Master's degree in Biology – Chemistry-Biology Department

Master 2 internship project
Year 2026-2027

Laboratory/Institute: DYNAMOP/IBS
Director: M. Weik
Team: SNAX
Head of the team: JP Colletier

Name and status of the scientist in charge of the project:
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HDR: yes

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Program of the Master's degree in Biology: Biochemistry & Structure

Title of the project: AI-based design of chromophore binding proteins.

Objectives (up to 3 lines): The objective is to develop a computational pipeline for the de novo design of proteins capable of binding chromophores. Leveraging the team's expertise, we will initially focus on two target chromophores: coenzyme B12 and carotenoids (see related publications). Beyond enabling selective binding and the generation of building blocks for new photoactive proteins, such a scavenging strategy could reduce the environmental impact associated with the industrial-scale extraction and purification of these valuable compounds (130 and 25,000 tons of B12 and carotenoids, respectively, are purified every year).

Abstract (up to 10 lines): Artificial intelligence (AI) is transforming structural biology by enabling the *de novo* design of proteins with tailored structures and functions. This project focuses on designing proteins that can selectively bind either vitamin B12, a bulky metal-containing cofactor, or canthaxanthin carotenoid, a hydrophobic pigment. The chemical differences between these molecules provide an ideal testbed for refining AI-driven binding-pocket design. The following steps will be incorporated into a specific design pipeline: backbone generation, ligand-aware sequence design, structure prediction and computational filtering. The approach will be validated by functional screening and structural characterisation of promising designs. The designed proteins could improve environmentally friendly extraction processes by reducing reliance on harsh solvents and energy-intensive steps.

Methods (up to 3 lines): The project will rely on state-of-the-art protein design software, including RFdiffusion, BoltzGen, NISE, and LaserMPNN, all of which are already available and routinely used by our team on a dedicated GPU workstation. The structures of the designed proteins will be experimentally determined by X-ray crystallography to validate their architecture and chromophore-binding properties.

Up to 3 relevant publications of the team:

Wilson et al., 2022, BBA Bioenergetics
Rios-Santacruz et al., 2025, Nature
Munro et al., 2026, biorxiv

Requested domains of expertise (up to 5 keywords):

structural biology, AI-based protein design, bioinformatics