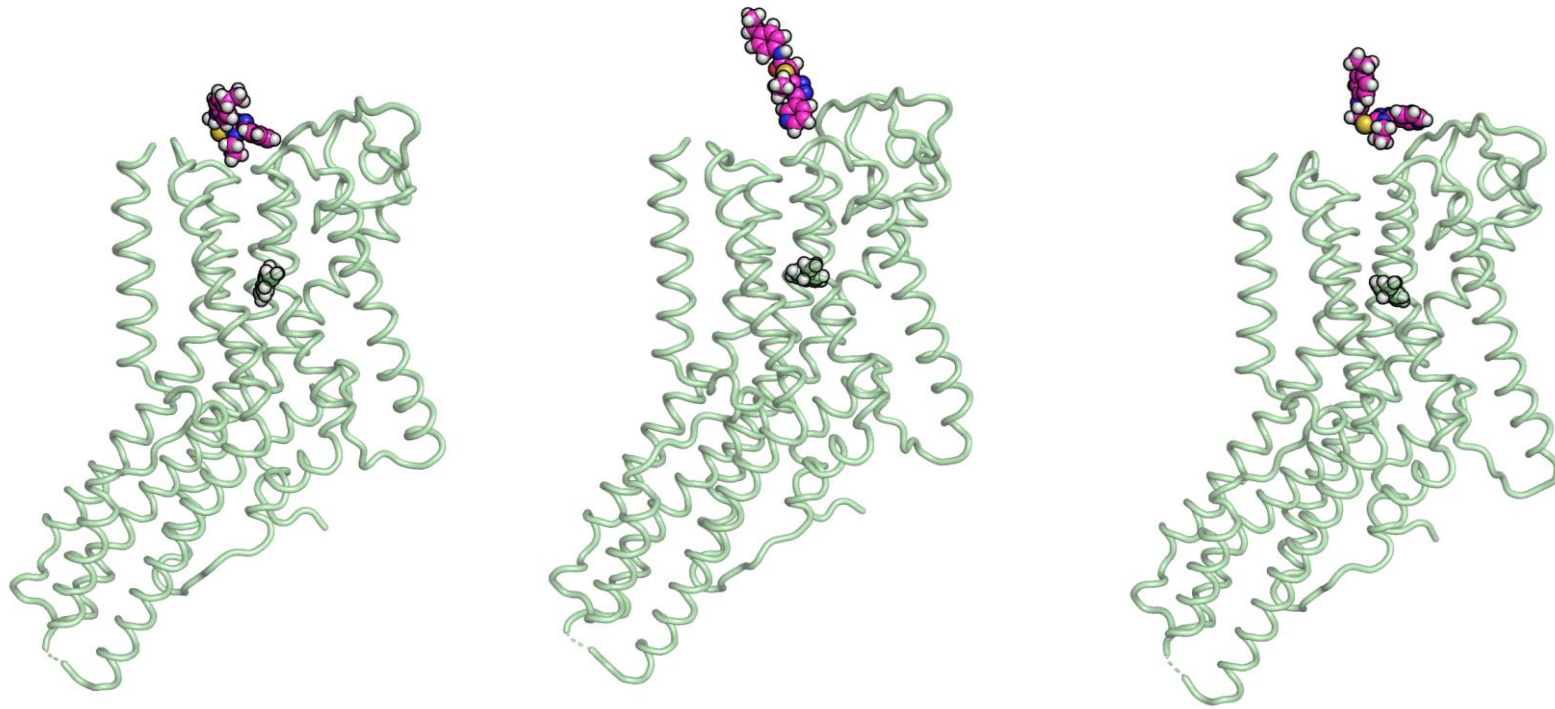


CAN WE IDENTIFY THE BINDING
POCKET OF A COMPLEX
MOLECULAR ASSEMBLY?

