



**CompBioMed**  
**Conference**

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**COMPBIOMED CONFERENCE 2023**

**12-15 SEPTEMBER 2023**

**[www.compbiomed-conference.org](http://www.compbiomed-conference.org)**

**Science Congress Center Munich,  
85748 Garching**



## CompBioMed Conference 2023 Programme

Time	Tuesday 12 September 2023	Wednesday 13 September 2023	Thursday 14 September 2023	Friday 15 September 2023		
08:30	Registration	Registration	Registration	CompBioMed – SEAVEA Hackathon		
09:00 09:15		Plenary Speaker: Ines Thiele	Plenary Speaker: Richard Law			
09:45	Welcome Address	Refreshments	Refreshments			
10:00 10:15	Plenary Speaker: Gunnar Cedersund	Organ Modelling and Simulation	AI/ML/QC		From Desktop to HPC...	Molecular Medicine
10:45	Refreshments					
11:00 11:30	Digital Twins and Personalised Medicine	In silico Themed Session	Lunch		Lunch	LRZ Tours
12:00 12:15	Lunch					
12:30 12:45		Lunch	Organ Modelling and Simulation		Computationally Intense Modelling in Immunology	From Desktop to HPC...
13:00 13:15	Digital Twins and Personalised Medicine					
13:30 13:45		Towards the Path to Exascale...	Refreshments		Refreshments	
14:00 14:15	Refreshments					Imaging and Visualisation
14:30 14:45		Refreshments	Closing Remarks and Prizes			
15:00 15:15	Refreshments				Poster Presentatons Including Food & Drink Reception	Poster Presentatons Including Food & Drink Reception
15:30 15:45		LRZ Tours				
16:00 16:15	LRZ Tours					
16:45 17:00		LRZ Tours				
17:30 17:45	LRZ Tours					
18:00		Board buses for brewery tour and conference dinner	Brewery tour		Beer Tasting	Conference Dinner
18:30	Brewery tour					
19:00	Beer Tasting					
19:30	Conference Dinner					
22:00	Buses return from conference dinner					

QR Code for online and detailed programme:



## Preface

We would like to welcome you to the third edition of the CompBioMed Conference (CBMC23). The Conference is taking place from 12<sup>th</sup> to 14<sup>th</sup> September at the Science Congress Center Munich. The conference will address all aspects of the rapidly burgeoning domain of computational biomedicine, from genome through organ to whole human and population levels, embracing data driven, mechanistic modelling and simulation, machine learning and combinations thereof. We welcome contributions from academic, clinical and industrial participants alike.

The conference is organised by the Centre of Excellence (CoE) in Computational Biomedicine (CompBioMed), aimed at nurturing and promoting the uptake and exploitation of high performance computing within the biomedical modelling community.

The congress center is a short walk down the road from Leibniz Supercomputing Centre (LRZ), a supercomputing centre on the Campus Garching near Munich, operated by the Bavarian Academy of Sciences and Humanities. LRZ operates the supercomputers SuperMUC and the next generation SuperMUC-NG. At the Science Congress Center Munich, we deliver an exciting programme of relevant symposia and world-renowned plenary and invited speakers, proposed and secured by our International Organising Committee.

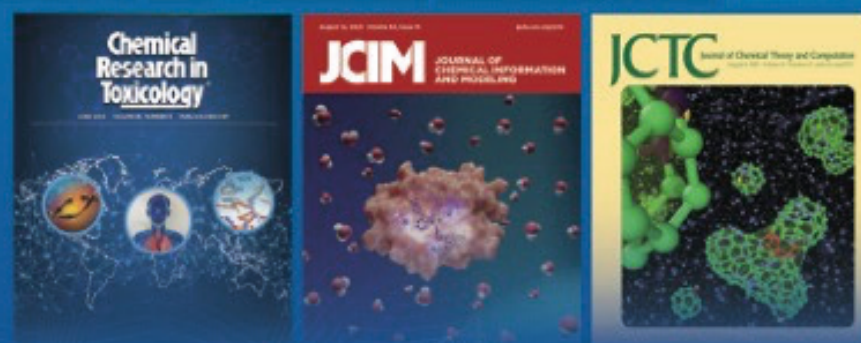
In addition to the scientific content, we are hosting two informal social events for delegates to enjoy. Firstly, tours of the LRZ supercomputing facilities have been arranged on Tuesday and Thursday, during the conference. We also have the conference dinner taking place on Tuesday evening next to the oldest brewery in the world, the Bayerische Staatsbrauerei Weihenstephan, including a guided tour of the brewery, beer tasting, and then the conference dinner at the nearby Braüstüberl.

