MD627 893 Seminar in Medical Microbiology

Department of Microbiology, Faculty of Medicine, Khon Khean University

Seminar title: Computational approaches for exploring antibody-antigen interactions

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Abstract

Emerging viruses pose a significant public health threat, making the development of new broad-spectrum antivirals a top priority. Computational approaches have become widely utilized in various aspects, such as predicting the binding interactions of antiviral drugs with active sites and forecasting antibody-antigen interactions for designing vaccines and therapeutic antibodies. Understanding computational tools has proven valuable in the development of computational pipelines, significantly reducing both costs and cycle times through computer-aided optimization. In this seminar, we demonstrate molecular docking and molecular dynamic simulation (MD) analysis to predict antibody-antigen interactions, explaining the binding interactions of mutant viruses and guiding the design of new antibodies.

In the first article of SARS-CoV-2 antibodies (Yanqi Jiao et al., 2023), they employed various computational tools, such as docking and MD, to predict interactions between mutant SARS-CoV-2 and existing antibodies. These methods can be used to anticipate and explain how mutations in the virus may reduce the neutralization effectiveness of antibodies.

In the second article of monkeypox virus (MPXV) antibodies (Yu H et al., 2023), they investigated two nanobodies, A1 and H8, which specifically target the A29 protein of MPXV. Using docking and MD computer-aided design, they predicted binding interactions and identified key residues to design new mutant antibodies. These new antibodies demonstrated a 10-fold increase in affinity compared to the original form.

In conclusion, both docking and molecular dynamics (MD) are valuable for predicting interactions, gaining insights into these interactions, and identifying improved therapeutic candidates. Utilizing both methods together can enhance and strengthen the development pipeline.

Reference

Yanqi Jiao, Y., et al (2023). Impact of E484Q and L452R Mutations on Structure and Binding Behavior of SARS-CoV-2 B.1.617.1 Using Deep Learning AlphaFold2, Molecular Docking and Dynamics Simulation. *International Journal of Molecular Sciences*, *14*. doi.org/10.3390/ijms241411564.

Yu H, et al., (2023). *In Vitro* Affinity Maturation of Nanobodies against Mpox Virus A29 Protein Based on Computer-Aided Design. *Molecules, 28(19), 6838.* doi.org/10.3390/molecules28196838.