



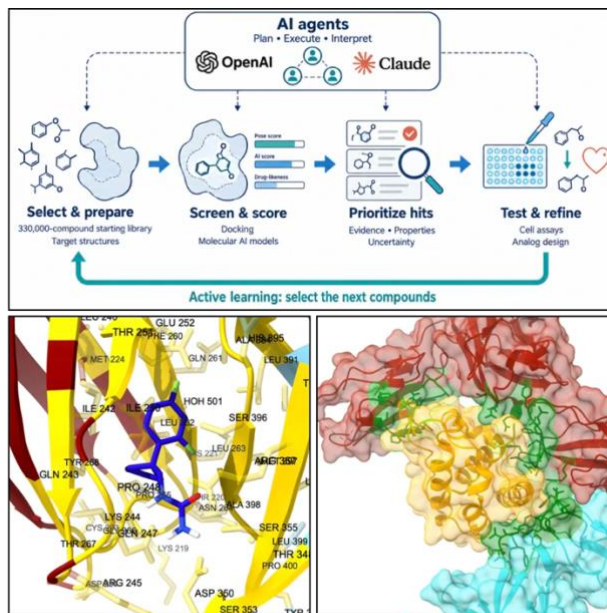
Hayat Lab at Uniklinik Aachen is seeking a:

Bachelor / Master thesis / HiWi (m/f/d)

Topic: Autonomous scientific orchestration of virtual screening

Participate in real-world AI-driven drug discovery: We are seeking an outstanding Bachelor/Master thesis student or HiWi for a fully funded international collaborative project to develop agentic AI systems for virtual screening and **discover a new generation of small-molecule drugs for heart disease**.

Agentic AI for Virtual Screening: You will help develop specialized AI agents that combine large language models, molecular foundation models, docking, and active learning to autonomously plan, execute, and improve screening campaigns. These systems will integrate molecular structures, docking results, biological knowledge, and scientific literature to prioritize compounds and guide the next screening round through adaptive, explainable decisions.



Top: Project outline. Cell assays will be conducted with a collaborator. **Bottom left:** Illustration of a cell docking simulation with a molecule in a pocket. **Bottom right:** 3D crystal structure of one of the target receptors.

Potential topics:

- Multi-agent virtual screening systems that coordinate molecular docking, ligand preparation, molecular property prediction, structural modeling, and hit prioritization
- Agentic active learning for ultra-large chemical libraries, enabling AI agents to iteratively select informative and promising compounds for the next screening round
- Intelligent orchestration of docking and scoring methods, allowing agents to select and combine classical docking, ML-based scoring, protein-ligand structure prediction, and consensus approaches depending on the target and screening results
- Explainable and evidence-based hit prioritization, combining molecular interactions, physicochemical properties and predicted activity into transparent screening decisions
- Integration of LLMs and molecular foundation models for autonomous planning and tool use across end-to-end virtual screening workflows, building on recent chemistry-agent systems such as ChemCrow and emerging multi-agent drug-discovery frameworks.

Desired Skills: Must have programming skills (Python). Experience with machine learning and deep learning (generative AI, large language models, reinforcement learning, active learning, or multimodal learning) and/or computational chemistry (molecular docking, cheminformatics, molecular dynamics, protein structure prediction, or virtual screening) are advantageous. Experience with scientific agents, tool use, or HPC/cloud computing is a plus.

We Offer: A highly interdisciplinary and collaborative research environment, access to state-of-the-art computational drug-discovery workflows and large-scale chemical libraries, opportunities to work at the intersection of AI agents, computational chemistry, and drug discovery, international collaborations, and competitive salary and benefits according to institutional guidelines.

Apply: Please submit a CV, brief motivation letter, and relevant supporting documents to shayat@ukaachen.de (Jun. Prof. Dr. Sikander Hayat, PhD)