Decode, design, deliver: machine learning revolutionizes target identification and therapeutic discovery

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Talk ***Decode, design, deliver: machine learning revolutionizes target identification and therapeutic discovery***

About

Timothy Jenkins is an Assistant Professor and Head of Data Science at DTU Bioengineering. After completing his BSc at James Cook University in Australia, he conducted his PhD at the University of Cambridge, exploring next-generation sequencing approaches and the impact of parasites on the human gut microbiome. He subsequently joined DTU as an HC Ørsted Postdoctoral Fellow and joined Professor Andreas Laustsen-Kiel's efforts in developing next-generation antivenom therapeutics. Shortly after, he took on the position of Assistant Professor and started a junior research group, the Digital Biotechnology Lab. Together with his team he focuses on leveraging data science, machine learning, and high-throughput *in vitro* approaches to develop new approaches for target identification and therapeutic discovery with a particular focus on neglected diseases, such as snakebite envenoming. Tim also heads the DTU Bioengineering Data Science Hub and was recently selected for the inaugural cohort of *The Young Academy of Technology, Science, and Innovation.*

Abstract

Machine learning (ML) is ushering in a new era in target identification and therapeutic discovery, with profound implications across various scientific domains. In the realm of proteomics, we have leveraged the power of ML to develop a leading-edge deep learning model called InstaNovo. This model enables high-precision *de novo* peptide sequencing, eliminating many of the constraints of conventional methods and opening up new opportunities in antibody sequencing, identification of neo-epitopes in cancer, and the exploration of the dark proteome. However, beyond target identification, ML is also proving promising in the rapid discovery and development of therapeutics. Particularly with the rise of generative *de novo* protein design, design of functional binders entirely *in silico* has been brought within reach. We have taken advantage of these developments, to design minibinders (small binding proteins primarily comprised of beta sheets and alpha helices) that can neutralise snake venom toxins. Though further validation is needed, these findings hold promise for the rapid development of next-generation therapeutics.