

The research commercialisation office of the University of Oxford, previously called **Isis Innovation**, has been renamed **Oxford University Innovation**

All documents and other materials will be updated accordingly. In the meantime the remaining content of this Isis Innovation document is still valid.

URLs beginning <u>www.isis-innovation.com/</u>... are automatically redirected to our new domain, <u>www.innovation.ox.ac.uk/</u>...

Phone numbers and email addresses for individual members of staff are unchanged

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Virtual Assay – Software to evaluate the safety and efficacy of medicines and drugs

Flexible, robust and user-friendly software for the prediction of safety and efficacy of medicines, for users without specialist expertise in programming or computer modelling.

Everyone is different

No two individuals respond to a drug in exactly the same way. Due to sometimes subtle variability at a physiological level, what works for one person may not work for another, even before taking into account any additional complicating factors. This is one of the most significant challenges faced by the pharmaceutical industry; clearly it is neither practical nor desirable to test a new medicine on the entire population to ensure it is both safe and effective.

Safety and Efficacy of Medicines

Ensuring a medicine is effective and does not have potentially harmful or unexpected side-effects requires a huge amount of rigorous testing before the drug can be approved for clinical use. Even then, unforeseen problems can occur due to patient population variation or exacerbation of other pre-existing diseases.

"Virtual" Screening

To overcome this, *in silico* modelling of cell physiology is becoming increasingly important in both efficacy and safety pharmacology testing. Consequently, it is attracting significant attention from both the commercial sector and regulatory bodies.

Calibrated model populations

Virtual Assay starts with well-understood cellular biology models and modulates the variables to generate a range, or population, of models, which will respond differently to the same inputs. These populations are then calibrated against experimental data. Once calibrated, these populations can be used to analyse the effects of different pharmaceutical agents on cellular response at the population level.

Key advantages

 Tight coupling between modelling and specific experiments

- Users can produce models constructed with their own experiments
- Quantitative prediction of the effects of drugs on cellular function
- Mechanistic explanation of the causes of drug effects by predicting them and identifying the main determinants of the effects

- Takes into account inter-subject variability in the modelling and simulation
- Consultancy services also available

Prizes and awards

Oliver Britton was awarded the 2014 3Rs winner prize by the National Centre for the replacement Refinement & Reduction of Animals in Research and was also one of the four finalist in the 2014 UK ICT Pioneers awards for his research in Population of Models.

The software development has been supported by the EPSRC Impact Acceleration Account.

Publications

Experimentally–calibrated population of models predicts and explains inter–subject variability in cardiac cellular electrophysiology. O. Britton, A. Bueno–Orovio, K. Van Ammel, HR. Lu, R. Towart, DJ. Gallacher and B. Rodriguez





Figure 2: AP changes

population of models.

induced by Flecainide in the

Figure 1: Representative AP traces for one model from the experimentally-calibrated population.



Figure 3: Virtual Assay software



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