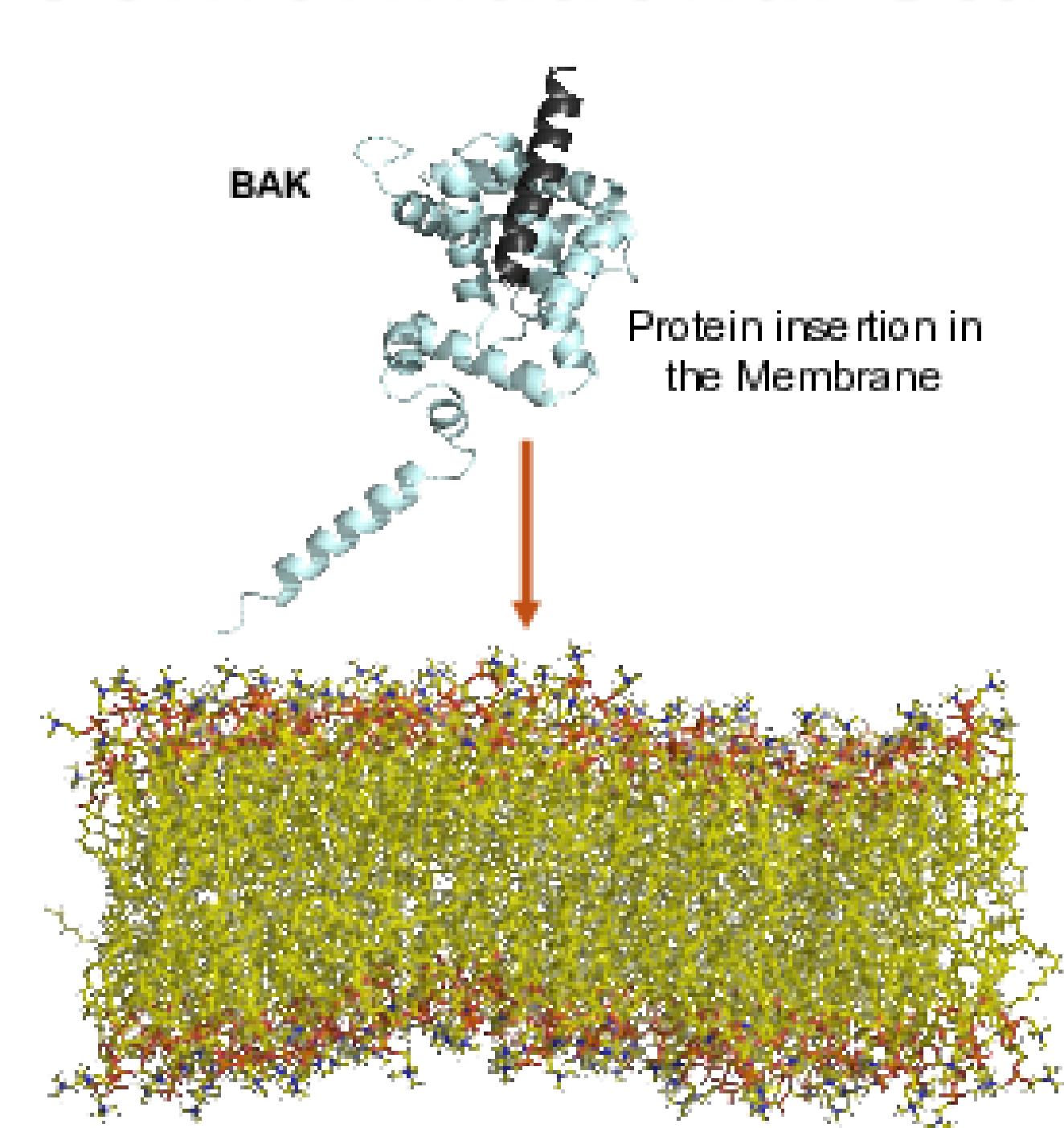


Unveiling experimental advances through atomistic simulations: Highlights from the Modelling of Biological Systems and Drug Design IQTC-UB Research Group

