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SAE Media Group Proudly Presents the 7th Annual Conference...

AI in Drug Discovery

**Harnessing the power of AI to maximise innovation
and efficiency across the drug pipeline**

Hilton London Kensington, UK

9 - 10
MAR
2026

HIGHLIGHTS FOR 2026:

- **DISCOVER** how Eli Lilly, Astellas Pharma, and Novo Nordisk use next-gen AI and automation to accelerate real-time drug discovery workflows
- **NETWORK** with senior experts from GSK, AstraZeneca, Novartis, and UCB as they share advances in AI-driven target identification, molecular design, and translational research
- **LEARN** from Sanofi, Recursion, and Insilico Medicine how machine learning is streamlining discovery-to-clinic, reducing late-stage attrition, and improving outcomes
- **JOIN** Roche, Orion Pharma, and Servier leaders to map the next five years of AI innovation, from ethics to autonomous labs and data integration

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2026 SPEAKERS:



Peter Clark,
VP Computational Drug Design,
Novo Nordisk



James Lumley,
Head of Cheminformatics,
GSK



Dr Pedro J. Ballester,
Royal Society Wolfson Fellow and Associate
Professor, Department of Bioengineering,
Imperial College, **University of London**



Lewis Vidler,
Senior Director – Structure Based Drug Design,
Eli Lilly and Company



Tim Hohm,
Associate Director Digital Science
Ext Partnerships, **Novo Nordisk**



Graeme Robb,
Director, Computational Chemistry,
AstraZeneca



Haruna Iwaoka,
Head, Advanced Modelling and Assays,
Innovation Lab,
Astellas Pharma



Le (Muller) Mu,
MLOps Lead, Computational Sciences
Center of Excellence, gRED,
Roche



Reiko Wada,
Senior Scientist,
Astellas Pharma



Anna Macintyre,
Senior Data Scientist,
Novo Nordisk



Simone Fulle,
Head CADD, Basel,
Novartis



Martin Redhead,
Associate Vice President Primary
Pharmacology,
Recursion



Paul Mortenson,
Senior Director, Computational
Chemistry and Informatics,
Astex Pharmaceuticals



Teresa De Haro,
Principal Scientist,
UCB



Martin Butterschoen,
Researcher,
University of Oxford



Venkatesh Pilla Reddy,
Senior Director, Global PKPD
and Pharmacometrics,
Eli Lilly



Christoph Grebner,
Senior Principal Scientist,
Sanofi



Dr Petrina Kamya,
Global Head of AI Platforms,
VP Insilico Medicine, President,
Insilico Medicine Canada Inc.



Sammeli Liikkanen,
Director, Digital Medicine,
Orion Pharma



Dr Yogesh Sabnis,
Lead Chemist,
UCB



Thierry Dorval,
Head of Data Science and
Data Management, **Servier**

Our Past Attendees Include:



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A LETTER FROM THE CHAIR

Dear Colleagues,

It is with great pleasure that I invite you to SAE Media Group's AI in Drug Discovery conference, taking place on 9–10 March 2026 in London.

This year's event will showcase how AI and machine learning are transforming every stage of drug R&D—driving efficiency, innovation, and new possibilities across the sector. As the field continues to evolve rapidly, we recognise that unlocking the full potential of AI requires not only technical progress but also advances in data generation, quality, and automation. That's why our 2026 programme expands its coverage to highlight these critical enablers.

We will deep-dive into the latest breakthroughs in AI-driven target identification, computational drug design, cheminformatics, and generative AI. The agenda also features real-world case studies on clinical progress, as well as honest discussions about the challenges of advancing AI-designed molecules through the pipeline.

This conference is your opportunity to engage with global leaders, share insights, and help shape the future of AI in drug discovery.

As Chair of this conference, I look forward to welcoming you to this must-attend event in London this March.