The organisers would like to thank all the authors, speakers and participants who will make this conference interesting and informative. Special thanks to our session chairs and reviewers who dedicated their time to evaluate a large number of submissions. We also thank all of our sponsors for their support and encourage you to read their material included in this programme and in the conference bags.

We thank you all for your participation in CBMC23 and for supporting our conference series, we hope that you will find it worthwhile and inspiring.



Prof. Andrea Townsend-Nicholson  
Professor of Biochemistry & Molecular Biology  
University College London



# STATE OF THE ART RESEARCH FROM ACS PUBLICATIONS

## GENERAL INFORMATION

### Social Events

- 12<sup>th</sup> Sept: 16:15 - 17:45: **LRZ Supercomputing Facility Tours** (Registration required), Leibniz-Rechenzentrum
- 12<sup>th</sup> Sept: 18:30 - 22:00: **Brewery Tour, Beer Tasting, Conference Dinner** (Registration required), Bräustüberl Weihenstephan
- 13<sup>th</sup> Sept: 17:30 -19:00: **Poster Session including Food & Drink Reception** (Open to all attendees), Science Congress Center
- 14<sup>th</sup> Sept: 13:00-13:45: **LRZ Supercomputing Facility Tours** (Registration required), Leibniz-Rechenzentrum

### Local Sights

- Leibniz-Rechenzentrum (LRZ), including supercomputers SuperMUC and SuperMUC-NG, is just down the neighbouring street on Boltzmannstraße 1, 85748 Garching bei München.

### Travel

- It will take 30 min by bus to get from the conference centre to Bräustüberl Weihenstephan on 13 September.
- The Munich town centre (Marienplatz) is also roughly 30 min taking the underground. A day pass to reach the centre of Munich costs 11 euros (Zone M-2). For 2 to 5 people, a group ticket is available for € 19.40.
- The underground station and bus station are about 2min/150m, from the Science Congress Center.

### Internet (WiFi)

Free WiFi will be provided throughout the Science Congress Centre.

### Insurance

The organisers accept no liability for personal injuries sustained, or for loss or for damage to property belonging to participants, incurred either during or as a result of the congress.

### Mobile Phones

As a courtesy to all meeting attendees and speakers, phones, pagers and other electronic devices must be operated in silent/vibration mode during sessions. No phone conversations are permitted during sessions.

**Tuesday 12 September**

**Tuesday 12 September 8:30-9:45**

**Registration**

**Tuesday 12 September 9:45-10:00**

**Welcome Address**

Room: Terra

**Tuesday 12 September 10:00-10:45**

**Plenary Session 1 - Gunnar Cedersund**

Multi-organ, multi-level, and multi-timescale digital twins of individuals

Room: Terra

**Tuesday 12 September 10:45-11:00**

**Refreshments**

**Tuesday 12 September 11:00-12:30**

**In Silico Themed Session 1**

Room: Jupiter

Session Chair: Jazmin Aguado-Sierra (Barcelona Supercomputing Center, Elem Biotech SL)

11:00-11:20 Clinical translation of virtual exposure-QTc studies

Georg Rast

11:20-11:35 The new version of PlayMolecule: a platform for computer aided drug discovery

Mariona Torrens Fontanals

11:35-11:50 Effect of pronation form on the risk of lateral ankle ligament sprain

Samuel Spriggs, Marlène Mengoni

11:50-12:05 In-Silico Characterisation of the Relaxation Behaviour of Bovine Discs

Philippe Marguerette Alfeche Alipat, Nagitha Wijayathunga, Ruth Wilcox, Marlène Mengoni

12:05-12:20 Overview of Achievements in Computational Medicine at the Sano Centre

Marian Bubak, Maciej Malawski, Alex Crimi, Ahmed Abdeen Hamed, Przemyslaw Korzeniowski, Piotr Nowakowski, Jose Sousa

**Tuesday 12 September 11:00-12:35****Digital Twins and Personalised Medicine 1**

Room: Terra

Session Chair: Peter Coveney (UCL, University of Amsterdam)

