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Machine learning to accelerate therapeutic antibody development

Antibody therapeutics are fundamental to healthcare, acting as best-in-class therapies for diseases ranging from cancers to viruses. However, the antibody development pipeline is plagued by high failure rates (nearly 80%), long timescales (averaging close to a decade) and high costs (at least hundreds of millions of dollars). My research aims to accelerate antibody development through machine learning.

Antibodies are proteins produced by our immune systems to defend against foreign pathogens. Their ability to bind strongly and specifically to a target, such as a tumour or viral surface protein, is also what makes them ideal candidates for therapeutics. While target binding affinity lies at the heart of therapeutic antibody development, additional properties affecting safety and developability must also be considered. For example, certain antibody sequences may have a higher risk of inducing an immune response when administered in patients (immunogenicity), and others reduced stability and therefore shelf-life.

Traditionally each property would need to be optimised one-by-one, experimentally and often in a trial-and-error manner. Computational approaches can however optimise multiple properties simultaneously. Laying the foundations to achieve this, I am developing machine learning models to predict properties, including binding affinity and immunogenicity, from antibody structure and sequence. These methods are generalisable and can be applied to antibody therapeutics for any target or disease.

Computational multi-property optimisation holds great promise not only to reduce timescales and costs of therapeutic antibody development, but also to improve clinical trial success rates, safety and therefore patient outcomes.