Yours sincerely,



Peter Clark,
VP, Computational Drug Design,
Novo Nordisk

08.00 Registration & Coffee

08.50 Chair's Opening Remarks

Peter Clark, VP Computational Drug Design, **Novo Nordisk**

09.00 Opening Address: Developing Actionable, Lab-Tractable Generative Designs to Accelerate Candidate Discovery



- Bridging in silico and in vitro workflows by generating molecular designs that align with real-world synthesis constraints and experimental feasibility
- Leveraging structure-based and ligand-based generative models to propose novel compounds optimised for activity, selectivity, and developability
- Accelerating iteration cycles through AI-guided design prioritisation, reducing reliance on brute-force screening and enhancing early candidate quality

James Lumley, Head of Cheminformatics, **GSK**

AI/ML FOR TARGET IDENTIFICATION AND EARLY DISCOVERY

09.30 Session Reserved for Lead Sponsor

10.00 Applications of AI in a Structure-Rich Environment

- Using proprietary structural data to evaluate and improve state-of-the-art co-folding models
- Characterising binding sites with a novel protein language model to generate debiased training and test sets for protein-ligand structure prediction
- Seamlessly integrating predictive and generative models into FBDD

Paul Mortenson, Senior Director, Computational Chemistry and Informatics, **Astex Pharmaceuticals**

10.30 Morning Coffee & Networking Break

11.00 Practical Applications of AI in Drug Discovery: Bridging Biology and Chemistry



- Integrating AI methodologies in biological data analysis
- Enhancing chemical compound discovery through AI-driven algorithms
- Case studies: successful AI implementations in drug discovery pipeline
- Future perspectives: the evolving role of AI in pharmaceutical research

Thierry Dorval, Head of Data Science and Data Management, **Servier**

11.30 Session Reserved for Sponsor

12.00 Mega-Scale Benchmark of De Novo Design Tools for Developing Protein-Based Therapeutics

- Recent explosion in the options available for generative AI-based protein design
- Comparing the in silico and in vitro success of out-of-the-box combinations of various tools, approaches and parameters
- Retrospective evaluation of experimental results to further optimise the selection of validation criteria

Anna Macintyre, Senior Data Scientist, **Novo Nordisk**

12.30 Large Language Models in Drug Discovery: From Design to Chemical Reasoning

- Exploring LLMs' potential in generating, analysing, and optimising chemical structures with improved efficiency
- Advancing chemical reasoning from large language models for molecular design
- Transforming drug discovery workflows by conversational AI

Christoph Grebner, Senior Principal Scientist, **Sanofi**

13.00 Networking Lunch

14.00 Holistic de Novo Design: Integrating Human Insight, AI, and Physics to Accelerate Drug Discovery at UCB



- Combining human design, AI, and physics-based methods to enhance drug discovery
- Using high-performance computing and predictive tools for synthesizable compounds
- A centralised platform for data-driven decision-making and collaboration
- Improved compound design, enhanced DEL readouts, and successful application of FEP+ in solving medium-resolution cryo-EM structures

Teresa De Haro, Principal Scientist, **UCB**

14.30 Session Reserved for Sponsor

15.00 Biasing and Debiasing Protein-Ligand Complex Prediction for Drug Discovery

- Highlighting how biases in training data and model architecture can distort protein-ligand interaction predictions, impacting drug discovery outcomes
- Exploring biasing techniques used to guide models toward chemically relevant interactions and improve predictive focus
- Presenting methods to identify and mitigate unwanted biases, such as data augmentation, adversarial training, or reweighting schemes
- Reviewing how balancing biasing and debiasing enhances model generalisability, leading to more accurate and robust candidate screening

Martin Buftenschoen, Researcher, **University of Oxford**

15.30 Afternoon Networking Break

16.00 Session Reserved for Sponsor

FOUNDATION MODELS AND AI INFRASTRUCTURE

16.30 Enabling AI in Drug Discovery - the Path Towards Self-Serviceable MLOps in Pharma Research

- Breaking silos: Enabling cross-disciplinary collaboration with intuitive, self-service AI tools
- Scaling success: How Roche pRED evolved MLOps from managed service to self-service over five years
- Accelerating discovery: Empowering scientists to turn hypotheses into insights faster and drive new therapies to patients.

