



# Potency predictions for drug design

How would you leverage cutting-edge machine learning techniques to create and integrate 3D-generative models with potency predictions for innovative drug design?

Submit your [scientific proposal](#) for a chance to be selected to conduct your proposed research plan as part of your PostDoc project at the research facilities of Boehringer Ingelheim in Biberach, Germany, one of the leading pharmaceutical companies worldwide. This opportunity is open for submissions through May 13, 2025, 11:59 pm PST.

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## What is the context of the opportunity that we are currently offering?

Generative molecular design has predominantly been anchored in two-dimensional (2D) methodologies. Despite the growing integration of three-dimensional (3D) post-processing techniques, the development of inherently 3D-generative models remains nascent. This discrepancy introduces a significant gap in predictive models for target-specific objectives operating in the 2D world and the 3D-target binding site of the hit or lead compound.

Recent advancements have seen first ventures into the realm of 3D-generative modeling. However, the synthesizability of the generated molecules remains a major bottleneck, significantly hampering the practical application of these methods. With the wealth of internal data and project-specific filters to restrict the chemical space explored, this bottleneck can be mitigated in the pharmaceutical industry.

For this PostDoc grant, we invite you to submit your research plan that focuses on the development and combination of 3D-generative models and potency predictions for drug design. A successful research proposal to our question will focus on these topics:

1. How to develop a 3D-generative algorithm for pharmaceutical drug design by using or combining novel machine learning approaches?
2. How would you integrate machine learning, physics-based methods in an early-stage of a project with limited experimental data points?
3. In addition, how would you combine various computational chemistry methods that can leverage data to enhance potency predictions?

With your solution, you will be able to benefit from the ecosystem of a large pharmaceutical player and at the same time contribute to better drug design with improved predictive models. [Apply now](#) to join Boehringer Ingelheim as part of the prestigious PostDoc grant program **opn2TALENTS**.

## What potential solutions could be in scope?

- Critically assessing the added value of 3D-based generative modelling compared to 2D-based approaches
- Tailored reward functions towards specific design objectives
- Dynamically incorporating new in-house data, thereby continuously improving predictive accuracy
- Establishing potency models using a range of different Computational Chemistry methods

## What potential solutions would be out of scope?

- Generative molecular design solely focused on the 2D-world
- Proposals that would take more than 2 years to complete

## What will be the reward to the winner?

As a winner of this call, you will have the unique opportunity to pursue your own submitted research project as a fully resourced two-years PostDoc (with the option for a one-year extension), in the Computational Chemistry group at Boehringer Ingelheim, Biberach, Germany. As part of an international team of world-class scientists working on computational drug design you will learn the processes and challenges of drug discovery in the pharmaceutical industry from the inside.

You want to learn more about living in Biberach

Find out more [here](#)

At Boehringer Ingelheim, you will have access to a fully equipped state-of-the-art research facility including access to all relevant tools and HPC-enabled technologies. You will benefit from mentoring through our internal experts, have the chance to attend international conferences, and publish your results in high-ranking journals. You will be part of the vibrant PostDoc and data science and AI community at Boehringer Ingelheim in Biberach.

In addition, you can benefit from the rich packages for employee benefit. Our most important asset in achieving our global vision is our people. We prioritize the growth of our people through mentoring, coaching, skill-building, leadership development, and academic support. Our infrastructure promotes wellness with sports groups, health counseling, onsite medical services, and regular check-ups. Achieve work-life balance with flexible work hours, remote working, childcare support, counseling, and convenient amenities. We ensure financial health with employer loans, private insurances, access to discounts, and a company pension scheme. You can also benefit from our excellent healthy on-site catering and the opportunity for take-away meals. We offer relocation support and interim accommodation to make joining us easy.

## What are the requirements to participate in this call?

Your proposal outlining your own research plan should contain a clear description of the planned combination of computational chemistry methods focused on 3D-based generative modelling, and a strategy of training potency models with fewer data points and tailored reward functions towards design objectives while generating molecules in 3D.