11:00-11:20 Digital Twins for Health Consortium: An International Alliance for Human Digital Twins Research

Jun Deng

11:20-11:35 Novel Digital Twin Pipeline of the Human Ventricular Activation Sequence Using Realistic Purkinje Networks for in Silico Clinical Trials

Lucas Arantes Berg, Julia Camps, Blanca Rodriguez

11:35-11:50 In silico assessment of the effects of micro-vessel flow obstructions on initial aggregate formation

Christian Johannes Spieker, Gabor Zavodszky, Alfons Hoekstra

11:50-12:05 Towards Personalised Treatment in Septic Shock via Bayesian Inversion of a One-Dimensional Vascular Model

Finneas Jacob Robson Catling, Kim H. Parker, Alun D. Hughes, Steve Harris, Anthony C. Gordon

12:05-12:20 Comparison of Equilibrium and Non-Equilibrium Approaches for Relative Binding Free Energy Predictions

Shunzhou Wan, Agastya Bhati, Peter Coveney

12:20-12:35 Interstitial Fluid Pressure in Heterogenous Solid Tumors: A Computational Study

Hooman Salavati, Pim Pullens, Wim Ceelen, Charlotte Debbaut

**Tuesday 12 September 12:30-13:30****Lunch****Tuesday 12 September 13:30-14:25****In Silico Themed Session 2**

Room: Jupiter

Session Chair: Jazmin Aguado-Sierra (Barcelona Supercomputing Center, Elem Biotech SL)

13:30-13:50 Predicting the impact of serial and parallel stenosis in bifurcations lesions on disease physiology with Computational Modeling: Simulating the impact of removing one stenosis on the signal decay of Fractional Flow Reserve of the other

Jens Flensted Lassen

13:50-14:10 Perspective on regulatory considerations for computational simulation applied to clinical decision making in the treatment of cardiac lesions

Tinen Lee Iles

14:10-14:25 A Novel Method to Model Coronary Bifurcations from X-ray Angiography Nada Ghorab
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<b>Tuesday 12 September 13:30-15:30</b>
<b>Digital Twins and Personalised Medicine 2</b>
Room: Terra Session Chair: Peter Coveney (UCL, University of Amsterdam)
13:30-13:50 In silico trials in cardiovascular healthcare: The future of diagnosis and treatment in cardiac disease Hector Martinez-Navarro, Blanca Rodriguez
13:50-14:10 The Acute Myeloid Leukemia Digital Twin Ilya Shmulevich
14:10-14:30 Digital Twins for Optimizing Therapeutic Interventions in Oncology Thomas Yankeelov, Thomas Yankeelov, David Hormuth II, Ernesto Lima, Guillermo Lorenzo, Chengyue Wu
14:30-14:50 Digital Twins for Cancer: A Growing and Global Effort Eric Stahlberg
14:50-15:10 Digital twinning the human retina Philip Luthert, Simon Walker-Samuel, Moussa Zouache
15:10-15:25 Digital Twins: The Virtual Future of Medicine Peter Coveney

<b>Tuesday 12 September 14:25-15:50</b>
<b>Towards the Path to Exascale Computing</b>
Room: Jupiter Session Chair: Valeriu Codreanu (SURF)
14:25-14:45 Distributing software the EESSI way Caspar Martijn van Leeuwen
14:45-15:05 New Processors for Exascale Computing in Computational Biology Igor Pasichnyk
15:05-15:20 HemePure HIP porting Loris Lucido, Okba Hamitou
15:20-15:35 Coupling Biomedical Codes with MUSCLE3 - Case Study with HemeLB Jon McCullough, Lourens Veen, Peter Coveney
15:35-15:50 Towards a platform agnostic HemeLB_GPU Ioannis Zacharoudiou, Jon McCullough, Xiao Xue, Sharp Lo, Balint Joo, Peter Coveney

<b>Tuesday 12 September 15:45-16:15</b>
<b>Refreshments</b>

<b>Tuesday 12 September 16:15-17:45</b>
<b>LRZ Tours</b>
Location: LRZ

<b>Tuesday 12 September 17:45-22:30</b>
<b>Conference Dinner</b>
Location: Bräustüberl Weihenstephan
18:00 - Buses depart from the Congress Centre to Weihenstephan
18:30 - Brewery tour (30 min)
19:00 - Beer tasting (30 min)
19:30 - Dinner (2h30min)
22:00 - Departure back to Garching
22:30 - Arrival at Garching

