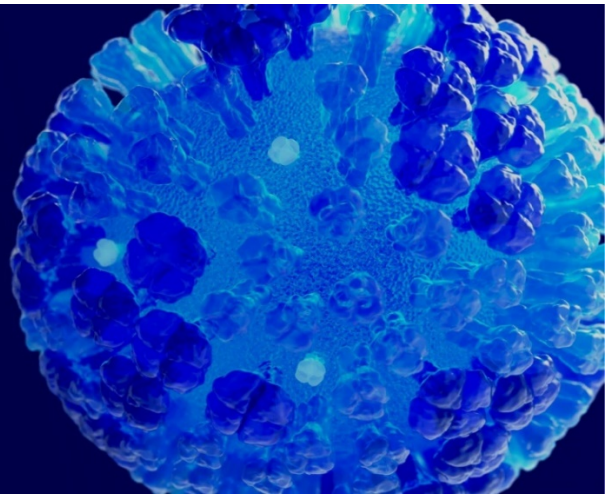
HPC & Data in Drug Design & Delivery



Ben Corry
(ANU)

Sean Smith
(NCI)

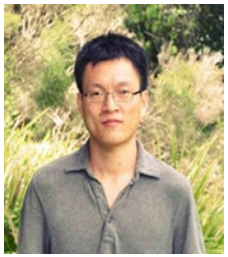
Andrew Howard
(NCI)

Maciej Cytowski
(Pawsey)

Katya Pas
(Monash)

Megan O'Mara
(UQ)

Alan Mark
(UQ)



Haibo Yu
(UoW)

Thomas Balle
(USyd)

David Chalmers
(Monash)

Olexandr Isayev
(CMU)

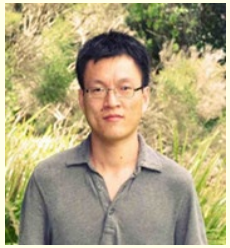
Ricardo Mancera
(Curtin)

Esben Bjerrum
(Odyssey Therapeutics)

Fiona McRobb
(Schrodinger)

HPC and Data in Drug Design and Delivery is a collaborative graduate teaching initiative for the Australian computational biological science research community. Below you find some brief professional bio details of the stellar teaching team. In each case, the name is linked to their website and the video thumbnail links to a short excerpt from their live online teaching sessions delivered as part of the course! To enrol as an Australian postgraduate student or researcher in the field, please follow click HERE.

Ben Corry is Professor at the Research School of Biology, Australian National University. He gained his PhD from the ANU in 2003, before holding successive ARC research fellowships at UWA. He returned to the ANU in a faculty position in 2012, where he held an ARC Future Fellowship. His research utilises molecular simulation to understand the structure and function of proteins as well as transport in synthetic systems, with applications in drug design and water treatment.	
Sean Smith is Director of the Australian National Computational Infrastructure (NCI) and conjointly Professor at the Australian National University (ANU). He gained his PhD at the University of Canterbury in New Zealand. He undertook postdoctoral research at Universität Göttingen and at UC Berkeley. He has held academic and management appointments at The University of Queensland, Oak Ridge National Laboratory, UNSW Sydney and ANU.	
Andrew Howard is Associate Director Cloud Services of the National Computational Infrastructure at the Australian National University. Andrew has many decades of hands-on technical, diplomatic and logistics experience covering a wide range of standard and bespoke technologies, languages and applications within Industry, government and academia nationally and internationally. He currently chairs the judging panel of the SuperComputing Asia Data Mover Challenge and the APAN Program Committee and Co-Chairs the Cloud Security Alliance: HPC Cloud Security, APAN E-Culture and Asia Pacific Research Platform working groups.	
Dr Maciej Cytowski joined Pawsey Supercomputing Centre in 2017 as a Supercomputing Application Specialist. He is presently Head of Scientific Services at Pawsey. He gained his PhD in Computational Science at the Polish Academy of Science. He is a mathematician and computational scientist with expertise is optimisation and development of application on massively parallel and accelerated HPC systems.	

