Project title: Uncovering Clinical Drug Sequencing Patterns Using AI and Longitudinal EHR Data

Project Summary:

Drug combination therapies are increasingly used to improve efficacy, overcome resistance, and reduce toxicity, but their clinical impact is highly dependent on the **sequence of administration**, which is poorly captured in existing computational models. Electronic health records (EHRs) contain rich longitudinal prescription and treatment data that, if systematically mined, could reveal real-world patterns of **drug sequencing** at scale. This project will develop an end-to-end pipeline to **extract and model the temporal order of drug combinations** from structured and unstructured EHR data, enabling the training of **order-aware AI models** for drug combination prediction.

First, we will design scalable algorithms to identify sequential drug exposures in EHRs by linking prescription timestamps, dosage changes, and treatment episodes, while applying large language models (LLMs) to clinical notes for additional temporal signals. Second, we will construct a large, disease-stratified dataset of sequence-annotated drug combinations, harmonised with molecular, pharmacological, and clinical covariates to support mechanistic interpretation. Third, we will develop deep learning architectures that incorporate **order of drug administration as a core feature**, extending Bayesian frameworks to model uncertainty in synergistic potency and efficacy for each combination. Finally, we will validate the models using held-out EHR subsets and external clinical datasets from oncology and cardiovascular indications.

By linking real-world treatment sequences to advanced AI modelling, this project will deliver **the first generalisable, uncertainty- and order-aware AI** for drug combination prediction trained on clinical practice, accelerating the discovery of effective, evidence-based treatment regimens.

Supervisory Team:

Name: Prof Dennis Wang, Chair in Data Science

Institution/Department: National Heart and Lung Institute and Imperial-X

Email: dennis.wang@imperial.ac.uk

Phone number: 07887970464

Name: Prof Paul Huang, Group Leader of Molecular and Systems Oncology

Institution/Department: Institute of Cancer Research

Email: paul.huang@icr.ac.uk

Phone number: 02071535554

Number of research degree students previously supervised to completion: 10

Clinical Specialities:

- **Medical Oncology**
- **Clinical Oncology**
- **Other specialities with an interest in medical informatics will be considered.**