Laboratoire de Chemoinformatique
UMR 7140 Chimie de la Matière Complexe
Université de Strasbourg/CNRS
4, rue Blaise Pascal, 67000 Strasbourg, France

Strasbourg, 20/10/2025

Post-Doc Position at the Laboratory of Chemoinformatics, Strasbourg

The Laboratory of Chemoinformatics (UMR 7140 CNRS/Strasbourg University), a well-established academic research team located on the Esplanade Campus of the University of Strasbourg and member of the ENACT consortium (https://cluster-ia-enact.ai/, dedicated to the development of novel AI approaches) is recruiting a post-doctoral research fellow for a period of 24 month, with a net monthly salary of €2000-2300, depending on the candidate's expertise. The position will be open in 2026.

The candidate, with a solid PhD level background in scientific computing, is expected to share with our team his or her extensive expertise in neural network architectures and machine learning - deep or shallow, multiobjective and multitask learning. Knowledge of physics and chemistry will be important in the cooperative endeavor to develop AI-powered predictive models of chemical properties of compounds and reactions, in deep collaborations with the chemoinformatics team, and potential experimental partners. His or her role will be to assess the current research of the chemoinformaticians from a scientific computing expert's point of view, suggesting novel and more appropriate optimization algorithms/neural net architectures/hardware solutions, while chemoinformaticians will scrutinize the chemical soundness and pertinence of algorithmic predictions. Research topics will include generative models for novel chemical structures - insisting on the current bottleneck of current approaches: chemical feasibility, modeling of chemical reactivity, biological activity predictions. Keeping in mind that raw experimental data is typically too sparse for deep learning, research will focus on physics-inspired AI models, trying to "bridge" missing data by learning from proxies obtained by high-quality physico-chemical simulations.

Fluency in English is an absolute must to fit our multinational team, fluency in French is appreciated. Open-mindedness and team-working are a must, as the candidate will have to integrate knowledge beyond the typical skills of a computer scientist.