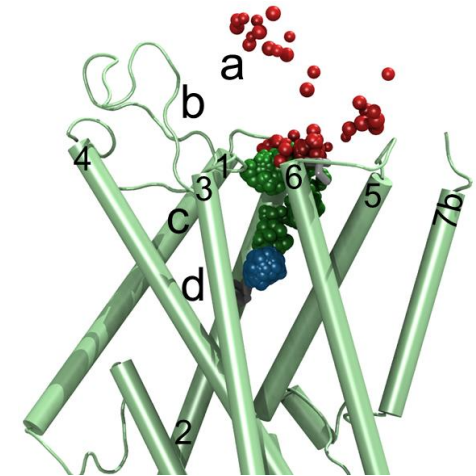
Binding Simulation



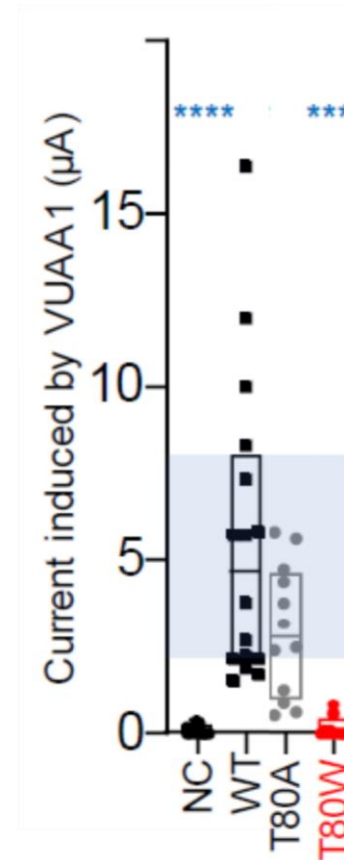
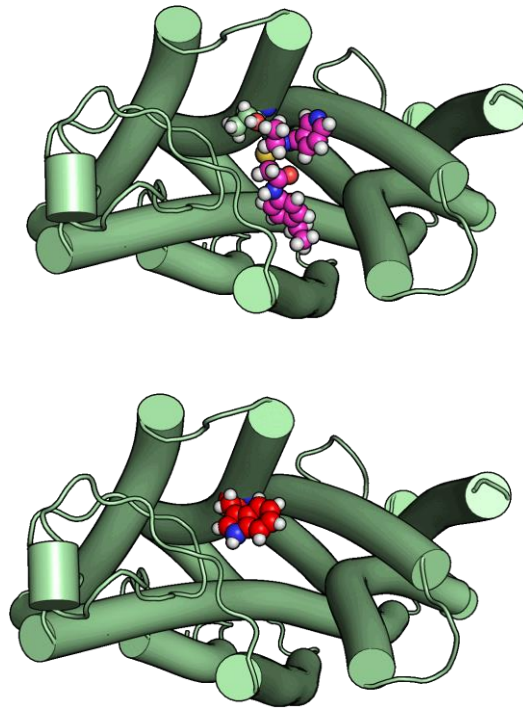
Binding Simulation / Results



22 independent simulations (31 μ s)
288 000 atoms (ff14SB/lipid14/gaff2)



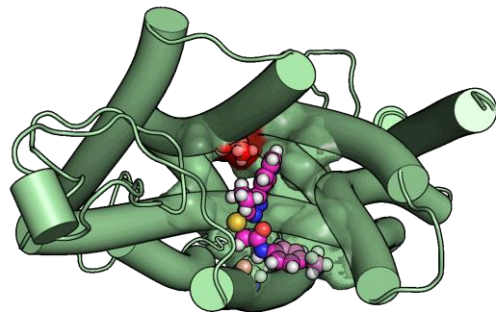
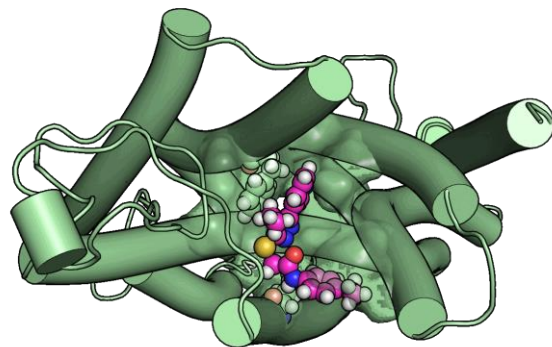
In Vitro evaluation Entry



