Saarland University is a campus university with an international reputation for research excellence, particularly in computer science and in the life sciences and nanosciences. The university is also distinguished by its close ties to France and its strong European focus. Around 17,000 students, studying over one hundred different academic disciplines, are currently enrolled at Saarland University. Saarland University is officially recognized as one of Germany's family-friendly higher-education institutions and with a combined workforce of more than 4000 it is one of the largest employers in the region.

The **Center of Bioinformatics** is inviting applications for the following position commencing **01 December 2025**

Doctoral Research Position (m/f/x)

Reference number W2726, salary in accordance with the German TV-L salary scale[1], pay grade: E13 TV- L, duration of employment: 3 years, volume of employment: 100 % of standard working time.

Workplace/Department:

Data Driven Drug Design, Center of Bioinformatics, Saarland Informatics Campus, Saarland University

Job requirements and responsibilities:

This PhD position is part of the EU Horizon project **RADAR** (Renewable and safe aromatic compounds as replacement for substances of concern, https://radarproject.webflow.io/), which aims to develop renewable, safe alternatives to fossil-based aromatic chemicals such as bisphenol A and alkylphenols. These compounds are widely used in surfactants, flame retardants, and plastics, but pose significant environmental and health risks. RADAR will apply the Safe and Sustainable-by-Design (SSbD) framework to create novel biobased molecules with reduced toxicity and improved sustainability profiles.

As a PhD student in the Volkamer Group at Saarland University, you will contribute to the development of computational tools for the design of safe and sustainable molecules. Your main responsibilities will include:

- Developing generative artificial intelligence (AI), including machine and deep learning, models for molecular design and redesign, integrating hazard, synthesizability, and synthetic route data.
- Applying structure-based modeling (e.g., docking, molecular dynamics) and machine learning to predict off-target effects and endocrine activity.
- Expanding the AI models into a holistic SSbD framework by incorporating performance and sustainability data from other RADAR work packages.
- Collaborating with interdisciplinary teams across Europe, including chemists, toxicologists, and industrial partners.
- Publishing results in peer-reviewed journals and presenting at international conferences.

---

[1] TV-L = collective agreement on remuneration of public sector employees in the German *Länder*

Your academic qualifications:

- Completed scientific university studies in MSc. in chem-/bioinformatics, or computational chemistry, computer science, or a related field
- Language skills (according to GER): English C2
- Strong programming skills (ideally Python or C++) and experience with version control systems such as GitHub.
- Experience with cheminformatics and molecular modeling tools and libraries (e.g., RDKit)
- Solid expertise in machine learning, particularly deep learning and generative molecular design, using frameworks such as PyTorch, TensorFlow, and/or scikit-learn
- Strong background in chemistry, with an understanding of how molecules are built and how they interact, to apply AI tools effectively to real chemical problems.
- Experience with molecular generative design frameworks (e.g., REINVENT), i.e. tools that address what molecules might we design?
- Familiarity with AI-based retrosynthesis and reaction-prediction platforms (e.g., IBM RXN for Chemistry, ASKCOS), i.e. tools that address how could we make this molecule?
- Proven ability to apply ML models to biological or chemical datasets

The successful candidate will also be expected to:

- Interest in applying computational skills to chemical safety and sustainability
- Ability to work independently and as part of a multidisciplinary team
- German is a plus but not required

What we can offer you:

- A flexible work schedule allowing you to balance work and family, among other things the possibility of teleworking
- Secure and future-oriented employment with attractive conditions
- A broad range of further education and professional development programmes (for example language courses)
- An occupational health management model with numerous attractive options, such as our university sports programme
- Supplementary pension scheme (RZVK)
- Discounted tickets on local public transport services ('Job-Ticket' of the saarVV)
- Job bike leasing (JobRad)

We look forward to receiving your **meaningful online application** (in a PDF file) by **15.10.2025** to **stefanie.wessinger@uni-saarland.de**. Please include the reference number **W2726** in the subject line of the e-mail.

If you have any **questions**, please contact us for assistance. Your contact:
Frau Stefanie Wessinger
Administrative Assistant, Data Driven Drug Design, Center for Bioinformatics
Tel.: +49 (0)681 302-50800