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## Wednesday 13 September

**Wednesday 13 September 8:30-9:00**

**Registration**

**Wednesday 13 September 9:00-9:45**

**Plenary Session 2 - Ines Thiele**

The role of whole-body metabolic modelling in computational medicine

Room: Terra

**Wednesday 13 September 9:45-10:00**

**Refreshments**

**Wednesday 13 September 10:00-12:15**

**Organ Modelling and Simulation 1**

Room: Terra

Session Chair: Andrew Narracott (University of Sheffield)

10:00-10:20 Patient-Specific Cardiac Anatomy Modeling for In Silico Trials

Abhirup Banerjee, Marcel Beetz, Vicente Grau

10:20-10:40 Physics-based modelling and machine learning synergies in cardiac twin technology

Mathias Peirlinck

10:40-11:00 Computational Challenges in Musculoskeletal Modelling and Simulation

Sara Oliviero, Alessandra Aldieri, Cristina Curreli, Giorgio Davico, Antonino Amedeo La Mattina, Domitille Marie Princelle, Marco Viceconti

11:00-11:15 Explore the effect of muscle forces on femur during normal gait using a virtual population of older women

Zainab Altai, Erica Montegiori, Ivan Benemerito, Xinshan Li

11:15-11:30 High Resolution Simulation of Basilar Artery Infarct and Flow Within the Circle of Willis

Jon McCullough, Ioannis Zacharoudiou, Sharp Lo, Peter Coveney

11:30-11:45 Towards Virtual Surgeries of Nasal Cavities Using High-Performance Computing

Moritz Waldmann

11:45-12:00 Proof of concept for assessing AVF maturation with in-silico hemodynamic models of arteriovenous fistulas in patients with end-stage renal disease Lidia Martínez-Dalmau, Andy Olivares, Oscar Camara, José Ibeas, Miriam Caravaca
12:00-12:15 Three-dimensional analysis of stroke scenarios in the circle of Willis using HemeLB_GPU Ioannis Zacharoudiou, Jon McCullough, Sharp Lo, Xiao Xue, Peter Coveney

<b>Wednesday 13 September 10:00-12:20</b>
<b>AI/ML/QC</b>
Room: Jupiter Session Chair: Natalia Jiménez (CGG)
10:00-10:20 Quantum Computing: Enabling Practical Quantum Computing Through Co-Design Peter Eder
10:20-10:40 Economical Scaling for Extreme AI Workloads Gillian Royle
10:40-10:55 De Novo Drug Design Using Simulation and AI David Wright, Jarryl D'Oyley, Will Gerrard, Alex Punter, Georg Schusteritsch, Raphael Chantreau, Parminder Ruprah, Vid Stojevic
10:55-11:15 Crystal Fit and Search: Finding the Diamond in the Rough Christian J. Burnham, Niall J. English
11:15-11:35 SGPocket: Predict protein-ligand binding site using graph convolutional neural network Kevin Crampon, Xavier Vigouroux, Stephanie Baud, Luiz Angelo Steffemel
11:35-11:50 Building a Machine Mind by Integrating Explicit and Tacit Knowledge for personalised medicine Jose Sousa
11:50-12:05 Integrating knowledge and machine learning for classification using binary data: A case study on mortality prediction of mechanically ventilated COVID-19 patients Moein Einollahzadeh Samadi, Andreas Schuppert
12:05-12:20 A formal and experimental exploration of joint eigenanalysis for optimal binary classification: leveraging covariance and Hessian matrices on health datasets Agus Hartoyo, Jan Argasinski, Aleksandra Trenk, Kinga Przybylska, Anna Blasiak, Alessandro Crimi