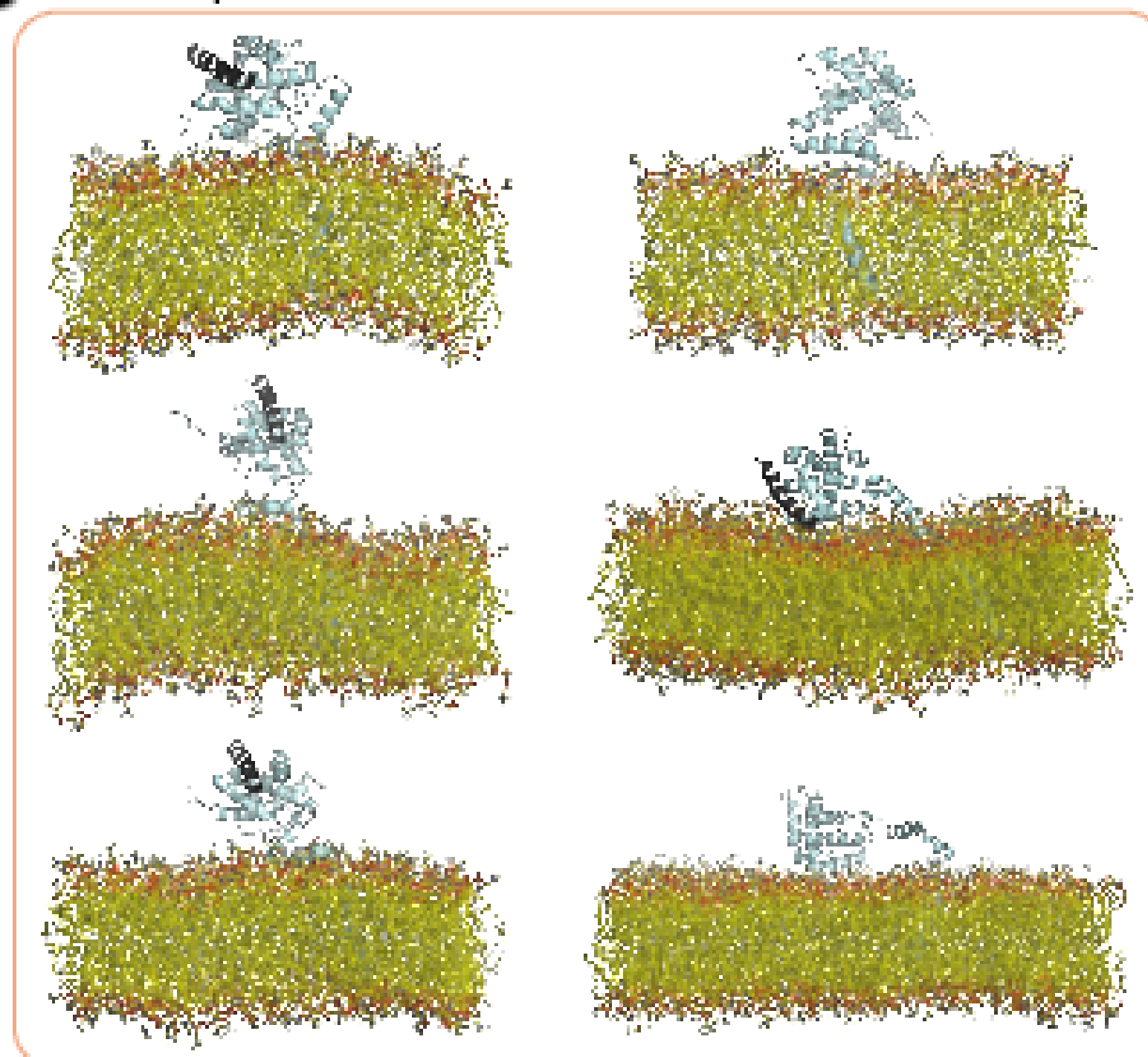
Objectives and principal lines of Research:

The Modelling of Biological Systems and Drug Design IQTC-UB research group focuses on advancing computational approaches to understand and design inhibitors targeting key proteins implicated in cancer, Alzheimer's disease or COVID-19, among others. Our research integrates molecular modelling, molecular dynamics, and structure-based drug design to characterize protein-ligand interactions at the atomic level. Using the AMBER and GROMACS simulation packages, we perform large-scale molecular dynamics studies to evaluate complex stability, conformational dynamics, and binding free energies via the MMGB/PBSA method. We further develop and apply computational tools to enhance virtual screening efficiency and improve the fragment-dissolved molecular dynamics (fdMD) methodology, enabling more precise and reliable modeling of molecular interactions. Combining theoretical insights with advanced algorithms and novel approaches, our group aims to accelerate the discovery and optimization of bioactive compounds with improved binding affinity, selectivity, and therapeutic potential, contributing to the development of innovative strategies in modern drug discovery. Thereby, bridging theoretical predictions to experimental advances.