Le (Muller) Mu, MLOps Lead, Computational Sciences Center of Excellence, gRED, **Roche**

17.00 Supercomputing & Quantum Horizons: Accelerating Pharma's Next Leap

- Exploring why mid-sized pharma must rely on external HPC infrastructure over in-house builds
- Showcasing LUMI and LUMI v2 supercomputing capabilities for pharma R&D
- Highlighting the Orion use case: unlocking new performance gains with HPC
- Framing the roadmap: quantum computing developments and practical next steps

Sammeli Liikkanen, Director, Digital Medicine, **Orion Pharma**

17.30 Chair's Closing Remarks and End of Day One

Peter Clark, VP, Computational Drug Design, **Novo Nordisk**

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08.30 Registration & Coffee

08.50 Chair's Opening Remarks

Peter Clark, VP Computational Drug Design, Novo Nordisk

DATA EFFICIENCY, LAB AUTOMATION & DEEP LEARNING

09.00 Opening Address: Autonomous Agents in the Field of Drug Discovery, How Useful Are They? And Where Are We Likely to See the Biggest Impact?

- Reviewing where autonomous agents are delivering value in drug discovery today
- Exploring how agents can automate target selection, compound screening, and data analysis
- Understanding the roadblocks and current limitations such as trust, transparency, and integration and potential approaches for overcoming them
- Outlook on where autonomous agents are poised to make the biggest impact next

Dr Petrina Kamyra, Global Head of AI Platforms, VP Insilico Medicine, President, Insilico Medicine Canada Inc.

09.30 Session reserved for gold sponsor

10.00 Panel Discussion: The Lab of the Future: Closing the Loop Between AI and Automation

- Orchestrating experiment design, execution, and analysis in real time
- Integrating robotic systems with AI decision engines for autonomous workflows
- Building feedback-driven cycles and enhancing data quality and speed through sensor fusion and process control

Lewis Vidler, Senior Director – Structure Based Drug Design, Eli Lilly and Company
Haruna Iwaoka, Head, Advanced Modelling & Assays, Innovation Lab, Astellas Pharma
Reiko Wada, Senior Scientist, Astellas Pharma

10.30 Morning Coffee & Networking Break

AI FOR CHEMISTRY, SCALE-UP, AND REPURPOSING

11.00 Case Study: Mahol-A-Ba: Integrating AI, Robotics, and Human Expertise for Next-Generation Drug Discovery

- Combining AI-driven analysis, robotic execution, and expert insight to accelerate and enhance discovery workflows
- Adapting the platform to advanced cell models and simulations in line with FDA and NIH guidelines to reduce animal use
- Advancing toward autonomous robot control guided by AI-evaluated experimental results for greater quality and efficiency

Haruna Iwaoka, Head, Advanced Modelling & Assays, Innovation Lab, Astellas Pharma

11.30 Session Reserved for Sponsor

12.00 Operationalising AI at Scale: From Proof-of-Concept to Cross-Portfolio Integration

- Establishing MLOps systems for model versioning, testing, and monitoring
- Fostering collaboration between domain scientists and data experts
- Driving internal adoption through user-friendly platforms and success metrics

Simone Fulle, Head CADD, Basel, Novartis

12.30 Networking Lunch

AI IN TRANSLATIONAL & CLINICAL SCIENCE

13.30 AI and ML in Clinical Pharmacology: Unlocking the Strategic Value of PK/PD Modelling

- Enabling data-driven decisions on dose selection, trial design, and patient safety through AI-enhanced pharmacology models
- Reducing late-stage attrition by improving the predictability of clinical outcomes from preclinical data
- Driving faster, more cost-effective development pathways by embedding PK/PD insights into portfolio-level strategy

Venkatesh Pilla Reddy, Senior Director, Global PKPD and Pharmacometrics, Eli Lilly

14.00 Session Reserved for Sponsor

14.30 Applying AI to Decode Biology

- Unlocking complex biological mechanisms through AI-driven data integration and modelling
- Accelerating target and biomarker discovery by linking omics, imaging, and clinical data
- Driving translational insights that connect molecular biology to therapeutic outcomes