<b>Wednesday 13 September 12:15-13:15</b>
<b>Lunch</b>

<b>Wednesday 13 September 13:15-14:15</b>
<b>Organ Modelling and Simulation 2</b>
Room: Terra Session Chair: Andrew Narracott (University of Sheffield)
13:15-13:30 A 0D model of lower limb haemodynamics: sensitivity analysis Magdalena Otta, Ian Halliday, Piotr Kica, Janice Tsui, Chung Lim, Maciej Malawski, Andrew Narracott
13:30-13:45 Coupling 3D Electromechanics of the Heart with 3D Fluid Mechanics of Blood Vessels in a Virtual Human Sharp C. Y. Lo, Alberto Zingaro, Mariano Vazquez, Peter V. Coveney
13:45-14:00 Model Order Reduction and Sensitivity Analysis for complex ocular simulations inside the human eyeball Thomas Saigre, Christophe Prud'homme, Marcela Szopos
14:00-14:15 The Interplay of Hemodynamics, Reactivity Kinetics, and Clot Permeability: Effects on the Platelets Mass Transfer Niksa Mohammadi Bagheri, Gabor Závodszy, Alfons Hoekstra

<b>Wednesday 13 September 13:15-14:45</b>
<b>Computationally Intense Modelling in Immunology</b>
Room: Jupiter Session Chair: Timothy Elliot (University of Oxford)
13:15-13:45 Decoding T cell recognition: Unravelling the intricacies of adaptive immunity Hashem Koohy
13:45-14:05 A 2D to 3D Simulation Workflow Demonstrator for Intervertebral Disc Degeneration Investigation and Diagnosis Maria Paola Ferri, Socayna Jouide El Kaderi, Dimitrios Lialios, Sai Natarajan, Estefano Matias Muñoz-Moya, Laia Codó Tarraubella, Josep Lluís Gelpi
14:05-14:25 Prediction of clinical haematotoxicity in oncology combinations from human bone marrow MPS: a translational quantitative systems toxicology approach. Massimo Lai, Nuria Folguera Blasco, Khan Kainat, Benedicte Recolin, Natacha Bohin, Riaz Basha Shaik, Emilyanne Leonard, Carmen Pin, Sonja Gill
14:25-14:45 In Silico Testing of Hypotheses for the Effect of Smoking on Somatic Evolution in the Healthy Human Lung Hugh Selway-Clarke

<b>Wednesday 13 September 14:15-15:15</b>
<b>Surrogate Modelling</b>
Room: Terra Session Chair: Gábor Závodszky (University of Amsterdam, Budapest University of Technology and Economics)
14:15-14:35 Efficient Reduced Order Modeling for Coupled Problems in Cardiac Electrophysiology Elena Zappon
14:35-14:50 Shear induced diffusion of platelets revisited Franck Raynaud
14:50-15:05 Registration-based reduced-order modelling for blood flow simulation Dongwei Ye, Valeria Krzhizhanovskaya, Alfons G. Hoekstra

<b>Wednesday 13 September 15:15-15:45</b>
<b>Refreshments</b>

<b>Wednesday 13 September 15:45-17:30</b>
<b>Imaging &amp; Visualisation</b>
Room: Terra Session Chair: Elisabeth Mayer (Leibniz Supercomputing Centre)
15:45-16:05 Immersive Visualization of Biomedical Data in Omniverse Peter Messmer
16:05-16:20 Virtual Reality, Biomedicine and Game Engines - Creating an Immersive and Interactive Biomedical Visualisation Elisabeth Mayer, Jon McCullough, Peter Coveney
16:20-16:35 Visualization of full human HemeLB simulations with Intel OSPRay Studio Jon McCullough, Elisabeth Mayer, Johannes Gunther, Salvatore Cielo, Peter Coveney
16:35-17:30 Hands-On Session - Imaging and Visualisation Elisabeth Mayer Hands-On imaging and visualisation session: Participants are invited to join the hands-on session of the imaging and visualisation session, where they can experience and experiment with different immersive visualisation workflows. There will be three workstations set up for visualisations for Virtual Reality (VR) with VR-headsets and different software ranging from Nvidia's Omniverse to Unreal Engine.