Conformational Studies

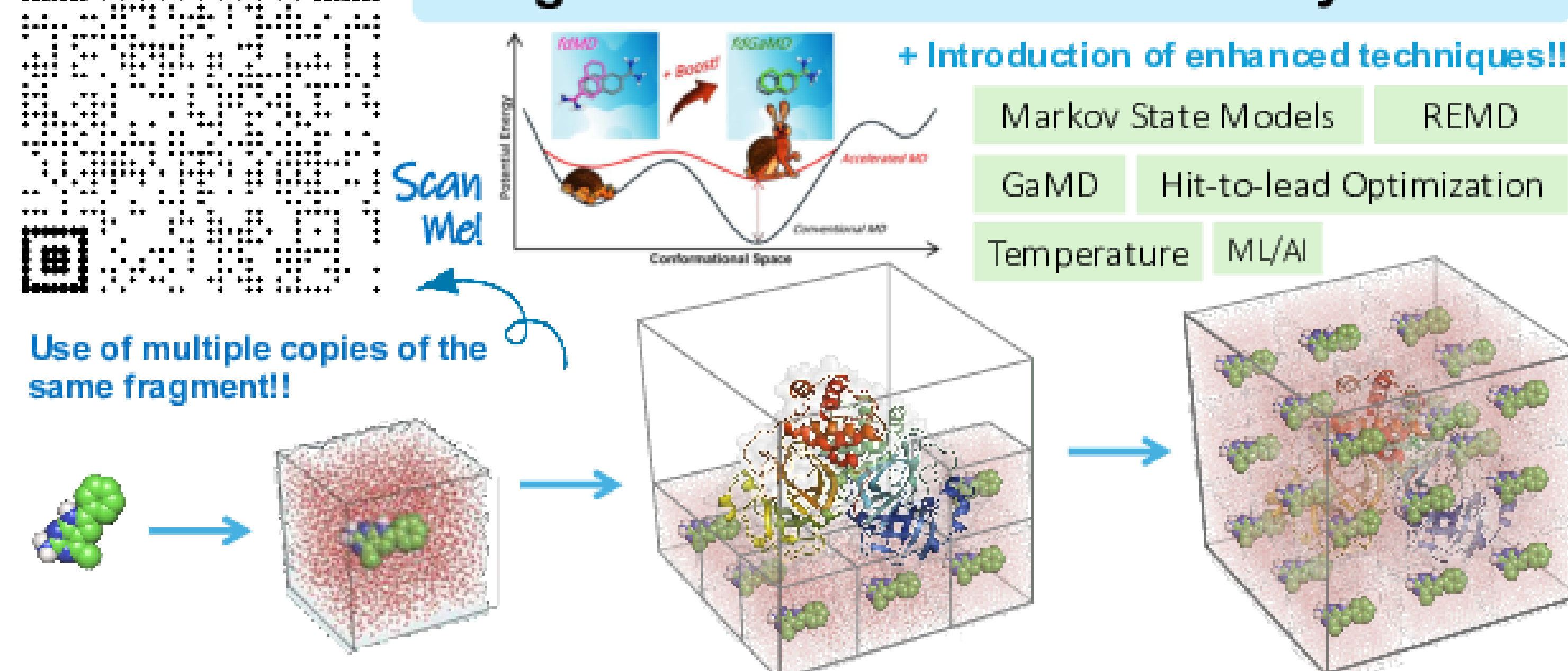


Stable protein-membrane conformations obtained from MD

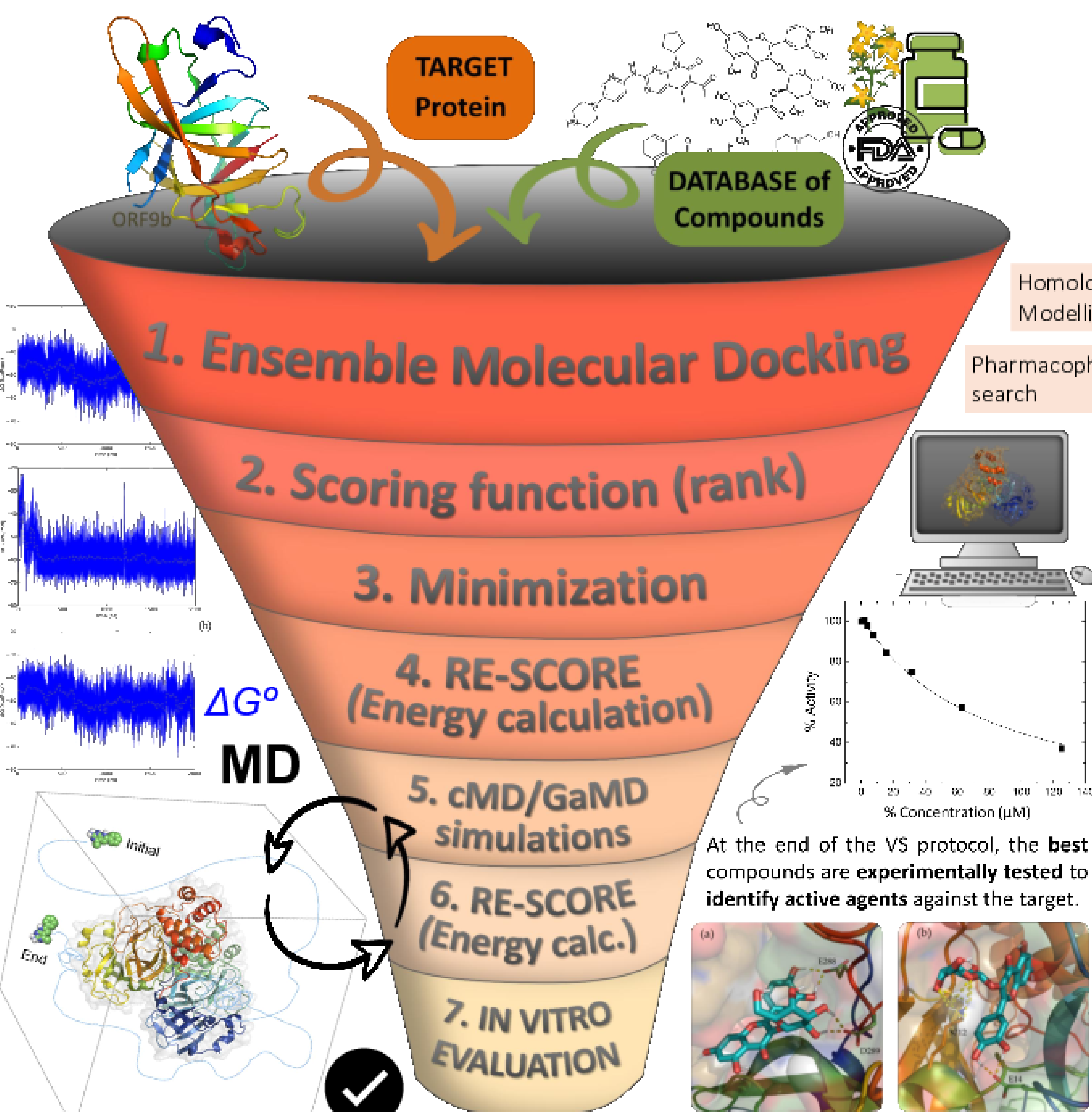