Additional requirements:

- Doctoral degree (PhD) in computational (medicinal) chemistry, computer-aided drug design or a related field. Track record of scientific innovation, as demonstrated by scientific publications, patents, relevant presentations, or software code.
- Demonstrated experience in structure- and ligand-based drug design methods (e.g., docking, QSAR, classic molecular dynamics, etc.)
- Familiar with all aspects of protein-ligand interactions.
- Solid python programming knowledge and good code quality is a must.
- Additional knowledge on machine learning (e.g., scikit-learn, Pytorch, and generative chemistry) and free energy calculations is beneficial.
- Outstanding creativity, critical thinking, and analytical as well as problem-solving skills.
- Enthusiastic, self-motivated, and result-driven with a strong desire to achieve scientific excellence and the will to challenge the status quo.
- Strong communication and presentation skills, capable of conveying project information in a clear manner to discipline experts

## What information should be included in your answer submission?

Please use our PostDoc grant application template to provide a 4–5-page non-confidential proposal (available for download on the following [site](#)). Please complement with your CV, publication list, and recommendation letters.

If confidential data exists that would strengthen the proposal, please indicate that information is available to share under a Confidential Disclosure Agreement (CDA). If we find the non-confidential concept proposal sufficiently interesting, we will execute a CDA for confidential discussions.

## What are the individual steps and timelines of the overall program?

Step 1	Please complete your application including a project proposal by May 13, 2025, 11:59 pm PST at the very latest. A full application package consists of your CV including references and a publication list. In addition, please submit the scientific project proposal based on our template (available for download from the following <a href="#">site</a> ). Please note that we will be unable to accept applications without a research proposal addressing our scientific question.
Step 2	We plan to finalize the review of all applications within two weeks by May 28, 2025.
Step 3	All final candidates will be invited for an opn2TALENTS interview week that will take place from June 23 to June 27, 2025. Even as we plan to give enough time for the finalists to prepare for their travel plans, we suggest that you block this time frame in your calendars already now. Please expect that you will be invited for only one day during this time frame. Depending on your location, please reserve more than one day for travel. All final candidates have the chance to present and discuss their research proposal at an internal meeting. Please prepare a PowerPoint version of your project proposal and be prepared for an in-depth scientific discussion of your ideas and approaches. Please also be prepared for additional interviews with members of the scientific team and our human resources department. Please address any questions you may have during this week as well.
Step 4	Beginning of July 2025, we plan to announce the final winner of the opn2TALENTS PostDoc grant.
Step 5	Sept 1, 2025, represents the earliest start date to work on your project at our Research and Development site in Biberach, Germany.

## How to apply?

- Check the outline of the “[opn2TALENTS grant opportunity](#)” on opnMe.
- Alternatively, you may click the “Get Application Template” banner.
- Follow the instructions to upload your submission document (requires login or registration).
- The upload allows you to attach additional application files such as your CV, publication list, and references. Please note that the maximum file size is 15MB per file.
- You will be able to access your final submitted collaboration proposal in your personal dashboard and follow its review status.
- Please also visit the [FAQ](#) section on opnMe.com to learn more about our opn2TALENTS program.

## What else is important to Boehringer Ingelheim?

- Our purpose is to transform lives for generations. Therefore, we developed three key principles for our PostDoc program which are determining our plans and actions: Drive cutting-edge science, new concepts and technologies; enrich Boehringer Ingelheim's innovation ecosystem with highly motivated, young fellows, who will help to build on science to develop new medicines; and train the next generation of leading scientists.
- Our campus community culture is great for sharing ideas and makes it easy to access technologies, meet experts, and approach leaders of all levels. There's a great spirit of freedom, fluidity, and fierce collaboration.
- Interactions are sound and informal. It's not particularly hierarchical, more team-based with a start-up attitude. We are always keen to help and speak up, open to positive change and new ideas that support our mission to improve lives.
- Our Speak-Up policy is an important part of our Code of Conduct. Only in this way we can continuously develop and improve as a company.
- Diversity, Equity, and Inclusion (DEI) is an integral part of Boehringer Ingelheim's identity; a key element of our culture and contributes to our 'Sustainable Development – For Generations'.
- Our core values of empathy, respect, passion, and trust nurture a diverse, collaborative, open and inclusive environment which is key to innovation, value creation and sustainable growth. With the inclusion of various experiences, backgrounds, and characteristics, Boehringer Ingelheim creates an openness to different approaches, solutions, and perspectives, all contributing to create "Value through Innovation".