Martin Redhead, Associate Vice President Primary Pharmacology, Recursion

15.00 Afternoon Networking Break

ADVANCES IN PREDICTIVE MODELING FOR DRUG-TARGET INTERACTIONS

15.30 Machine-Learning Scoring Functions for Structure-Based Binding Affinity Prediction: A 15-Year Perspective

- Reviewing the evolution of ML-based scoring functions from early linear models to modern deep learning architectures, highlighting key milestones and breakthroughs
- Comparing performance trends, limitations, and validation strategies across generations of models using benchmark datasets and real-world case studies
- Pointing out common pitfalls and limitations, and the latest efforts to mitigate them

Dr Pedro J. Ballester, Royal Society Wolfson Fellow & Associate Professor, Department of Bioengineering, Imperial College, University of London

THE FUTURE OF AI IN DRUG DISCOVERY

16.00 Closing Panel Discussion: Charting the Next 5 Years of AI in Drug Discovery

- Evaluating emerging technologies including causal AI, agent-based learning, and autonomous labs; establishing organisational shifts needed to fully capitalise on AI innovation
- Discussing regulatory, ethical, and public trust considerations
- Mapping the convergence of AI, data, and experimental science over the coming decade

Le (Muller) Mu, MLOps Lead, Computational Sciences Center of Excellence, gRED, Roche

Dr Yogesh Sabnis, Lead Chemist, UCB

Tim Hohm, Associate Director Digital Science Ext Partnerships, Novo Nordisk

16.30 Chair's Closing Remarks and End of Conference

Peter Clark, VP Computational Drug Design, Novo Nordisk



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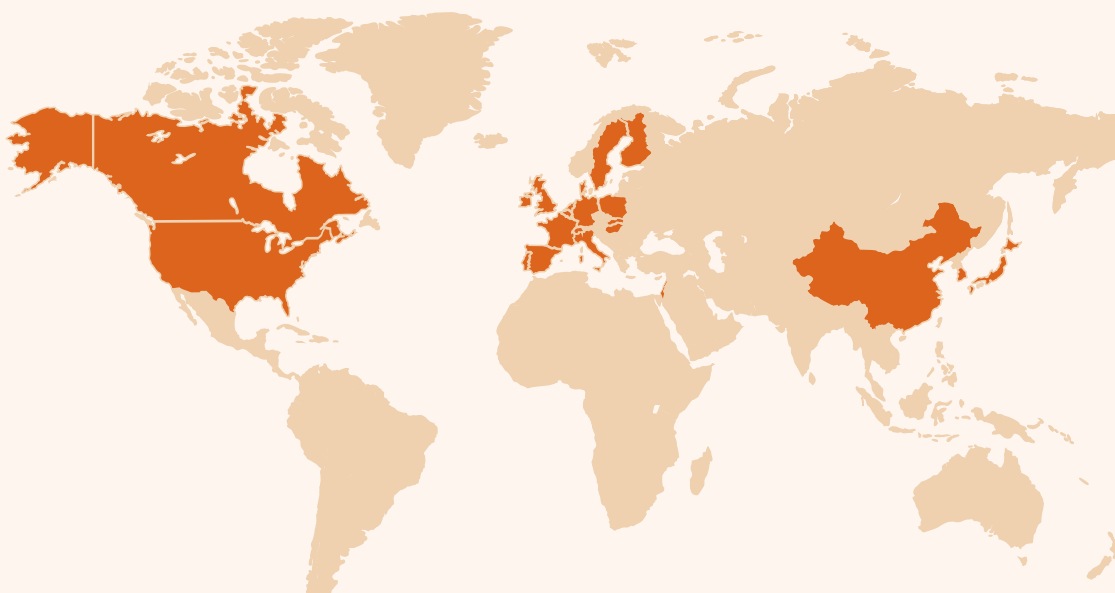
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PAST ATTENDEE

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