Taher Yacoub

Structural bioinformatics: drug discovery & method development

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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	9	15	6
international benchmarks organised	laboratories coordinated	methods evaluated under one protocol	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.
- Referent biologist in chemoinformatics in a consortium of CNAM, CGI, Université de Lyon and Sorbonne Université. Preparing SHREC 2027, a new benchmark on distant homologs.

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.

PUBLICATIONS

Yacoub T. *et al.* SHREC 2025: protein surface shape retrieval including electrostatic potential. *Computers and Graphics* 132, 104394, 2025. Corresponding author.

Storder M. *et al.* Engineering SIRPα conformational plasticity to reveal a cryptic pocket suitable for structure-based drug design. *bioRxiv*, 2025. Fourth author.

Yacoub T. *et al.* Color coding for the fragment-based docking, design and equilibrium statistics of protein-binding ssRNAs. *RECOMB 2024*, LNCS 14758, Springer. First author.

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, R · RDKit, PyTorch, scikit-learn, pandas, Matplotlib, Seaborn · Unix and Linux, Windows (WSL, MSYS2), HPC, GPU · Snakemake pipelines, 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