POSTDOCTORAL RESEARCH FUNDING
18 months – Starting date: 01/12/2026

Computational investigations of hemiindigoid photoswitches

Context. The goal of this theoretical project is to study hemiindigoid-type compounds for photopharmacological use by investigating the photoswitching properties of these molecular switches in water and physiological media. It is part of the HELIOPHORE project, funded by the national program PEPR LUMA. The work will be carried out in close collaboration with the experimental groups performing the synthesis and characterization of these systems. The primary mission of this position will be to provide theoretical support to understand and rationalize the behavior of these compounds, in order to potentially assist in the design of new more efficient derivatives.

Research activities. The study of the Z/E photoisomerization mechanism of hemiindigoids will require i) static mechanistic investigations through exploration of potential energy surfaces using multiconfigurational electronic structure approaches (e.g., CASSCF, CASPT2, MRSF-TDDFT), ii) nonadiabatic dynamics simulations (e.g., TSH), iii) accounting for environmental effects with explicit solvent (micro-solvation, QM/MM approach) and/or implicit solvent (PCM). Once the photoisomerization mechanistic picture is unraveled for this type of photoswitches, we will attempt to design rationally more efficient compounds for photoisomerization in water and under visible light irradiation. It will require identifying the most relevant substitution sites and studying the most promising new compounds. This task will involve frequent exchanges with the experimental collaborators.

Research environment. The postdoctoral researcher will work at the Laboratory of Quantum Chemistry and Physics of the EPE University of Toulouse and CNRS, within the Theoretical and Computational Photochemistry team under the supervision of Martial Boggio-Pasqua. He or she will have access to the laboratory's computing resources and the regional HPC (CALMIP). Participation in group meetings and conferences is expected throughout the 18-month project duration.

Expected skills. The candidate is expected to possess a strong background in theoretical chemistry, particularly in electronic structure methods. Knowledge of nonadiabatic molecular dynamics and excited electronic state calculations will be highly appreciated. Some experience with at least one electronic structure code (e.g., GAUSSIAN, MOLPRO, GAMESS) is required. An interest in interdisciplinary research (chemistry/pharmacology interface) and teamwork (theory/experiment collaboration) will be considered an asset. Proficiency in English is essential (scientific communication).

Monthly gross salary depending on experience: between 3041€ and 4216€.
Applications can be deposited on the CNRS employment portal:
https://emploi.cnrs.fr/Offres/CDD/UMR5626-MARBOG-002/Default.aspx#
Contact: martial.boggio@irsamc.ups-tlse.fr