Development of New Computational Tools

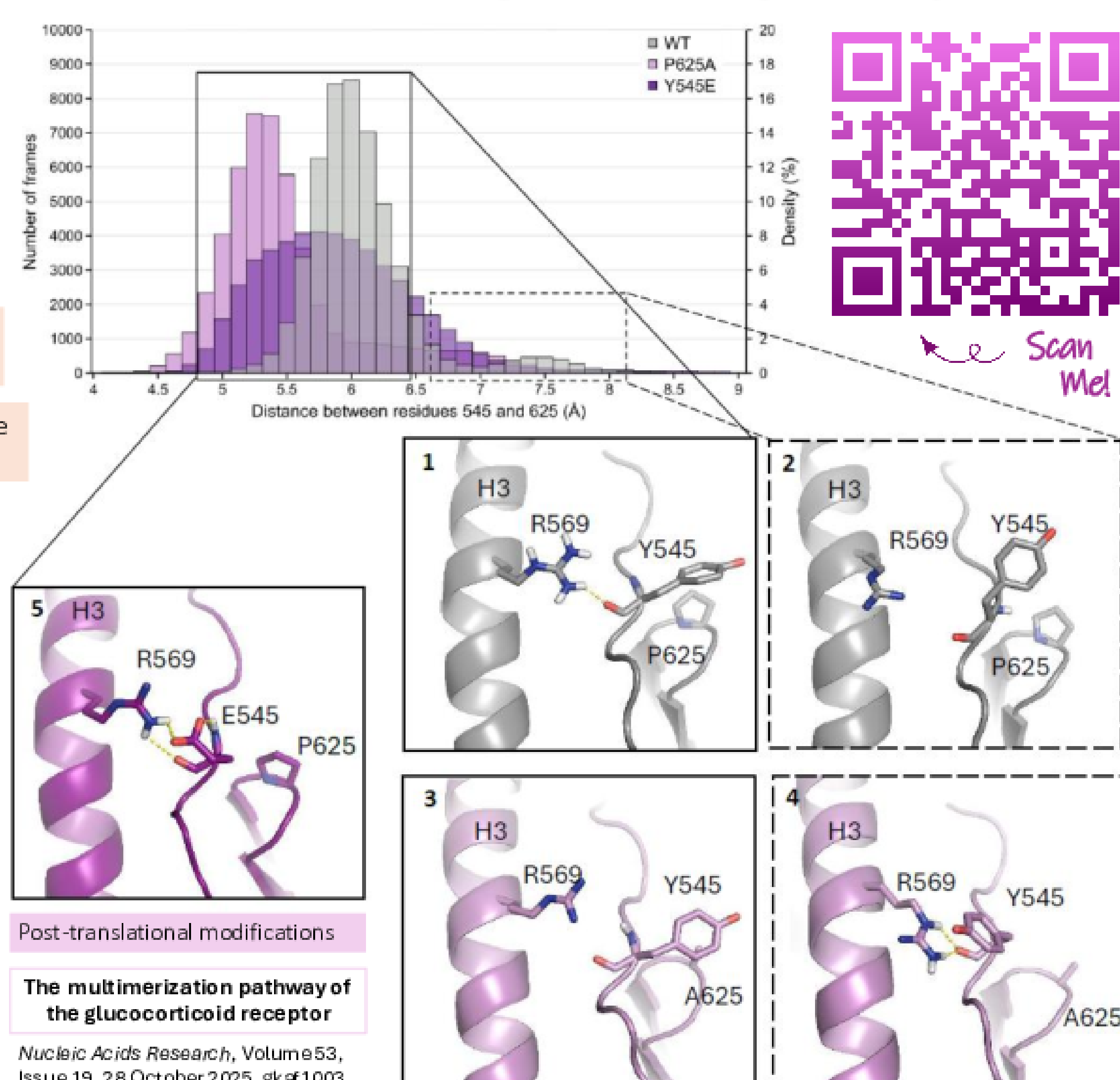
Fragment dissolved Molecular Dynamics



Development of New Inhibitors (V.S. Docking)



Molecular Modelling of Biological Systems



