

# "In Silico Human drug safety and efficacy" initiative.



The project "In silico human-based methodologies for evaluation of drug safety and efficacy" officially started on September the 1<sup>st</sup>, 2016. The main goal of this initiative is to accelerate the use of *in silico* methodologies for the evaluation of drug safety and efficacy in academic, industrial, regulatory and clinical settings. The coordinated action of these four sectors aims to improve the efficiency of drug testing through the use of human-based computer models, refined and evaluated, using experimental and clinical recordings. Through this project we will work towards the refinement, reduction and replacement of animals in the drug development process, and the development of a more reliable and accurate process for drug testing. The team is formed by a partnership across industry, academia, hospitals and regulatory agencies from 14 countries.

[The webpage of this project](#) is an open space to share knowledge, papers and models and a reference for experts on in silico methodologies for drug safety and efficacy.

We would like to encourage all partners to get involved and send news, papers and models related to in silico drug safety and efficacy to [insilicocardiotox@cs.ox.ac.uk](mailto:insilicocardiotox@cs.ox.ac.uk).

## NEWS & UPCOMING EVENTS

- [18th World Congress of Basic and Clinical Pharmacology \(WCP2018\).](#)  
Kyoto, 1- 6 July, 2018.
- [The VPH-CaSE. Frontiers of Simulation and Experimentation for Personalised Cardiovascular Management and Treatment conference.](#)  
London, 19-20 July, 2018.
- [World Congress in Computational Mechanics 2018.](#)  
New York, 22-27 July, 2018.
- [Virtual Physiological Human \(VPH\) Conference.](#)  
Zaragoza, 5-7 September, 2018.
- [21<sup>st</sup> International Conference on Medical Image Computing & Computer Assisted Intervention - MICCAI.](#)  
Granada, 16-20 September, 2018.
- [Computing in Cardiology 2018.](#)  
Maastricht, 23-26 September 2018.
- [Safety Pharmacology Society annual meeting.](#)  
Washington, 30 September- 3 October, 2018.
- [2018 SPS Regional Meetings.](#)  
Check meetings organised by the Safety Pharmacology Society.
- [Frontiers Topic on Safety Pharmacology - Risk Assessment QT Interval Prolongation and Beyond.](#)  
Frontiers Topic on "Safety Pharmacology - Risk Assessment QT Interval Prolongation and Beyond" is now finalised. It has received over 40400 views to date and includes 28 topics summarised in the editorial by Grandi, Morotti, Pueyo and Rodriguez.

## PAST NEWS & EVENTS

- [VPHi Barcelona Summer School.](#)  
Barcelona, 18 - 22 June 2018.
- [Webinar: Computational Cardiology: A novel non-invasive personalized approach to assess sudden cardiac death \(SCD\).](#)  
Webinar, Prof Natalia Trayanova, the Johns Hopkins University, 20 June, 2018.
- [Nordic-Baltic VPHI Workshop.](#)  
Tampere, 10-12 June, 2018. Organised by Tampere University and BioMediTech to facilitate collaborations on VPH-related activities.
- [Gordon Research conference Drug Safety in the Modern Development Landscape: Innovations from Industry, Academia, and Government.](#)  
Easton, 9-15 June, 2018. The Computational Cardiovascular Science team presented the latest research on In Silico human cell models predicting Safety and Efficacy of Drugs.
- [Cheltenham Science Festival.](#)  
Cheltenham, 9 June, the film "Building a Virtual Human" was presented by the High Performance Centre of Research Excellence in Computational Biomedicine Centre (CompBioMed).
- [Hay festival.](#)  
Wales, 30 May, 2018. Elisa Passini was an invited speaker at the Hay Festival presenting a journey into the Virtual Heart to understand how human-based computer models and simulations can be used to predict risk of cardiac side effects in patients taking drugs.
- [SelectBio Conference.](#)  
Cambridge, 24-25 May 2018. Matt Daniels, Oxford, presented at the conference a talk entitled: "Stem Cells and antibodies for drug discovery".
- [BMSS Webinar: Quantitative Systems Toxicology as a Tool for Explaining and Predicting Drug-Related Organ Toxicity.](#)  
Webinar, 11 April, 2018 International Society of Pharmacometrics (ISoP) Drug Safety Working Group.
- [The conversation.](#)  
The conversation, 26 March, 2018, an article on "Why computer simulations should replace animal testing for heart drugs", by Patricia Benito, Elisa Passini and Blanca Rodriguez.
- [NC3Rs Cardiovascular Showcase event.](#)  
London, 23 March. This event brought together a diverse group of scientists, including in silico experts, working to advance the application of the 3Rs in cardiovascular research and safety assessment.
- [NC3Rs international Prize.](#)  
London, 12 March. Elisa Passini won the 2017 3Rs Prize, awarded by the NC3Rs and sponsored by GSK.

## PUBLICATIONS

- [Population-based mechanistic modeling allows for quantitative predictions of drug responses across cell types.](#)  
Jingqi Q. X. Gong, Eric A. Sobie. Npj Systems Biology and Applications. 2017.
- [The Structural Basis of IKs Ion-Channel Activation: Mechanistic Insights from Molecular Simulations.](#)  
Smiruthi Ramasubramanian, Yoram Rudy, Biophysical Journal. 2018.
- [Automatic optimization of an in silico model of human iPSC derived cardiomyocytes recapitulating calcium handling abnormalities.](#)  
M .Paci, R.P. Pölönen, D. Cori, K. Penttinen, K. Aalto-Setälä, S. Severi, J. Hyttinen. Frontiers in Physiology. 2018.
- [In silico evaluation of arrhythmia.](#)  
X. Zhou, A. Bueno-Orovio, B. Rodriguez. Current Opinion in Physiology. 2018.
- [Unlocking data sets by calibrating populations of models to data density: A study in atrial electrophysiology.](#)  
B.A.J. Lawson, C.C. Drovandi, N. Cusimano, P. Burrage, B. Rodriguez, K. Burrage. Science Advances. 2018.
- [From ionic to cellular variability in human atrial myocytes: an integrative computational and experimental study.](#)  
A. Muszkiewicz, X. Liu, A. Bueno-Orovio, B.A.J. Lawson, K. Burrage, B. Casadei, B. Rodriguez. American Journal of Physiology-Heart and Circulatory Physiology. 2018.
- [In silico assessment of the effects of various compounds in MEA/hiPSC-CM assays: Modeling and numerical simulations.](#)  
E. Abbate, M. Boulakia, Y. Coudière, J.F. Gerbeau, P. Zitoun, N. Zenzemi. Journal of Pharmacological and Toxicological Methods. 2018.
- [Action Potential Recording and Pro-arrhythmia Risk Analysis in Human Ventricular Trabeculae.](#)  
Y. Qu, G. Page, N. Abi-Gerges, P. E. Miller, A. Ghetti, H. M. Vargas. Frontiers in Physiology. 2018.
- [Adult Human Primary Cardiomyocyte-Based Model for the Simultaneous Prediction of Drug-Induced Inotropic and Pro-arrhythmia Risk.](#)  
N. Nguyen, W. Nguyen, B. Nguyenton, P. Ratchada, G. Page, P. E. Miller, A. Ghetti, N. Abi-Gerges. Frontiers in Physiology. 2017.

