SORS: AI and simulation for Antibody drug discovery

Abstract

Following in the footsteps of computer vision and natural language processing, the use of deep learning in the fields of protein science and protein engineering is rapidly increasing. Antibodies, in particular, are not only crucial research subjects in drug discovery, vaccines, and immunology but also serve as excellent benchmarks for the effective application of deep learning in protein science due to the availability of big data on sequences, structures, functions, and physical properties.

Recently, in antibody drug discovery, AI and simulation have become essential for improving the efficiency of protein engineering, designing lead antibodies, and assessing and improving developability and immunogenicity. This presentation will provide an overview of these applications, incorporating our recent research to outline the current landscape, challenges, and future perspectives. This includes developing a methodology to assess "human-likeness" of antibody structures from two-dimensional images using a Variational Autoencoder as an anomaly detection problem, suggesting the potential to assess protein stability through ultra-short molecular dynamics simulations, and examples where point mutations have successfully stabilized proteins based on changes in free energy due to amino acid mutations.

Short Bio

Dr. Hiroki Shirai (Pharmaceutical Sciences) completed his master’s degree at Osaka University and has over 30 years of experience in computational drug discovery across multiple pharmaceutical companies. He acquired advanced skills in molecular simulation and protein informatics during a secondment to Haruki Nakamura's lab at Tanabe Seiyaku Co., Ltd., and later pursued further studies at the University of Cambridge under Professor Sir Tom Blundell.

Dr. Shirai led the Bioinformatics Group at Astellas Pharma Inc., where he achieved notable results at the global antibody structure prediction competition (AMAII; Los Angeles) and spearheaded international industry-academic collaboration on antibody informatics under the EBI industry programme based in the UK. He has served as the Vice Representative for Japan with the Asia Pacific Protein Association, as Vice President of the Protein Science Society of Japan, and Visiting Professor at the University of Tsukuba.

Dr. Shirai has also contributed to committees responsible for the development of the supercomputer "Fugaku." Currently, he serves as a Coordinator at the RIKEN Center for Computational Science, where he is responsible for promoting the use of high-performance computing in life sciences and actively working to develop a platform for antibody drug discovery by leveraging RIKEN's comprehensive capabilities.

Speakers

Speaker: Dr. Hiroki Shirai, Coordinator, Riken Center for computational science. Visiting Professor at the Faculty of Pharmaceutical Sciences, Kumamoto University. AI Advisor at Meiji Seika Pharma Co., Ltd. Executive Officer of the Protein Science Society of Japan. Auditor of the Japanese Antibody Society
Host: Víctor Guallar, Electronic And Atomic Protein Modelling Group Manager, Life Sciences Department, BSC
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