Ekaterina Pas is Professor in the School of Chemistry at Monash University. She gained her PhD at Universität Münster in Germany under the supervision of Prof Stefan Grimme. She undertook postdoctoral research at the Australian National University and Monash University before taking up her faculty position at Monash in 2007.	
Megan O'Mara is Professor of Computational Biophysics at the Australian Institute for Bioengineering and Nanotechnology, University of Queensland. She gained her PhD from the Australian National University in 2005. After postdoctoral research at the University of Calgary in Canada (2005–2008) and at UQ (2009-2011), she took up an ARC DECRA at UQ and held a joint appointment as Lecturer between the School of Chemistry and Molecular Biosciences and the School of Mathematics and Physics. Megan joined the Research School of Chemistry at ANU as Rita Cornforth Fellow and Senior Lecturer in early 2015.	
Professor Alan Mark gained his PhD at Australian National University in Chemistry. He held postdoctoral positions at the Research School of Chemistry at ANU (1987-1988) and at University of Groningen (1989-1990). In 1990, he moved to ETH Zurich and became Oberassistant in 1996. In 1998, he was appointed Professor of Biophysical Chemistry, University of Groningen. Alan's primary research interests include physical and computational chemistry and simulation of biomolecular systems. He is presently Emeritus Professor at School of Chemistry and Molecular Biosciences, University of Queensland.	
Haibo Yu is Associate Professor at School of Chemistry and Molecular Bioscience, University of Wollongong. He gained his PhD at the ETH Zürich. He then conducted postdoctoral training at the University of Wisconsin-Madison (2005-2007) and University of Chicago (2007-2010). He joined the School of Chemistry and Molecular Bioscience at the University of Wollongong in 2010.	
Thomas Balle is presently Associate Professor at the School of Pharmacy, University of Sydney. He gained his PhD in Medicinal Chemistry in 2002 at University of Copenhagen and conducted postdoctoral training there (2003-2006). He was Associate Professor at the Danish University of Pharmaceutical Sciences from 2006 to 2012 before he joined University of Sydney in 2012.	

Dr David Chalmers is Senior Lecturer at the Faculty of Pharmacy and Pharmaceutical Sciences, Monash University. He gained his PhD in Medicinal Chemistry from University of Melbourne and was Postdoctoral Research Fellow at the Washington University (1993-1996) before he joined Monash university. He is an accomplished computational scientist with broad research interests and outputs from computational and medicinal chemistry; drug design and discovery; molecular dynamics and modelling and so forth.	
Olexandr Isayev is Assistant Professor at the Department of Chemistry at Carnegie Mellon University. In 2008, Olexandr received his Ph.D. in computational chemistry. He was Postdoctoral Research Fellow at the Case Western Reserve University and a scientist at the government research lab. During 2016-2019, he was a faculty at UNC Eshelman School of Pharmacy, the University of North Carolina at Chapel Hill. Olexandr received the “Emerging Technology Award” from the American Chemical Society (ACS) and the GPU computing award from NVIDIA. The research in his lab focuses on connecting artificial intelligence with chemical sciences.	
Ricardo Mancera is Professor of Biophysical Chemistry and Computational Biophysics at Curtin University. He obtained his PhD in Theoretical Chemistry from University of Cambridge. Presently he heads the Biomolecular Modelling Group in the Curtin Medical School and is Program Lead in Biomolecular Structure and Interactions at the Curtin Health Innovation Research Institute (CHIRI). He is also a member of the Curtin Institute for Computation (CIC).	
Dr Esben Jannik Bjerrum completed his PhD in Computational Chemistry at Copenhagen University in 2008. He has since worked both in academia as a post.doc, in industry as an IT specialist as well as an self-employed pharma IT consultant. In 2017 his independent research resulted in several contributions to the chemistry deep learning renaissance. He joined Odyssey Therapeutics in 2022 where he currently works with development and usage of de novo design algorithms. He’s the lead blogger of cheminformania.com.	

Dr Fiona M. McRobb is Principal Scientist in the Drug Discovery Group at Schrödinger. She gained her PhD from Monash University in 2011 and held postdoctoral research position at UC San Diego from 2012 to 2014. She has joined Schrödinger since 2014.

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