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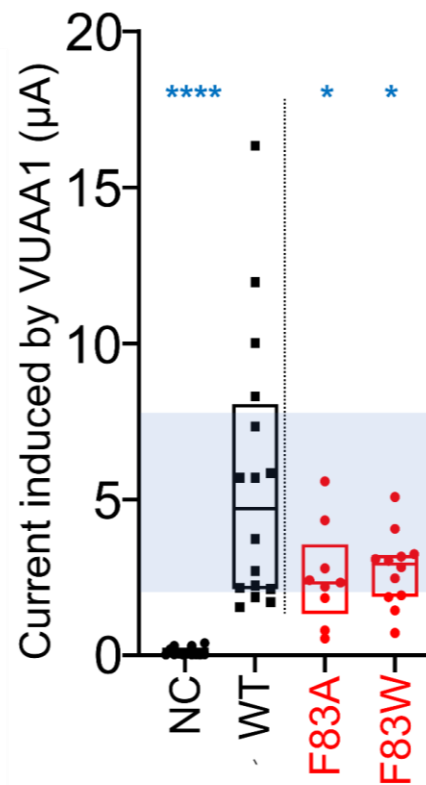
Une vision moléculaire du vivant
A molecular vision of life

In Vitro evaluation Binding Site

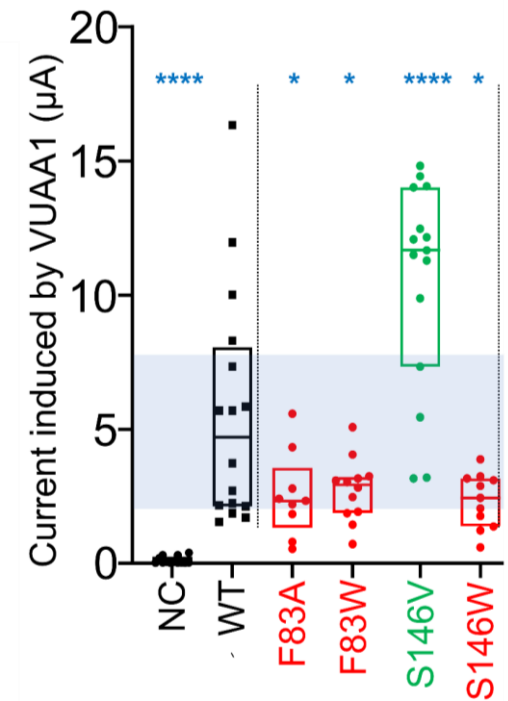
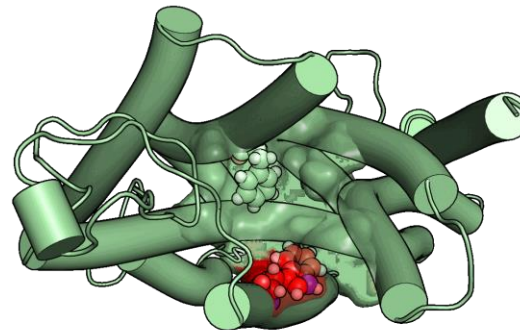
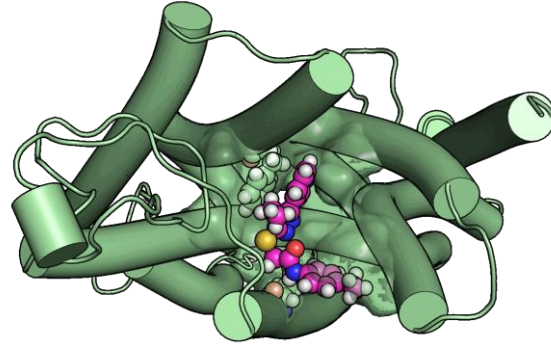