Collaborators

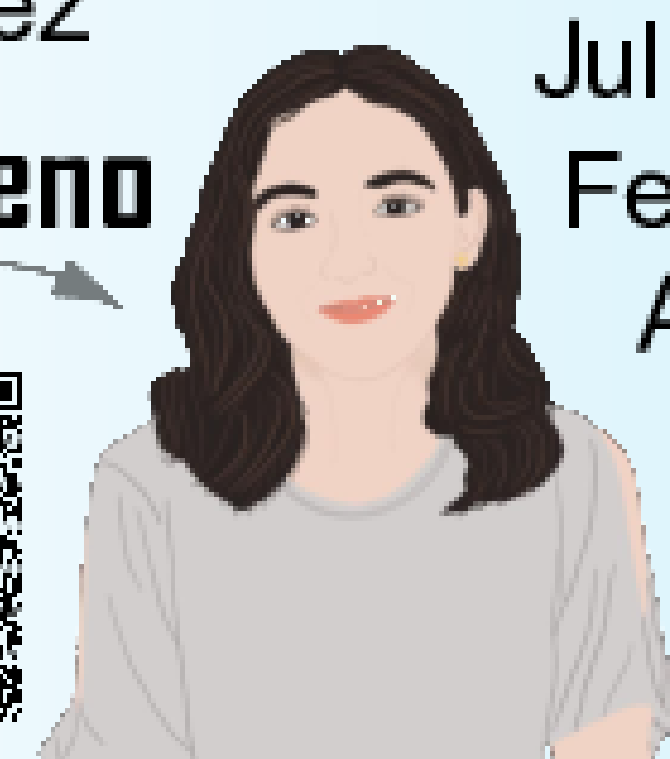
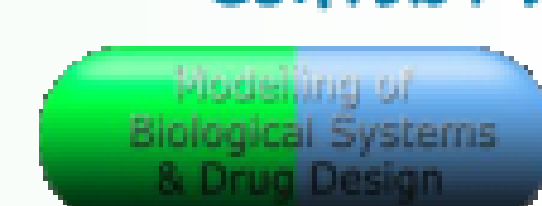
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Acknowledgements:

