Pistoia Alliance Cheminformatics Forum

Meeting Wednesday 18-Jun-25

Royal Society of Chemistry, Burlington House, Piccadilly, London W1J 0BA

Participant photos / brief biographies

Photo	Bio
	**Becky Upton** Becky was appointed as the Pistoia Alliance's first female President in June 2022. She is a long-time supporter of pre-competitive collaboration in life sciences and healthcare R&D and the critical role it plays in advancing science and is passionate about diversity in STEM. Becky is responsible for leading the Pistoia Alliance's strategy and defining its future within areas of increasing importance to the industry, such as data standards, emerging technologies, diversity and inclusion, sustainability, and precision medicine. Becky first engaged with the Pistoia Alliance on its Lab of the Future project whilst at VWR (now part Avantor) where she worked for over a decade in sales, business development, and scientific services. From here, she joined the scientific instrumentation and analytical services company, Pion, as Managing Director, before moving to the Alliance as a project manager. She later became Chief Portfolio Officer and within this role established the Alliance's first and thriving Diversity and Inclusion in STEM Leadership program. Becky re-joined the Alliance as President after a return to the commercial world as a Director at Impellam Group where she led the company's STEM services strategy. Becky has a PhD in Biochemistry from Imperial College and an MBA from Cranfield University.

Christian Baber

J. Christian Baber is the Chief Portfolio Officer of the Pistoia Alliance.

Christian is a chemist by training and holds undergraduate and PhD degrees in computational chemistry with a focus on AI techniques to assess the synthetic accessibility of *de novo* design compounds.

Christian continued this work with a post-doctoral fellowship on the automated design of targeted combinatorial libraries at the Department of Knowledge Engineering, Osaka University, Japan before moving into industry initially as a computational chemist and cheminformatician.

Christian has a wide breadth of R&D experience across companies ranging from startups to large pharma and diverse therapeutic areas with a focus on informatics and predictive modeling for drug discovery but has also managed development systems and lab & automation teams including compound management and high-throughput purification. Most recently, after spending the previous 6 years leading Scientific Computing & Informatics and R&D IT at Shire & Takeda, Christian led the global Scientific & Pharmaceutical Data, Informatics and Systems function in Janssen R&D.

In addition to his day job, Christian sits on several industry advisory boards, and has been a Director of the Pharmaceutical R&D Information Systems Management Executive (PRISME) forum and chair of the Finance sub-committee of the Pistoia Alliance Board of Directors.

Claire Bellamy

Claire is a senior manager at Pfizer.

Claire has extensive experience of working within Pharma R&D IT both as project lead and business relationship manager. After reading Chemistry at Nottingham University, Claire worked as a medicinal chemist before moving to AstraZeneca R&D IT. During her 13 years at AZ Claire worked across multiple projects but notably led the business analysis work and project managed the configuration of the global Med Chem ELN and Bio ELNs.

After gaining an MBA from Loughborough University, Claire worked for the Pistoia Alliance leading the HELM project which established HELM across the life science community as the preferred representation of complex biomolecules, gaining recognition by ISO and supported the EBI ChEMBL and PubChem teams to add HELM to their public datasets.

Currently Claire leads a team at Pfizer to capture and manage AI-ready proteomics data.

Darren Green

Darren has recently retired from GSK after a 33-year career which included roles in Cheminformatics & Data Science, Computational Chemistry, Combinatorial Chemistry, laboratory automation and informatics, Data Warehousing and Lean Sigma process optimisation.

He is now a consultant and Honorary Professor of Chemistry at University College, London.

Darren has a PhD in Theoretical Chemistry from the University of Manchester and is a Fellow of the Royal Society of Chemistry.

Jürgen Harter

Jürgen is the CEO & Founder MatriQx and is the former CEO, Cambridge Crystallographic Data Centre (CCDC).

Jürgen has been running the CCDC, a not-for-profit global data repository (for crystal structures) and internationally renowned structural science research centre as Chief Executive Officer until recently. He is presently focusing on setting up a new entrepreneurial venture called MatriQx - addressing the digital transformation of chemistry with AI/ML and high-quality data. He has three decades worth of experience within life sciences, biotech, information technology and business development.

His executive leadership expertise is extensive, paired with commercial acumen, a strong technical background and broad business skills, gained in organisations such as CCDC, Horizon Discovery, Exco InTouch, PerkinElmer Informatics (now Revvity), CambridgeSoft, Abcam and Biowisdom.

He holds a PhD in organic chemistry from the University of Cambridge (Prof. S.V. Ley) and carried out his postdoctoral research at the Unilever Centre for Molecular Informatics (Prof. R.C. Glen, and Prof. P. Murray-Rust). He cares passionately about digital transformation, big & smart data (and FAIR standards for both data and software), knowledge management, automation, scientific and business intelligence. Working with diverse and global teams he has successfully delivered many complex solutions, projects, and business systems (ERP / CRM / ELN / LIMS / mHealth platforms) spanning a range of business functions on an enterprise-wide & global level. He has worked with most of the Top 20 pharmaceutical companies and has a wide global network in the biotech, pharma, and the chemical industry sectors (incl. materials science). This is combined with many active links to information management and software development companies & vendors, as well as new AI companies & startups.

Jürgen passionately cares about driving excellence in people, science, and data quality. He likes to push value engineering, continuously raise automation levels, utilise transformative and innovative technologies - working with the global scientific communities, to create value & growth and advance science. He has been championing the building and establishing of digital drug design and digital drug development & manufacturing centres, based on high-quality structural chemistry data in combination with scientific software utilising artificial intelligence (machine learning, deep learning & neural nets, GenAI), and cheminformatics algorithms, and is passionate about the concept of ‘Digital First’ and ‘Digital Twins’.

David Drake

David has over 20 years' experience in Drug Discovery IT, including roles as Early Science Enterprise Architect, Enterprise Data Architect and currently Drug Discovery Capability Lead at AstraZeneca UK. David provides strategic thought-leadership and domain expertise on the future direction of the IT platforms & applications supporting Early Science.

As a previous Board member of the Pistoia Alliance, David is a dedicated supporter of pre-competitive collaboration and the value of working together to solve life science challenges.

David holds a DPhil in Chemistry from the University of Oxford and a Postgrad Diploma in Data Science, Technology, and Innovation (with Medical Informatics) from the University of Edinburgh.

John Wise

John is a consultant to the PRISME Forum and the Pistoia Alliance where his responsibilities include business development and member relations. He specialises in the coordination of pre-competitive collaborations in life science / biopharma R&D IT.

Previously, John has held Informatics leadership roles in a variety of organizations including the University of London, Sandoz (now Novartis), the Imperial Cancer Research Fund (now CRUK), Roche, Ipsen and Daiichi Sankyo. John has also worked in the technology supply side of the industry. In these roles, he has gained direct hands-on experience writing analytical software, teaching computation, delivering IT capabilities, and providing computer-based services to the discovery, non-clinical development, clinical development, and regulatory affairs domains of the life-science industry.

John graduated in physiology from the University of Oxford and received a post-graduate certificate in education from the University of London.

Ann Mai Wiseman

Anne Mai Wassermann is the Global Head of Cheminformatics at Johnson & Johnson Innovative Medicine. Her team partners closely with colleagues from In Silico Discovery, Chemistry, Screening, Cell and Genetics Medicine, IT, and Therapeutic Areas to deliver state-of-the-art informatics capabilities including support for encoded library platforms, predictive modeling, visualization, and design tools.

Prior to joining Johnson & Johnson, she held roles at Novartis, Pfizer, MSD, Bayer, and Odyssey Therapeutics. Anne Mai holds a PhD in Computational Life Sciences from the University of Bonn.

James Lumley

James has 25 years' experience applying molecular design methods and software engineering practices to aid small-molecule drug discovery. His initial career includes 10 years in Biotech applying small-molecule design methods, primarily as Head of Computational Chemistry, Arrow therapeutics (subsidiary of AstraZeneca). He has inventorship on multiple antiviral drug candidates including AZD-7295 and later Sisunatovir (RV521) as a ReViral Ltd cofounder. In 2010, James joined Eli Lilly responsible for global Cheminformatics support. He led projects delivering award-winning platforms, methods, and models including multiple CIO awards and an IT World Innovative Practice Award (Research Data 20 2020). He is currently Head of Cheminformatics at GSK.

Csaba Peltz

Spent 11 years in pharmaceutical R&D specializing in mass spectrometry and NMR spectroscopy. Joined Chemaxon in 2012 as part of the product development team. Held various roles within the product organization, including product owner/manager, product director responsible for portfolio-level strategy, and currently director of chemistry with a focus on science and market trends.
Holds an MSc in chemistry and computer sciences, and a PhD in chemistry with a specialization in theoretical mass spectrometry.

Ramil Nugmanov

Ramil Nugmanov is a Principal Scientist at Johnson & Johnson Innovative Medicine, specializing in AI-driven drug design, synthesis optimization, and cheminformatics. He is leading the advancement of innovative AI platforms for drug discovery, synthesis planning, and molecular activity/reactivity prediction, bridging deep learning, cheminformatics, and computational chemistry.
Before joining J&J, Ramil was an Associate Professor at Kazan Federal University, mentoring master's students and teaching courses on data mining, deep learning, and cheminformatics. Before, as a Senior Scientist, he developed generative models for molecular activity and reactivity prediction and contributed to open-source ML and cheminformatics tools.
With a Ph.D. in Organic Chemistry & Cheminformatics from the Arbuzov Institute of Organic and Physical Chemistry, Ramil combines deep scientific expertise with a passion for AI innovation in pharmaceutical research.

Jeremy Fry

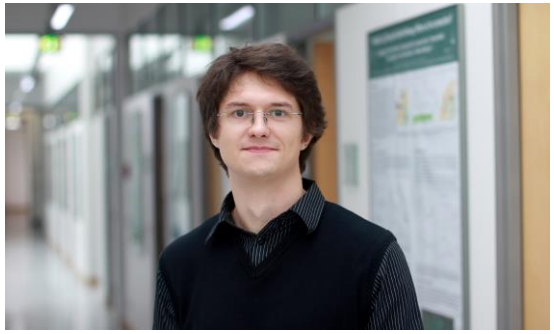
Jeremy describes himself as a physical and digital chemistry, with interests in promoting interdisciplinary research across the physical and life sciences, from laser spectroscopy and imaging, computational modelling, and digital chemical duals.

Jeremy obtained his BA in 1980 and DPhil in 1982 (under the supervision of Brian Howard) in Chemistry from the University of Oxford. Then 1982 – 1984 held a NATO/SERC fellowship at the Lawrence Berkeley Laboratory, University of California, (with Yuan T. Lee). He was appointed to a lectureship in at the University of Southampton in 1984, where he is now Professor of Physical Chemistry. From 2019 to 2024 he was the Head of the Computational Systems Chemistry Section, and 2021 – 2024 Head of Physical Chemistry Teaching.

Jeremy has heavily involved in the UK e-Science programme, (the CombeChem Project) which along with is role in the Digital Economy programme (IT as a Utility Network+) led to his role as PI of the AI for Scientific Discovery Network. He is a co-I on the Physical Science Data Infrastructure project, Physical Science Data Science Service, and the Alchemy AI Hub. His most recent project which evolved from a Basic Technology funded project to now working with the Rosalind Franklin Institute (RFI) is to develop further the laser driven high resolution soft x-ray microscope for biological imaging in the water window.

In the Royal Society of Chemistry, Jeremy is a committee member and former secretary of the Chemical Information and Computer Applications Interest group (CICAG), served on the Members and Communities Board (MCB), and earlier in his time at Southampton was the secretary and Chair of the Mid Southern Counties Local Section

Jeremy is vice president of the Physical and Bio-Physical Division of IUPAC, a member of the IUPAC Committee on Publications and Chemical Data Standards (CPCDS) and coordinates the projects for the Green Book (Quantities, Units and Symbols in Physical Chemistry).



Adrian Krzyzanowski

Adrian holds a Bachelor of Science in Biochemistry from Aberystwyth University, Wales, and a Master of Science in Chemistry, with a specialisation in Medicinal Chemistry, from Umeå University, Sweden. During his studies in Sweden, he gained hands-on experience in synthetic organic chemistry, working under the guidance of Professors Christian Hedberg and Mikael Elofsson. He further continued his studies in Germany, obtaining a doctoral degree in Chemical Biology at the Max Planck Institute of Molecular Physiology and the Chemical Genomics Centre in Dortmund. His doctoral research, supported by a scholarship from the German Association of the Chemical Industry, was conducted in the laboratories of Prof. Herbert Waldmann and Peter ‘t Hart. There, he focused on studying protein-protein interactions, developing modulatory cyclic peptides, and conducting molecular modelling and simulations of ligand-protein complexes, alongside cheminformatics-based data analysis related to molecular complexity. Adrian earned an engineering degree in Informatics from the Polish University of Humanities and Economics in Łódź. In 2023 he joined the GSK Cheminformatics Group.

David Lancaster

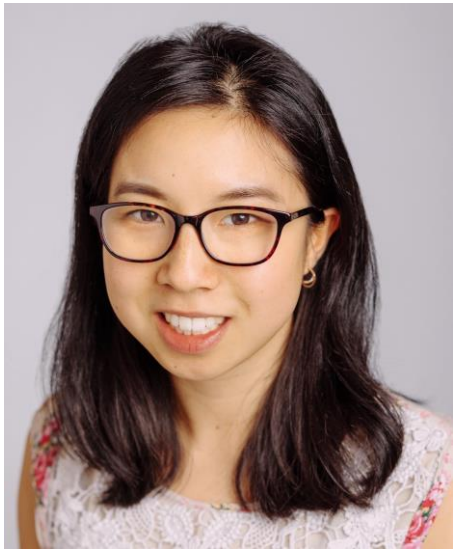
David Lancaster is a partner and Head of Intellectual Property Litigation in Quinn Emanuel's London Office.

David specialises in the litigation and resolution of disputes relating to intellectual property rights, including patents, trademarks, copyright, designs, and confidential information. David is highly experienced in representing clients in litigation before the English Courts and co-ordinating proceedings before European national courts and the European Patent Office. David is qualified as a barrister in both England & Wales and Ireland and advises clients in relation to the Unified Patent Court.

David has a technical background in biochemistry and acts for clients across a range of business sectors, including life sciences, telecommunications (including FRAND licensing), computing, financial services, energy, and manufacturing. David increasingly advises in relation to enforcement and risk mitigation strategies in the context of artificial intelligence.

Thomas Doerner

Thomas Doerner is an independent consultant for research informatics in life sciences and chemistry. Located at the interface of R&D and Informatics, Thomas helps his clients define, design, and implement solutions that enable scientists, foster more effective R&D, and lay the foundation to achieve better outcomes faster. Before he became self-employed in 2010, Thomas held various customer-facing technical roles at MDL and Elsevier. Thomas is an organic chemist by background and has a doctorate from the University of Heidelberg, Germany.



Susan Leung

Susan Leung is a Cheminformatics Data Scientist at AstraZeneca, working at the intersection of chemistry, data, and software to accelerate drug discovery. She specializes in molecular representations, chemical registration systems, and structure-based methods. Prior to joining AstraZeneca, she worked at Benevolent AI and completed her DPhil in Cheminformatics at the University of Oxford.

Gerde Blanke

After his Dr. rer. Nat. in theoretical chemistry at the HHU in Düsseldorf in 1991, Gerd Blanke had worked for MDL Information Systems and Symyx until 2010 when he opened his own business StructurePendium Technologies GmbH in Essen, Germany. He has specialized in the representation of chemical structures and reactions working on structure normalizations, registration of chemical structures and reactions, database mergers, and structure-based data analytics. Since 2021 he has hold the position of the Technical Director of the InChI Trust, being responsible for the further technical development of the IUPAC International Chemica Identifier.