<b>Wednesday 13 September 15:45-17:30</b>
<b>Ensemble workflows, verification, validation and uncertainty quantification (SEAVEA)</b>
Room: Jupiter Session Chair: Diana Suleimenova (Brunel University London)
15:45-16:05 AI-coupled HPC Workflow Applications, Systems and Software Shantenu Jha
16:05-16:25 Software Environment for Actionable and VVUQ-evaluated Exascale Applications toolkit Diana Suleimenova, Alireza Jahani, Yani Xue, Maziar Ghorbani, Derek Groen
16:25-16:40 Uncertainty Quantification of Hydrodynamic Impacts of Peripheral Arterial Disease on Abdominal Aortic Aneurysms Sharp C. Y. Lo, Jon W. S. McCullough, Xue Xiao, Ioannis Zacharoudiou, Peter V. Coveney
16:40-16:55 A lattice Boltzmann study on the stenosis of the aorta Xiao Xue, Jon McCullough, Sharp Lo, Ioannis Zacharoudiou, Peter Coveney
16:55-17:10 Using MUSCLE3 and EasyVVUQ to Perform Uncertainty Quantification of Fusion Plasma Core Transport Simulations David Coster
17:10-17:25 Quantifying Uncertainties in Route Selection: A Comprehensive Analysis of Health Facility Effects in South Sudan using EasyVVUQ Alireza Jahani, Derek Groen, Diana Suleimenova, Maziar Ghorbani, Arindam Saha, Yani Xue

<b>Wednesday 13 September 17:30-19:00</b>
<b>Poster Session, plus Food &amp; Drinks Reception</b>
Room: Poster Space
17:30-19:00 LIT-FED-SEARCH - A Federated Search Workflow for Large-Scale Real-World Biomedical Evidence Analysis Filip Katulski, Maciej Malawski, Ahmed Abdeen Hamed
17:30-19:00 Computational Medicine Toolkit for HPC Applications Karol Zając, Marek Kasztelnik, Jan Meizner, Piotr Nowakowski, Taras Zhyulin, Maciej Malawski, Lukasz Wronski
17:30-19:00 CircularRNA as potential biomarker - from computation fo molecular approach. Sabina Licholai
17:30-19:00 Efficient Computational Modelling of Additive Manufactured Spinal Implant Cameron Cullen
17:30-19:00 A Novel Method to Model Coronary Bifurcations from X-ray Angiography Nada Ghorab

17:30-19:00 Language Models and Protein Stability: Predicting Protein Thermostability with Deep Learning Models Adam Sułek, Jakub Jonczyk, Ahmed Abdeen Hamed, Maciej Malawski, Marek Wodziński
17:30-19:00 GPU Benchmarking on Fully Occupied Accelerated Cluster Nodes via Molecular Dynamics Software Packages Plamen Dobrev, Ivan Pribec, Gerald Mathias

**Thursday 14 September**

<b>Thursday 14 September 8:30-9:00</b>
<b>Registration</b>

<b>Thursday 14 September 9:00-9:45</b>
<b>Plenary Session 3 - Richard Law</b>
The future of AI enabled drug discovery Room: Terra

<b>Thursday 14 September 9:45-10:00</b>
<b>Refreshments</b>

<b>Thursday 14 September 10:00-12:00</b>
<b>From desktop to HPC and beyond in the clinic 1</b>
Room: Terra Session Chair: Phil Luthert (UCL)
10:00-10:20 HPC-based fluid simulations for the planning of left atrial appendage occluder implantations Oscar Camara
10:20-10:40 Wireless Endocardial Optimisation System for Cardiac Resynchronisation Therapy Angela Wing Chung Lee, Baldeep Sidhu, Justin Gould, Bradley Porter, Benjamin Sieniewicz, Mark Elliott, Vishal Mehta, Nadeev Wijesuriya, Abdoul Amadou, Gernot Plank, Ulrike Haberland, Ronak Rajani, Christopher Rinaldi, Steven Niederer
10:40-11:00 From Theory to Practice - A Medical Student's journey through Computational Medicine and Prospects for Computational Psychiatry using HPC Abdullah Ahmad

11:00-11:15 Bodylight.js - toolchain for in-browser simulation of simple and complex mathematical models Tomas Kulhanek, Jiri Kofranek
11:15-11:30 JupyterHub on Cyfronet PLGrid infrastructure as a tool for medical applications Kamil Burkiewicz, Marek Kasztelnik, Łukasz Flis, Bartosz Soból, Maciej Malawski
11:30-11:45 Enhancing Prostate Cancer Clinical Decision Support with ChatGPT-Enabled Real-World Evidence Jakub Klimczak, Maciej Malawski, Byung Suk Lee, Ahmed Abdeen Hamed
11:45-12:00 TIES - Relative Binding Free Energies With a Press of a Button Mateusz K. Bieniek, Gavin J. Pringle, Peter V. Coveney