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Une vision moléculaire du vivant
A molecular vision of life



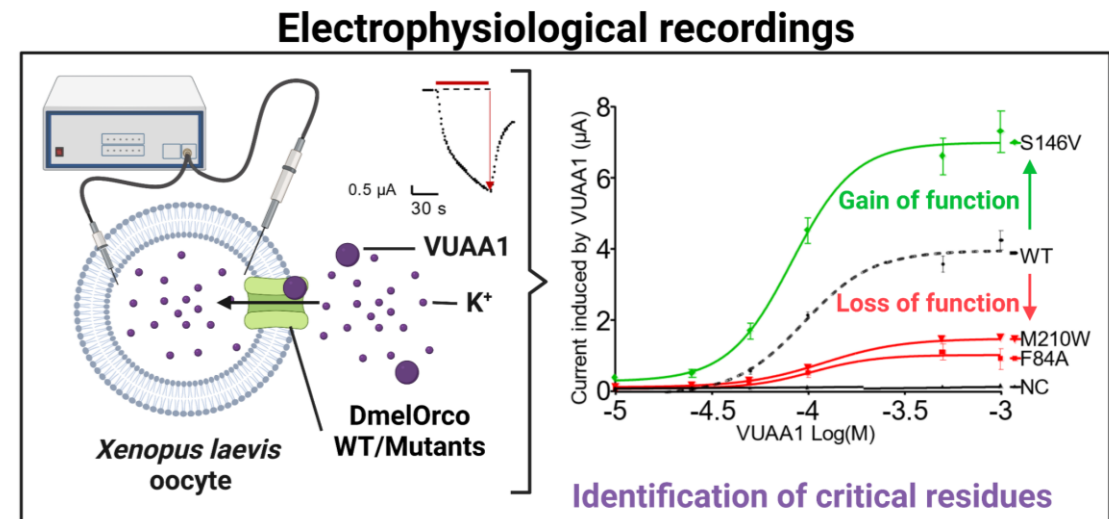
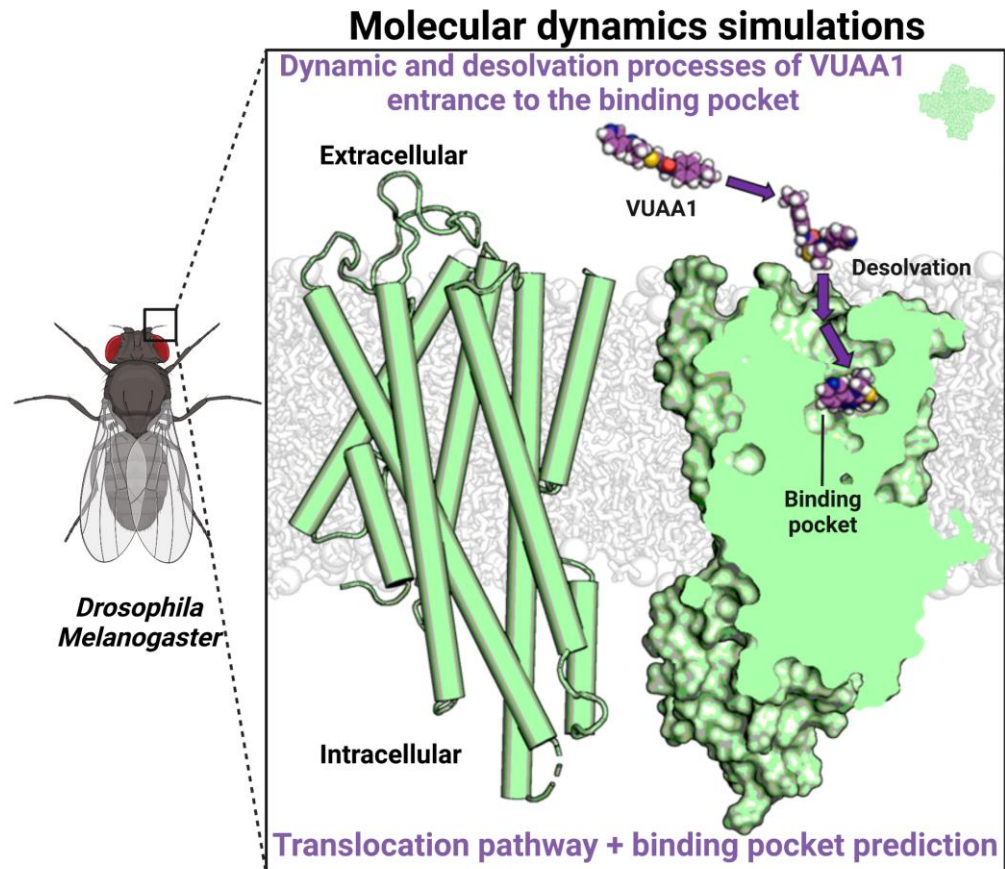
In Vitro evaluation Binding Site

