

## COMPUTATIONAL SCIENTIST IN DRUG DISCOVERY

# Company Description

At Oxcitas we are committed to slowing ageing and improving the chances of living longer and healthier lives. We are looking for a highly qualified and motivated individual to join our drug discovery team in Bilbao (Spain) and play an important role in our mission of harnessing the power of Al for a better understanding of the mechanisms underlying ageing and age-related diseases. If you are interested in tackling this challenge, passionate about Aldriven discovery, and would like to be part of a great dynamic team, this is the right place for you!

## Information

Deadline: 2024-04-30
Category: Academia

Province: Bizkaja

Company

**Oxcitas** 

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## Main functions, requisites & benefits

### Main functions

To contribute ideas and expertise to our drug discovery pipeline. To investigate novel drug-target interactions and elucidate the corresponding mechanisms of action. To develop algorithms together with the rest of our data science team in order to predict new therapeutic hypotheses. To provide domain expertise to product development activities. To work closely with the broader team on the development of our modelling software.

## Requisites

PhD in organic chemistry, molecular biology, pharmacology or similar discipline. Industry experience in the biotech/pharma sector would be a plus. Demonstrable ability in transforming biological principles into quantifiable hypotheses. Proven expertise in working with molecular modelling, computer-aided drug discovery/design, and lead optimisation techniques. Knowledge of medicinal chemistry principles and physico-chemical properties optimisation strategies. Experience understanding and working with molecular databases and familiarity with molecular modelling libraries (such as RDKit, OpenMM, etc.) for computational chemistry tasks. Strong data analysis skills and solid Python and/or R programming. Good communication skills (both in written and oral form) to collaborate effectively with the rest of the team. The working language is English. Nice to have: Knowledge of molecular docking and virtual screening approaches. Experience with bioinformatics tools and databases for protein sequence analysis and structure prediction. Familiarity with drug metabolism, pharmacokinetics and pharmacodynamics modelling. Understanding of biological pathways, signalling cascades, and disease mechanisms relevant to drug discovery. Experience with cloud computing and/or working-knowledge of machine learning approaches would be a plus.

### **Benefits**

The opportunity to learn about digital health. Being part of a team full of highly qualified young professionals/researchers. A flexible and inclusive work environment Professional growth and learning possibilities Being a key contributor to Oxcitas Al-powered solutions and digitals platforms.