<b>Thursday 14 September 10:00-12:00</b>
<b>Molecular Medicine 1</b>
Room: Jupiter Session Chair: Andrea Townsend-Nicholson (UCL)
10:00-10:20 Creating an Open Ecosystem for Data Driven Molecular Discovery Using Accelerating Therapeutics for Opportunities in Medicine (ATOM) Technologies Eric Stahlberg
10:20-10:40 Accelerating Drug Discovery by Combining Machine-Learning and Physics-Based Methods Agastya Bhati, Shunzhou Wan, Sean Black, Marco Klahn, Hannes Loffler, Andre Merzky, Mikhail Titov, Matteo Turilli, Jens Glaser, Ola Engkvist, Eric Stahlberg, Shantenu Jha, Peter V. Coveney
10:40-11:00 Advances in the Fragment Molecular Orbital (FMO) Method for High-Throughput Drug Design Alexander Heifetz
11:00-11:15 Machine Learning Surrogate Model for Molecular Pose Optimization in Drug Discovery Sean Black, Eric Stahlberg, Agastya Bhati, Shunzhou Wan, Peter Coveney
11:15-11:30 QM Methods for Exploring Molecular Interactions in Protein-Ligand Binding Reuben Martin, Alexander Heifetz, Andrea Townsend-Nicholson

<b>Thursday 14 September 12:00-13:00</b>
<b>Lunch</b>

<b>Thursday 14 September 12:45-13:45</b>
<b>LRZ Tours</b>
Location: LRZ

<b>Thursday 14 September 13:45-14:20</b>
<b>From desktop to HPC and beyond in the clinic 2</b>
Room: Terra Session Chair: Phil Luthert (UCL)
13:45-14:05 Personalised Treatment Effects: A Prototype Generic Software Kurinchi Selvan Gurusamy
14:05-14:20 CompBioMed Data Platform for FAIR Data Narges Zarrabi, Jazmin Aguado-Sierra

<b>Thursday 14 September 13:45-15:10</b>
<b>Molecular Medicine 2</b>
Room: Jupiter Session Chair: Andrea Townsend-Nicholson (UCL)
13:45-14:05 Development of Synthetic Retinoids for the Treatment of Neurodegenerative Diseases Ehmke Pohl
14:05-14:20 Long Time Scale Ensemble Methods in Molecular Dynamics: Ligand-Protein Interactions and Allostery in SARS-CoV-2 Targets Agastya P. Bhati, Art Hoti, Andrew Potterton, Mateusz Bieniek, Peter V. Coveney
14:20-14:40 Finding better molecules with Active Learning Hannes Loeffler
14:40-14:55 Large Scale Study of Ligand-Protein Relative Binding Free Energy Calculations: Actionable Predictions from Statistically Robust Protocols Agastya P. Bhati, Peter V. Coveney
14:55-15:10 Accurate Ligand-Protein Absolute Binding Free Energy Calculations at Large Scale: Equilibrium and Non-equilibrium Approaches Agastya P. Bhati, Shunzhou Wan, Peter V. Coveney
15:10-15:25 FEgrow: an open-source molecular builder and free energy preparation workflow Mateusz K. Bieniek, Ben Cree, Rachael Pirie, Joshua T. Horton, Natalie J. Tatum, Daniel J. Cole

<b>Thursday 14 September 14:20-15:30</b>
<b>Education, Training &amp; Public Awareness</b>
Room: Terra Session Chair: Carlos Teijeiro Barjas (SURF)
14:20-14:40 Materials Science and Biomedicine: Parallel Stories in Computation Alvaro Ridruejo

14:40-15:00 Building Learning Paths for High-Performance Computing Xavier Álvarez Farré, Carlos Teijeiro Barjas
15:00-15:30 Panel Discussion - Education, Training and Public Awareness of HPC in Biomedicine Carlos Teijeiro Barjas Panel discussion addressing current issues surrounding education, training and public awareness of HPC in biomedicine.

