Taher Yacoub

Structural bioinformatics: drug discovery & method development

Paris, France · +33 6 65 41 29 37 · taher@ycbtaher.fr · https://www.ycbtaher.fr
gitlab.com/ycbtaher · linkedin.com/in/taheryacoub · ORCID 0009-0006-1542-1264



Decide between several tools that solve the same problem
Speed up a computation that no longer copes with the load
Make it applicable to a real biological and pharmacological problem

TRACK RECORD

2 international benchmarks organised
9 laboratories coordinated
15 methods evaluated under one protocol
5 publications and preprints

First or corresponding author on three, including **RECOMB 2024**. Full list, talks and posters on **https://www.ycbtaher.fr** and ORCID.

EXPERIENCE

Postdoctoral researcher, computational modeling and machine learning — Feb 2024 – Feb 2027
GBCM (EA7528), CNAM, Paris · ANR GRADIENT · Supervisor: Prof. Matthieu Montès

- Organised the SHREC 2025 protein surface retrieval challenge: defined the protocol and the metrics, designed a class-balanced reference dataset with controlled difficulty and known confounders, and assessed the methods submitted by nine international laboratories.
- Compared learned and deterministic methods under the same protocol, analysed where each one fails, and turned that analysis into concrete proposals on descriptors and on evaluation design.
- Co-organised SHREC 2024 on shape complementarity in protein-protein interactions, measured against DockQ, TM-score and lDDT.
- Developed C and C++ methods detecting distant structural homologs at low sequence identity, for target identification and drug repurposing.

PhD researcher, fragment-based drug design and algorithm development — Nov 2020 – Jan 2024
I2BC and LIX (École polytechnique), CNRS · Fondation Vaincre Alzheimer · Supervisors: Dr Yann Ponty, Dr Fabrice Leclerc

- Designed ColorDocking, a color-coding and dynamic-programming algorithm for fragment-based docking and design, reproducing brute-force results at a fraction of the cost. Benchmarked on seven RNA-binding proteins, with in silico designs for BACE1 and BACE2.
- Established the physicochemical determinants of BACE1 against BACE2 selectivity, two homologs sharing over 90% sequence identity, across orthosteric and allosteric sites.
- Built an integrative protocol spanning modeling, chemistry and biology for selective molecule design.

SKILLS

Modeling and CADD · MOE, OpenEye, AutoDock and Vina, AlphaFold · structure-based and ligand-based design, pharmacophore modeling, QSAR, fragment screening

Simulation and structure · CHARMM27, CHARMM36, Amber · trajectory analysis (VMD) · PyMOL, MolProbity, protein surface and shape analysis · ChemAxon, pKa and logP

Benchmarking and evaluation · benchmark design, reference dataset construction, metric selection · comparative evaluation of learned and deterministic methods, failure analysis · coordination of external contributors

Computing and data · C, C++, Python · PyTorch, scikit-learn, pandas · Linux, HPC, GPU · Snakemake, Git, reproducible workflows · algorithm design

EDUCATION

2026 CNU qualification, section 27, computer science
2024 PhD, biochemistry and structural biology, Université Paris-Saclay (ED 577 SDSV)
2020 MSc, health engineering, drug design track, Aix-Marseille Université
2018 BSc, life sciences, Aix-Marseille Université

BEYOND RESEARCH

Teaching at CNAM and Paris-Saclay, from C programming to molecular modeling · Peer reviewer for SHREC 2026 and ICMSCT 2024 · Elected member of the ED 577 doctoral school and GBCM laboratory councils · French native, English professional