



**Date of publication of the job offer 29/09/22**

**Job title:** Postdoctoral Position, Machine Learning at the Computational Science Group of the Pompeu Fabra University. Ref. MELIS-INV-INDF-2022-15

### **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**

VLAIO project - G.deFabritiis

### **Official number reference/AE/Research Spanish Agency DOI**

VLAIO project

### **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 36.227,04€ approximately (plus Social Security costs) depending on the skills and experience.

### **Information on the application process**

The interested candidates must send their CV to the address: [recruitment.melis@upf.edu](mailto:recruitment.melis@upf.edu) with the reference MELIS-INV-INDF-2022-15.

Additional information of the Computational Science Group: [gianni.defabritiis@upf.edu](mailto:gianni.defabritiis@upf.edu).

**Deadline to submit applications 20/10/22**