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Job title: Postdoctoral Position, Machine Learning at the Computational Science Group of the Pompeu Fabra University. Ref. MELIS-INV-INDF-2022-22

The project

The aim of the project is to construct powerful molecular representations of chemical space to be used for property prediction and generative models. The project is in collaboration with the Pharma company Janssen and will have access to private datasets.

Job description

- Implementing the state-of-the-art deep neural architecture such as equivariant transformers extending previous work on TorchMD-NET
- Build foundation models of three-dimensional molecular structures using unsupervised learning approaches from which specific downstream task can be trained in a supervised and data efficient manner
- Integration of conformational flexibility into the model
- Generating quantum mechanical datasets
- Develop a generative model which is dependent on structural information to propose new molecule candidates

Project and Institution that finance the contract

Collaboration Agreement JANSSEN – UPF – Universiteit Antwerpen, finançat per l'Agentschap voor Innoveren & Ondernemen de Bèlgica ("VLAIO").

Skills and Experience:

The candidate will preferably have a profile in computer science, chemistry, physics, medicinal chemistry, or similar discipline.

Very good knowledge of at least a machine learning framework, preferably PyTorch or Jax and very good knowledge of Python and git.

We seek exceptional candidates with a passion for using computation and machine learning to solve real problems.



Experience in previous machine learning projects is a requirement.

The capability to think out of the box, the ambition to work in very innovative projects and very good communication skills in English.

Very good publication record.

Benefits of the opening

2 years contract with a gross salary/year of 39.380,04€ approximately (plus Social Security costs) depending on the skills and experience.

Information on the application process

The interested candidates must send their CV, PhD degree and ID document number (DNI, NIE or passport) to the address: recruitment.melis@upf.edu with the reference MELIS-INV-INDF-2022-22.

Additional information of the Computational Science Group: gianni.defabritiis@upf.edu.

Deadline to submit applications 20/12/22