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2 PhD fellowships in Machine Learning for Biology and Drug design

The Department of Computer Science (DIKU) invites applicants for two PhD fellowships in *Neuro-symbolic Machine Learning for Biology and Drug design*.

Start date is (expected to be) 1 September 2026 or as soon as possible thereafter.

The projects

PhD1: Project in tractable, neuro-symbolic foundations for biomolecular machine learning.

The PhD project is part of TRANSFORMBIO, a collaboration between the BioML group at the University of Copenhagen (PI: Wouter Boomsma) and the University of Edinburgh (Co-PI: Antonio Vergari), focused on developing tractable neurosymbolic AI for biological sequence modeling.

The core challenge is that current foundation models for biology - despite their impressive performance - lack the ability to perform reliable, flexible probabilistic inference. They cannot exactly evaluate arbitrary conditional distributions or guarantee that predictions conform to known biological constraints. The PhD student will work on two main problems. First, developing probabilistic circuits (PCs) as expressive and tractable alternatives to variational autoencoders for protein family modeling, enabling flexible conditioning on observed amino acids and exact likelihood computation while maintaining competitive predictive performance. Second, developing scalable methods for constrained decoding in biological sequence models, ensuring outputs always respect structural or grammatical biological constraints such as codon-length rules or transmembrane topology. The position offers a collaborative international environment, including a research stay in Edinburgh.

Project in Literature-Aware Neuro-symbolic Modeling of Interactions. The PhD project is a collaboration between the

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Fakta

Application due: 5/21/2026

Start date: 9/1/2026

Position type: Ph.D. positions

Workplace: Faculty of Science

Workplace: Department of Computer Science

Homepage:

diku.dk/

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BioML group at the Department of Computer Science (PI: Wouter Boomsma) and the Pharmaceutical Informatics group at the Department of Drug Design and Pharmacology (Co-PI: Alexander Hauser), focused on developing a neurosymbolic AI framework that integrates biomedical literature with 3D molecular structure for interpretable reasoning about protein–ligand interactions. The core challenge is that current AI systems treat scientific text and molecular geometry as separate knowledge sources: large language models process literature without grounding statements in 3D structure, while structure-based models ignore the mechanistic insight present in scientific text. This project bridges that gap, with a focus on G protein-coupled receptors (GPCRs) - a pharmacologically important protein family with a rich structural and ligand literature. The PhD student will work on extracting and jointly representing biochemical and geometric knowledge from the GPCR literature, designing a neurosymbolic architecture based on probabilistic circuits that combines natural-language evidence with molecular geometry, and validating the resulting model on GPCR binder rediscovery tasks - with the longer-term goal of proposing novel binders. The PhD is part of a cohort of PhD students in the Center for Pharmaceutical Data Science Education (CPDSE), providing the PhD student with a uniquely interdisciplinary environment spanning AI methodology and pharmaceutical sciences.

Who are we looking for?
We are looking for candidates within the fields of machine learning, computational biology, or related areas at the interface of AI and the life sciences. Applicants can have a background from computer science, bioinformatics, computational chemistry, physics, or mathematics. Experience with deep learning, probabilistic modeling, natural language processing, or structural biology is an advantage. No single background is required - we welcome candidates who combine strong technical skills with curiosity about biological or pharmacological questions.

Our group and research- and what do we offer?
Both PhD projects will be hosted at the Department of Computer Science (DIKU) in the BioML group, led by Professor Wouter Boomsma (email: wb@di.ku.dk). The group currently comprises three PhD students and two postdocs, and focuses on developing machine learning methodology for the biological sciences, with recent emphasis on representation learning and biomolecular foundation models.

PhD 1 will be co-supervised by Antonio Vergari, Reader (Associate Professor) at the School of Informatics, University of Edinburgh, who leads the APRIL lab. His research focuses on efficient and reliable deep probabilistic reasoning, and he holds an ERC Starting Grant on trustworthy ML. The PhD student will have the opportunity to spend

part of their studies in Edinburgh as part of this collaboration.