James Webster

James Webster is the team leader of the Computational Drug Discovery Developer Team (CD3T) within the Drug Discovery Unit (DDU) at the University of Dundee. His main research interest is in cheminformatics and bioinformatics and their applications to problems in chemical biology.

James completed his doctoral studies at the University of Sheffield within the cheminformatics group developing new methods for reaction based de novo design. He then worked in industry at Evotec (U.K.) working on method development for multi-modal generative design - spanning small molecules to full scale protein design.

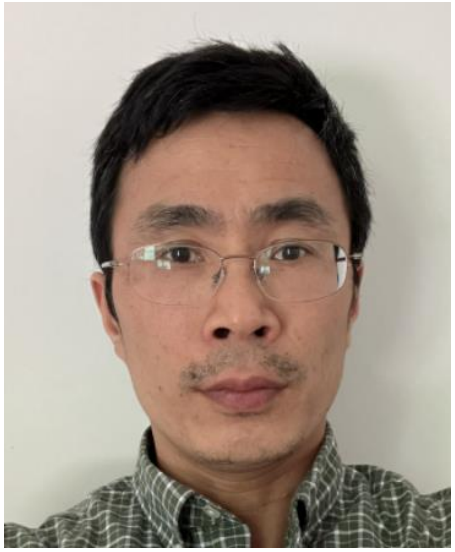
At the DDU his research is focussed on utilising modern Design of Experiments (DoE) and AI/ML approaches to reimagine drug discovery and reduce the “time-to-hypothesis.”

Robet Owen

Robert Owen leads the Chemistry Solutions group within the Scientific Software Engineering (SSE) organization as part of Pfizer Digital's R&D Creation Center. His group focuses on delivering custom software solutions and supporting the required infrastructure to enable chemists within Pfizer's as well as supporting initiatives across the wider research organization. Robert completed his doctorate with Laura Kiessling at the University of Wisconsin – Madison where he focused on developing new tools to understand multivalent interactions. Following a post doc with William Roush at the University of Michigan focused on total synthesis of Peloruside A, Robert joined Pfizer as a medicinal chemist at their research site in Ann Arbor. After time in Sandwich and Cambridge UK, Robert moved to a more technology focused role within Pfizer's research organization and within Pfizer Digital.

Matthew Sage

Dr. Matthew Sage is Senior Product Manager for the Cheminformatics applications at BIOVIA, with over 20 years of experience working with customers in Implementation Project management, Database administration, End User and Administrative training, Custom Software solution deployment and more recently, he has been responsible for the Cheminformatics offerings from BIOVIA. Namely the scientific sketchers, chemistry storage and searching capabilities, Pipeline Pilot Chemistry and the Chemistry aspects in BIOVIA's ELNs. Matthew has a PhD from the University of Bath, UK in Medicinal Chemistry and Molecular Modelling.



Tony Yuan

Tony (Yongwen) Yuan is the President and founder of Scilligence, a leading provider of integrated cheminformatics and bioinformatics software solutions for life sciences R&D. With over two decades of experience in cheminformatics and scientific software development, Tony has been instrumental in advancing tools that streamline data management and accelerate discovery in the pharmaceutical and biotech industries.

Tony has 25 years of software development experience in cheminformatics and bioinformatics. Prior to founding Scilligence in 2011, Tony worked as a cheminformatician at Novartis in Cambridge for 3 years, and as a software developer at Cambridgesoft for 7 years, where he contributed to key products including ChemDraw, Chem3D, and ChemScript. He holds a master's degree in Cheminformatics, and bachelor's degree in chemical engineering.

Nicolas Triballeau

Nicolas Triballeau is Director Drug Discovery - Chemistry at Revvity Signals. With 17 years of experience in drug discovery, he has not only provided direct project support and led teams but has also played a significant role in establishing scientific standards and ontologies. Nicolas holds a master's degree in chemical engineering with a specialization in organic chemistry, a Pharm.D. and a Ph.D. in Drug Design from the University of Paris.