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ANGERS UNIVERSITY LERIA- Laboratoire d'Etude et de Recherche en Informatique d'Angers	Junior Contract Researcher Post-doctoral contract in public law Category : A

Presentation of the University of Angers

In the heart of a region recognized for its quality of life, the University of Angers, the 3rd largest employer in the region, offers an environment conducive to the development of its staff and students. The UA is a multidisciplinary university, welcoming more than 25,000 students spread over 3 campuses and 2 relocated campuses (in Cholet and Saumur). It has 8 components (5 UFR, 1 IUT, 1 internal engineering school and 1 internal business and management school), and 31 federative research units and structures. Thanks to the many innovative projects it carries out and its openness to the world, the AU allows everyone to evolve in a stimulating environment. Its annual budget is €156 million (including €123 million in payroll). The UA has 1134 teachers and teacher-researchers, 882 administrative and technical staff and nearly 2000 individual contractors and is looking for involved and daring actors. You recognize yourself in this job offer ? Join us !

Contract features:

Starting date : Mars 2024
Contract duration : 18 months French law work contract
Work quota : 100%
Monthly wage : 2969.59€ gross
Location : Angers University, LERIA Laboratory

Name of research project : $^{G\text{-}}$GENOCOD

Description of the research project in which the research activities entrusted to the officer take place:

In chemistry, the discovery of new molecules often results from the refinement of an already known effective compound through chemical reactions to enhance its properties. The emergence of a truly new molecule is a rarer phenomenon. It is around this objective that a theme has developed focusing on the de novo generation of molecules with desired properties. Among the challenges in this research area are the size of the search space and the difficulty of generating synthesizable molecules.

Molecules can be represented as graphs, where vertices are labeled according to the type of atom, and edges are labeled according to the type of bond. This is a problem of generating a graph structure, where the goal is the combination of one or more functions to optimize and constraints to satisfy. Thus, the $^{G\text{-}}$GENOCOD project (Graph-Generation for Novel Compound Discovery), although applied to chemistry, addresses a much broader problem of generating complex graph structures with a very large space of composed actions.

The $^{G\text{-}}$GENOCOD project follows EvoMol, an evolutionary algorithm for molecule generation developed by an interdisciplinary team from LERIA and MOLTECH. While EvoMol achieves benchmark results, significant challenges that $^{G\text{-}}$GENOCOD aims to address remain:

1. The first will be conditioned by the goal of realism (generating synthesizable molecules). This objective is crucial for real-world applications. Methods derived from the goal-conditioned RL approach will enable the attainment of strong synthesizability properties while being explainable.
2. The second will be conditioned by the selection of optimal actions to achieve the desired chemical properties ("properties conditioned"), i.e., the choice of actions on the graph is currently random. One would expect an intelligent method (here, reinforcement learning: RL) to apply a policy of selecting actions that has worked in the past, as a chemist would add a known chemical function to enhance a target property.
3. The third objective will finally be to evolve towards the ability to generate molecules according to several defined objectives (multi-objective optimization).

Provisional project schedule:

A- WP0: Requirements elicitation: 02/01/2024 – 15/05/2024
B- WP1: Molecular context acquisition: 01/04/2024 – 15/07/2024
C- WP2-C: RL algorithms: 02/05/2024 – 30/09/2024
D- WP2-D: methodological study: 01/09/2024 – 15/11/2024
E- WP3: Bottom-up synthesizability: 02/11/2024 – 31/05/2025
F- WP4: Scientific communication : 01/10/2024 – 31/12/2025

Expected results :

Academic:
- Publication of a Popular Science article, conference papers in AI (e.g., IJCAI, UAI, AAAI, ICTAI, SAC), and an article in a transdisciplinary review.
- Organization of a scientific seminar in the field of chemoinformatics.
- Progress facilitating the submission of an ERC project.

Applied:
- Industrial-relevant advancements in the field of chemistry and the application of AI to chemistry.
- Public and corporate workshops (e.g., Science Festival, Angers Technopole morning sessions).

Definition of research activities and tasks to be accomplished:

- Literature review in the field of reinforcement learning and the generation of graph structures, both in general and applied to chemistry.
- Python development of a molecular context acquisition module.
- Python development of reinforcement learning algorithms (Deep RL: Deep Reinforcement Learning),
- Scientific experiments.
- Writing scientific articles (ranked from B to A*, Q1/Q2 journals) in English

Expected skills :

Knowledge :

- Reinforcement learning
- Graph theory
- Theorems and proofs of convergence
- Probabilistic reasoning

Know-how:

- Python development
- Development using scikit-learn, PyTorch
- Writing scientific articles in LaTeX

Soft skills:

- Efficient and responsive
- Autonomous
- Proactive
- Rigorous

Qualifications

PHD degree of less than 3 years
Specialty : Computer Science, Artificial Intelligence

Présidence de l'Université d'Angers – Direction des ressources humaines
40 rue de Rennes I BP 73532 I 49035 ANGERS cedex 01
Tél. 02 41 96 23 94 ou 02 41 96 23 58 I recrutement@univ-angers.fr

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Recruitment procedures and contact :

You must submit your CV, cover letter and doctoral degree by mail at :
nicolas.gutowski@univ-angers.fr copy to : recrutement@univ-angers.fr

Deadline for applications: **21/01/2024**
This job description is available until the closing date for applications.
On that date, it will no longer be available on the website.

If needed, your contact for any further information:
nicolas.gutowski@univ-angers.fr

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