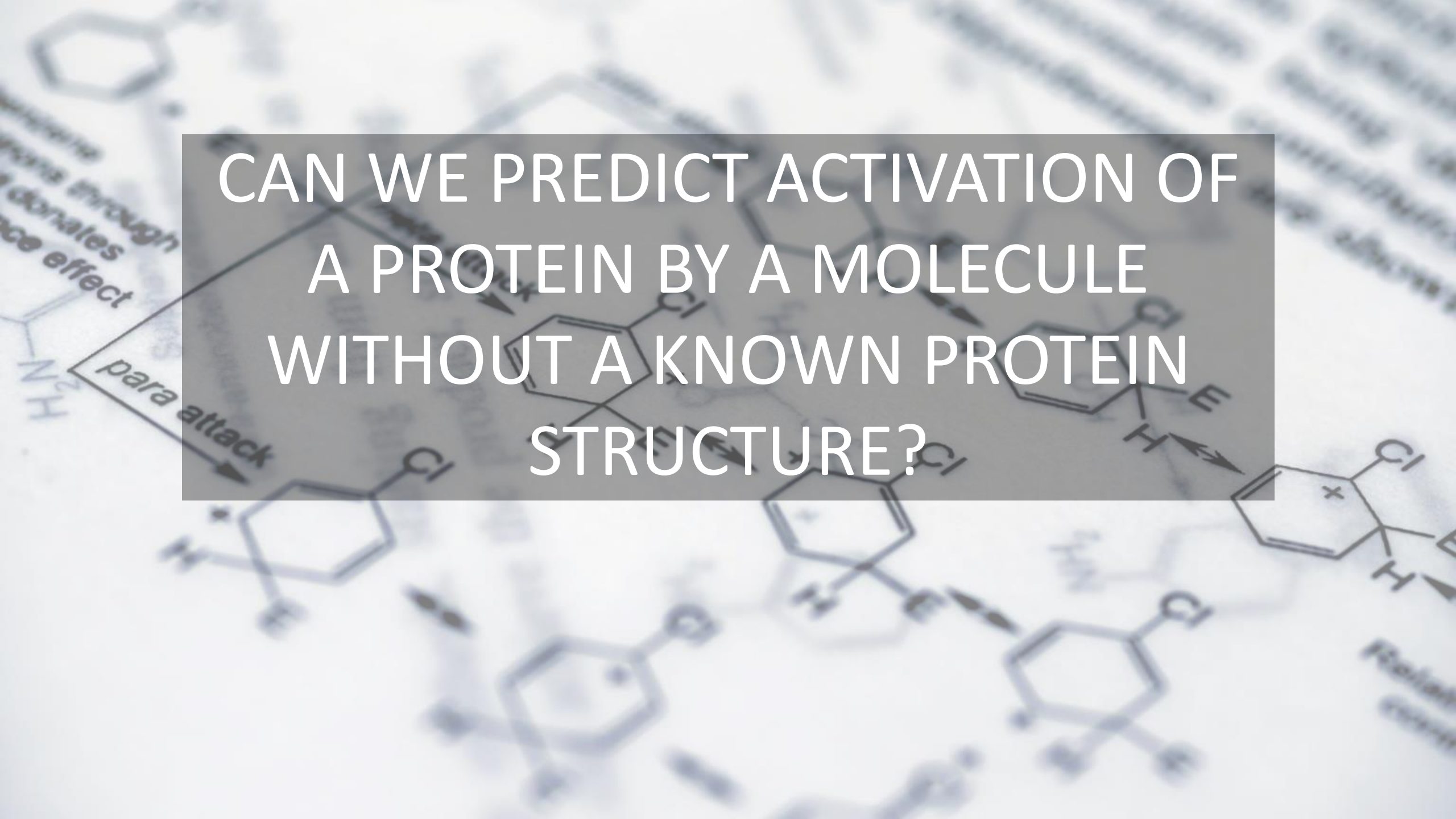


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Une vision moléculaire du vivant
A molecular vision of life

Translocation pathway in Orco



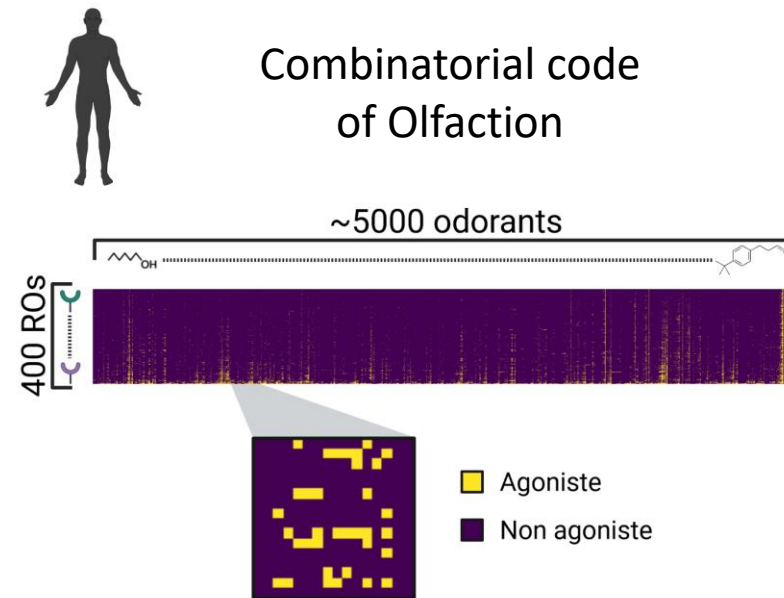
The background features a collage of chemical diagrams and reaction schemes. On the left, there are labels such as "para attack" and "resonance effect" with arrows pointing to various molecular structures. The structures include benzene rings with substituents like chlorine (Cl) and hydrogen (H), and other organic molecules. The overall theme is organic chemistry and reaction mechanisms.

CAN WE PREDICT ACTIVATION OF
A PROTEIN BY A MOLECULE
WITHOUT A KNOWN PROTEIN
STRUCTURE?