PhD 2 will be co-supervised by Alexander Hauser at the Department of Drug Design and Pharmacology (ILF), specialising in computational biology of GPCRs, including large-scale virtual screening and structure-based drug discovery. This position establishes a direct collaboration between the two groups within the Center for Pharmaceutical Data Science Education (CPDSE), providing the PhD student with a uniquely interdisciplinary environment spanning AI methodology and pharmaceutical sciences.

For both projects, our research facilities include access to high-performance computing infrastructure, including Denmark's Gefion supercomputer, and a collaborative cross-disciplinary network within the BioML group.

The PhD programme

Qualifications needed for the regular programme
To be eligible for the regular PhD programme, you must have completed a degree programme, equivalent to a Danish master's degree (180 ECTS/3 FTE BSc + 120 ECTS/2 FTE MSc) related to the subject area of the project. For information of eligibility of completed programmes, see General assessments for specific countries and Assessment database.

Terms of employment in the regular programme
Employment as PhD fellow is full time and for maximum 3 years.

Employment is conditional upon your successful enrolment as a PhD student at the PhD School at the Faculty of Science, University of Copenhagen. This requires submission and acceptance of an application for the specific project formulated by the applicant.

Terms of appointment and payment accord to the agreement between the Danish Ministry of Taxation and The Danish Confederation of Professional Associations on Academics in the State. The position is covered by the Protocol on Job Structure.

Responsibilities and tasks

- Carry through an independent research project under supervision
- Complete PhD courses corresponding to approx. 30 ECTS / ½ FTE
- Participate in active research environments, including a stay at another research institution, preferably abroad
- Teaching and knowledge dissemination activities
- Write scientific papers aimed at high-impact journals
- Write and defend a PhD thesis on the basis of your project

We are looking for the following qualifications:

- Professional qualifications relevant to the PhD project
- Relevant publications
- Relevant work experience
- Other relevant professional activities
- Curious mind-set with a strong interest in neurosymbolic AI and its applications in the biological sciences
- Good English language skills

Application and Assessment Procedure

Your application including all attachments must be in English and submitted electronically by clicking APPLY NOW below.

Please include:

1. Motivated letter of application (max. one page)
2. Your motivation for applying for the specific PhD project.
3. Curriculum vitae including information about your education, experience, language skills and other skills relevant for the position
4. Original diplomas for Bachelor or Master and transcript of records in the original language, including an authorized English translation if issued in another language than English or Danish. If not completed, a certified/signed copy of a recent transcript of records or a written statement from the institution or supervisor is accepted.
5. Publication list (if relevant)
6. Reference letters (if available)

The deadline for applications is 21 May 2026, 23:59 CET. We reserve the right not to consider material received after the deadline, and not to consider applications that do not live up to the abovementioned requirements.

The further process
After deadline, a number of applicants will be selected for academic assessment by an unbiased expert assessor. You are notified whether you will be passed for assessment.

The assessor will assess the qualifications and experience of the shortlisted applicants with respect to the above-mentioned research area, techniques, skills and other requirements, and conclude whether each applicant is qualified. The assessed applicants will have the opportunity to comment on their assessment. You can read about the recruitment process at http://employment.ku.dk/faculty/recruitment-process/.

Questions
For specific information about the PhD fellowship, please contact the principal supervisor.

General information about PhD study at the Faculty of SCIENCE is available at the PhD School's website

The University of Copenhagen wishes to reflect the surrounding community and invites all regardless of personal background to apply for the position.

Apply for position

Use your talent in a professional setting

The University of Copenhagen gives you the opportunity to develop your talent at the highest level. As one of Europe's leading universities, we strive for the highest academic level in research, education, and innovation, as well as in the functions that support the university's core activities. Whether you are looking for a scientific, technical, or administrative role, you will meet high expectations. We recruit talented employees and empower them to realise and develop their full potential.

Tilgængelighedserklæring