

Two post-doctoral research positions in anti-cancer biologic design using explainable AI and generative AI

Two post-doctoral research positions are available in AI-inspired drug design in the Biomedical Computing Group headed by Professor Jagath Rajapakse (<https://personal.ntu.edu.sg/asjagath/>) at Nanyang Technological University, Singapore, for a period of three years starting from 1 July 2025.

The project investigates the design of biologics (peptides and antibodies) as anticancer therapeutic agents by using explainable AI (XAI) and generative AI (genAI). First, we build predictive AI models such as large language models (LLM) for predicting binding affinities of biologics. Second, we use XAI approaches such as integrated gradients for identifying the features of predictive models and the mechanism of action of biologics. Third, using these features as constraints, we will use genAI techniques such as LLM and diffusion models to generate biologics with anti-cancer properties. The candidate will develop necessary predictive AI, XAI and genAI methods for design of anti-cancer biologics.

The postdoctoral candidate is to have a PhD in a related field and experience in deep learning architectures and frameworks like Pytorch/Tensorflow. Candidates with Master degrees with a strong related background will also be considered. Interested candidates must email their CVs to asjagath@ntu.edu.sg. Only shortlisted candidates will be notified.

References:

1. C. Wang, G. A. Kumar, and J. C. Rajapakse, "Drug discovery and mechanism prediction with explainable graph neural networks," *Scientific Reports*, Vol. 15, Issue 1, pp. 179, January 2025, IF = 3.8, DOI: <https://www.nature.com/articles/s41598-024-83090-3>
2. C. Wang, H. H. Ong, S. Chiba, J. C. Rajapakse, "GLDM: Hit molecule generation with constrained graph latent diffusion model," *Briefings in Bioinformatics*, 2024, Volume 25, Issue 3, May 2024, IF = 6.8, bbae142, DOI: [10.1093/bib/bbae142](https://doi.org/10.1093/bib/bbae142)