Cracking the Combinatorial Code of Olfaction

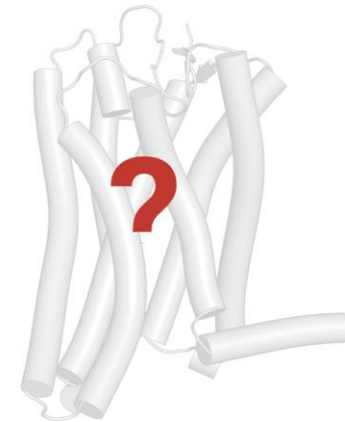


M. Lalis & M. Hladiš



The majority of Odorants-ORs pairs remains unknown

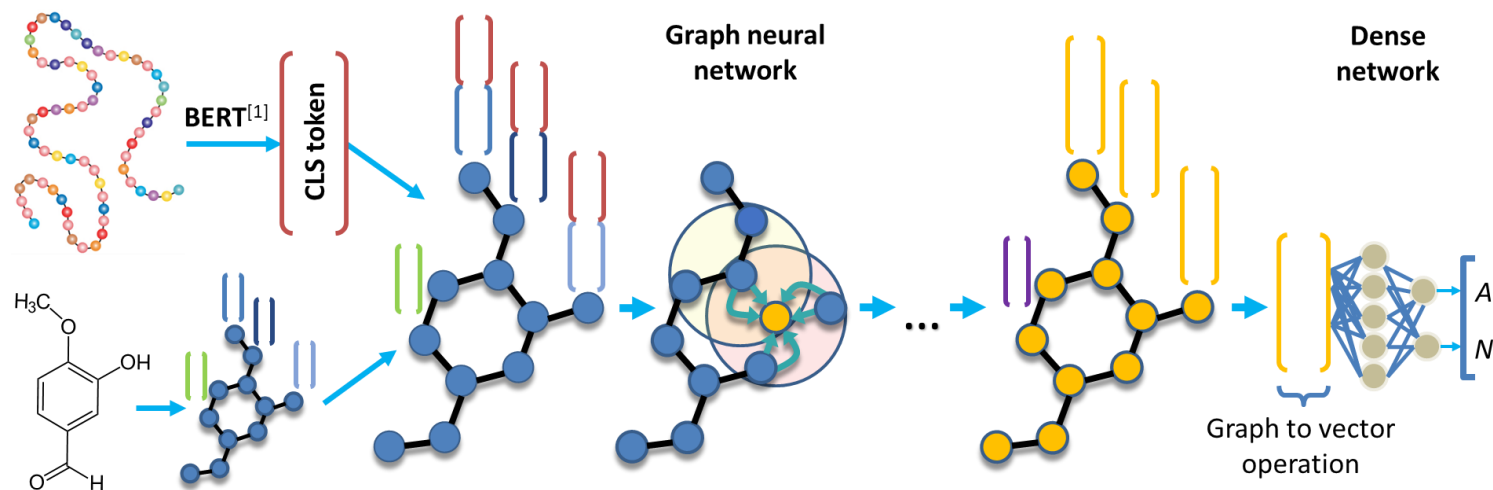
No experimental structure for all ORs



Cracking the Combinatorial Code of Olfaction



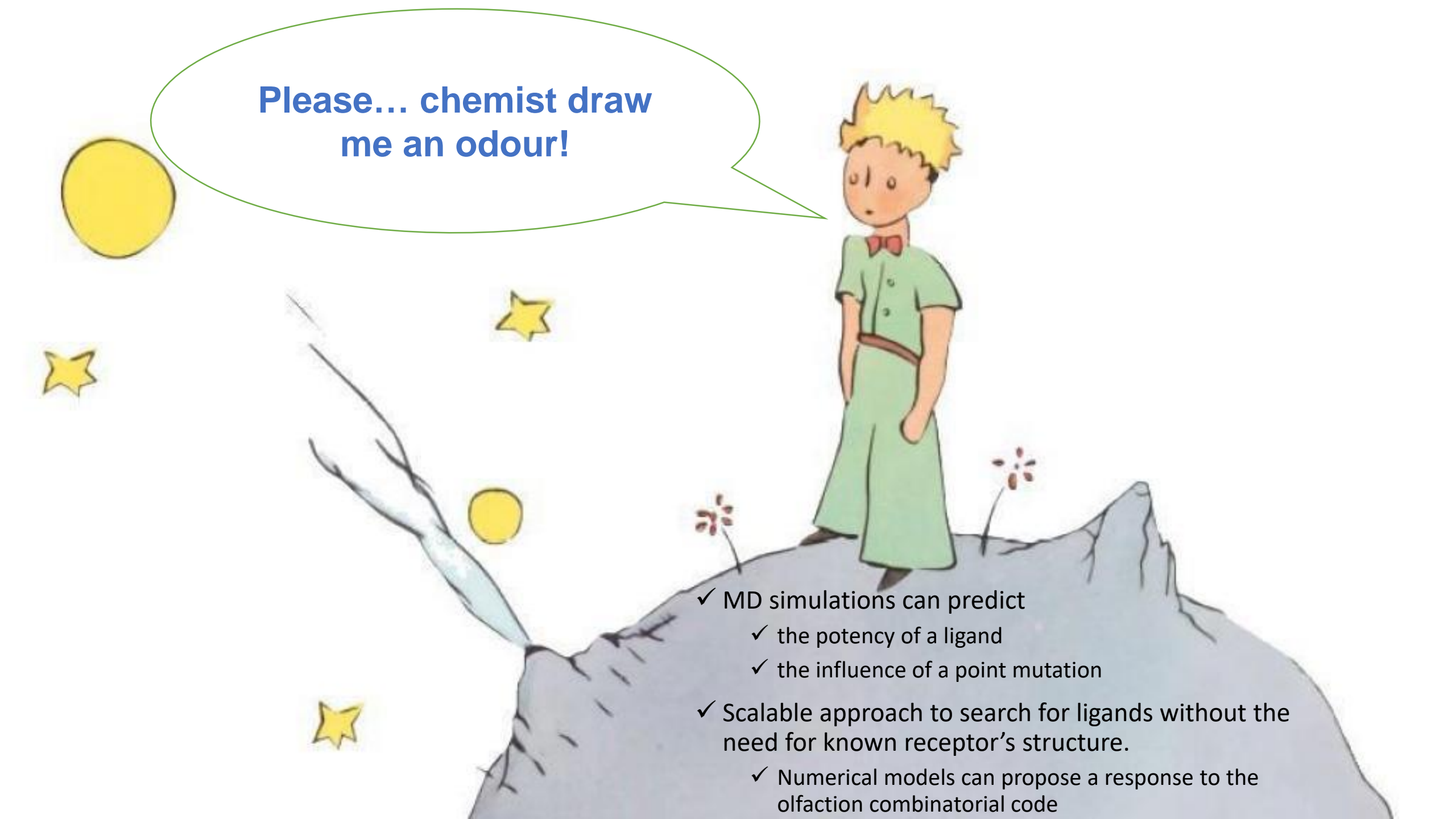
M. Lalis & M. Hladiš



Matching receptor to odorant with protein language and graph neural networks

Matej Hladiš, Maxence Lalis, Sebastien Fiorucci, Jérémie Topin

Published: 01 Feb 2023, Last Modified: 01 Feb 2023 ICLR 2023 poster Readers:  Everyone Show Bibtex Show Revisions

The illustration shows The Little Prince standing on a grey, rocky planet. He has spiky yellow hair and is wearing a green short-sleeved shirt, a red bow tie, and green trousers. A large green speech bubble originates from him, containing the text 'Please... chemist draw me an odour!'. The background is white with several yellow stars and a yellow sun. A blue comet with a long tail is visible on the left side of the planet. There are a few small red flowers on the planet's surface.

Please... chemist draw me an odour!

- ✓ MD simulations can predict
 - ✓ the potency of a ligand
 - ✓ the influence of a point mutation
- ✓ Scalable approach to search for ligands without the need for known receptor's structure.
 - ✓ Numerical models can propose a response to the olfaction combinatorial code