



# Job Description

<b>Job title</b>	Senior Computational Chemist
<b>Reports to</b>	Director of Computational Sciences
<b>Department</b>	Chemistry
<b>Location</b>	Cambridge (UK) - remote working possible
<b>Date last updated</b>	October 25, 2022

## Job Purpose

The primary duties of this post are to apply computational chemistry expertise to accelerate drug discovery programs. Working in collaboration with internal and external partners in a multidisciplinary integrated drug discovery environment, this key member of the team will lead and support, computationally, the development of the Dunad discovery platform.

## Responsibilities

- Work collaboratively within multi-disciplinary drug discovery teams to design molecules with improved potency, selectivity, functional activity and ADME/Tox profiles.
- Apply a full range of computational chemistry and cheminformatics methods to accelerate and guide the discovery of new drug candidates. These may include docking, covalent docking, quantum mechanics, structure and ligand-based virtual screens, molecular dynamics, library design, protein modelling, and more.
- Apply data science techniques and/or ML algorithms for extracting relevant information from internal and external datasets, build predictive models for biological activities and compound properties, and effectively find/visualize trends & patterns in the experimental data.
- Maintain up-to-date knowledge of literature and recent developments in the fields of computational chemistry, data analysis, and cheminformatics. Evaluate and apply new computational methods to drug discovery workflows and contribute to increasing the impact of informatics tools on drug discovery at Dunad.
- Occasionally perform informatics activities such as maintaining databases, web services and software applications used by the scientific teams.
- Work collaboratively with external partners and CROs.
- Define, implement, and communicate computational strategies to the scientific teams and senior management.

## Experience & knowledge:

- PhD, MSc or equivalent in Chemistry, Computational Medicinal Chemistry or a related discipline.
- Directly related experience in industry or academia.
- Extensive knowledge of chemistry, medicinal chemistry, drug discovery and related discipline.



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- Previous track record of scientific accomplishment with experience in small molecule ligand-based and structure-based design, covalent compound design, virtual screening, quantum mechanical techniques and molecular dynamics.
- Familiarity with data analysis and data visualization (data science) in a drug discovery environment.
- Knowledge of multiple state-of-the-art drug design tools (e.g., Maestro, Schrodinger), pipelining software (e.g., Knime), and data analysis software (e.g., Spotfire).
- Familiarity with cheminformatics toolkits, computer programming and scripting languages (Python and Bash).

Highly qualified candidates will also bring to Dunad:

- Experience working across multiple target-types and disease areas
- An appreciation of relevant scientific disciplines that are related to drug discovery and early development such as target validation, pharmacology, SBDD, LBDD, ADME, structural biology and drug safety/toxicology

## Person Specification:

- Demonstrated history of successful team collaboration and of communicating complex scientific information both orally and in writing to audiences with various scientific backgrounds (e.g., biology, biophysics, DMPK).
- Demonstrated experience successfully delivering results in a fast-paced environment in which priorities may change quickly.

## About Dunad Therapeutics

Dunad Therapeutics is a biopharmaceutical company developing small molecule covalent therapies based on novel insights from chemistry and protein degradation. Dunad's proprietary, tunable platform is designed to discover and develop orally bioavailable, including CNS-accessible, therapeutics with greater specificity and improved pharmacologic attributes compared with current therapies.

Founded in 2020, Dunad is headquartered in Cambridge, UK, with operations in Cambridge, Massachusetts and Toronto, Ontario, and is backed by founding investor Epidarex Capital as well as BioGeneration Ventures (BGV) and Novartis. For more information, please visit: [www.dunadtx.com](http://www.dunadtx.com)

*Dunad Therapeutics is committed to being an equal opportunity employer. We do not discriminate in recruitment, hiring, training, promotion, or other employment practices for reasons of race, color, religion, gender, national origin, age, sexual orientation, gender identity or expression, marital or veteran status, disability, or any other legally protected status.*