<b>Thursday 14 September 15:45-16:15</b>
<b>Refreshments</b>

<b>Thursday 14 September 16:15-17:00</b>
<b>Plenary Session 4 - Amanda Randles</b>
Unlocking the Potential: Advancing Vascular Digital Twins for Transformative Healthcare Room: Terra

<b>Thursday 14 September 17:00-17:30</b>
<b>Closing Remarks and Prizes</b>
Room: Terra

**Friday 15 September**

<b>Friday 15 September 9:00-16:30</b>
<b>CompBioMed-SEAVEA Hackathon (Satellite Event)</b>
Room: Hörsaal Session Chair: Diana Suleimenova (Brunel University London)



# Addressing All Neurodegenerative Diseases

## Novel neuroprotective small molecules with disease modifying potential

Nevrargenics Ltd is a UK-based neuroscience company specialising in the discovery and development of novel medicines for the treatment of all neurodegenerative disease, such as Alzheimer's and Parkinson's diseases, Multiple Sclerosis, and Amyotrophic Lateral Sclerosis. These diseases are a major medical challenge and is having an ever-increasing impact upon the lives of patients, carers and indeed, upon society as a whole.

Our understanding of the root causes of these diseases are still, to date, very limited, resulting in a lack of effective treatments which focus upon treating some of the symptoms rather than tackling the real causes and being able to reverse the diseases themselves.

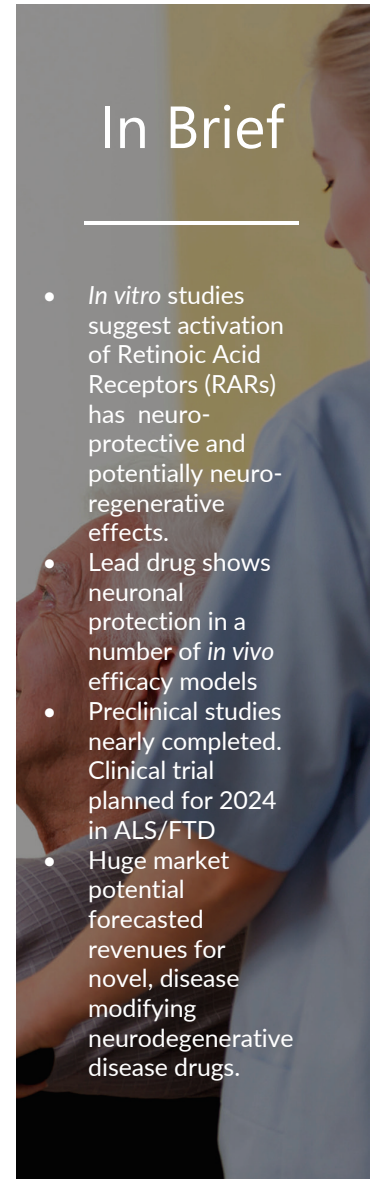
### Background

With a history going back 15 years, involving >150k man hours of research, 9 PhD students and 2 post-doctoral researchers split between two closely collaborating research groups based at Aberdeen and Durham Universities in the U.K., we have designed, synthesised and identified new synthetic retinoid drug candidates with disease modifying potential for establishing new treatment approaches. Our strategy is to employ a new type of molecule: dual-acting retinoic acid receptor modulators, as the basis for developing a series of new rationally designed, effective disease reversing treatments, meeting that most severe of unmet needs represented by all the neurodegenerative diseases.

Our business model is to drive high caliber Research & Development, and execute novel therapeutics through a focused commercial drug development approach, matched and supported by, progressing our underlying understanding of neurodegenerative disease mechanisms through ongoing research.

### Market Opportunity

Global healthcare spending expected to increase \$10 trillion by 2022 (Deloitte, 2019). Neurological disorders are a major, worldwide unmet need, with nearly 1 billion people affected (WHO). Progressive loss of nerves results from degeneration of brain tissues and nerves. Around 7 million deaths occur annually due to neurodegeneration, making it THE major unmet need and a cost in Europe alone of around €140 billion per annum and rising. There is a definite and urgent need for novel therapeutics, especially with disease modifying potential.



## In Brief

- *In vitro* studies suggest activation of Retinoic Acid Receptors (RARs) has neuro-protective and potentially neuro-regenerative effects.
- Lead drug shows neuronal protection in a number of *in vivo* efficacy models
- Preclinical studies nearly completed. Clinical trial planned for 2024 in ALS/FTD
- Huge market potential forecasted revenues for novel, disease modifying neurodegenerative disease drugs.

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