



TITLE: Optimal Design of High Dimensional Experiments

SPEAKER: Joff Jones¹

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ABSTRACT: In-vitro assay development is vital to ensure that assays are sensitive and robust for the purposes of target and hit discovery. Often, many factors need to be optimised and historically this has been handled by performing sequential experiments. However, iterative experiments can be extremely slow, particularly for cellular assays that take days or weeks.

We will present how High Dimensional Experimentation can effectively accelerate the preclinical drug discovery process. HDE utilises optimal Design of Experiments (DoE), lab automation, and high-capacity microtiter plates to optimise many factors in one experiment. In this talk, we present three complementary approaches to implement DoE for HDE. First, using results from a simulation study, we show how to wisely choose between implementing 2nd or 3rd order DoEs to fit models that maximize prediction accuracy. Building on this, we next describe a novel variant of the coordinate exchange algorithm that extends traditional design optimisation by explicitly accounting for spatial variability on two-dimensional plates. We also compare our method's performance with less effective alternative approaches for handling spatial effects. Finally, we show how agentic AI can be used to generate DoEs based on expert know-how, effectively democratising DoE for biologists.

BRIEF SPEAKER BIO: Joff Jones is a Senior Statistician at AstraZeneca, where his role is to ensure selection of the right design and the right analysis across preclinical in-vitro and in-vivo experiments. He collaborates with multi-disciplinary teams of biologists, lab scientists, data scientists, & bioinformaticians to carefully design experiments and analysis strategies that can accurately and reliably address the question of interest. He leads the implementation of optimal Design of Experiments in Drug Discovery to deliver higher quality data, faster.