

REGISTER BY 27 NOVEMBER AND SAVE £400
REGISTER BY 10 JANUARY AND SAVE £200
REGISTER BY 31 JANUARY AND SAVE £100

SAE MEDIA
GROUP

SAE Media Group Proudly Presents the 6th Annual Conference...

AI in Drug Discovery

Transforming drug discovery and development
with the power of machine learning

Hilton London Kensington, UK

10 - 11
MAR
2025

HIGHLIGHTS FOR 2025:

- **ENGAGE** in discussions on the latest advancements in computational drug design methodologies with leaders from Novartis, GSK, UCB Pharma and Sanofi.
- **GAIN** insights from senior industry experts on methods for accelerating AI integration within existing processes and the art of balancing exploration vs exploitation in drug discovery.
- **EXPLORE** the impacts of generative AI, LLMs and causal AI through case studies presenting brand new clinical data from Insilico Medicine and PrecisionLife.
- **LEARN** how to optimize your data generation, and quality from leading biotech's Recursion and Iambic Therapeutics.

CHAIRS FOR 2025:



Maureen Makes,
VP Engineering,
Recursion



Peter Clark,
VP Computational Drug Design,
Novo Nordisk

FEATURED 2025 SPEAKERS INCLUDE:

- **Fabian Heinemann**, Head Central Data Science EMEA, **Boehringer Ingelheim**
- **James Lumley**, Head of Cheminformatics, **GSK**
- **Lewis Vidler**, Senior Director - Structure Based Drug Design, **Eli Lilly and Company**
- **Henrik Mobitz**, Director, CADD, Global Discovery Chemistry, **Novartis**
- **Prakash Rath**, Augmented Drug Design Engineering Lead, **AstraZeneca**
- **Le Mu**, PM and Tech Lead for Roche pRED-MLOps, Senior Scientist / Solution Architect, **Roche**
- **Hannah Bruce Macdonald**, Associate Principal Scientist, **Charm Therapeutics**
- **Petrina Kanya**, VP AI, and Head of Insilico Medicine Canada, **Insilico Medicine**

Sponsored by:



www.ai-indrugdiscovery.com

Register online or fax your registration to
+44 (0) 870 9090 712 or call +44 (0) 870 9090 711

SMI Group Ltd trading as SAE Media Group



SAE Media Group Pharma
@SAEMGPharma
#AIDrugDis

A LETTER FROM OUR CHAIR...

Dear Colleagues,

It is with great pleasure that we invite you to SAE Media Group's AI in Drug Discovery conference, taking place on the 10-11 March 2025 in London.

As part of SAE's leading series of Drug Discovery conferences, this year's event will showcase how AI/ML are driving efficiency and innovation within drug R&D. Despite exponential progress, many barriers remain to unleashing the full potential of AI and this year we have extended our domain coverage to discuss the role enhancing data generation, quality and automation will play in increasing the power of AI.

Aside from this, we will deep-dive into the latest advancements in AI/ML driven target identification, computational drug design, cheminformatics and generative AI. As well as reviewing the clinical progress of AI-designed drug candidates, and the challenges associated with progressing these molecules through the pipeline.

The 2025 conference is the perfect opportunity to discuss the use of AI through the drug discovery process. As the Chairs of this conference, we look forward to welcoming you to this must-attend event in London this March.

Yours Sincerely,



Maureen Makes,
VP Engineering,
Recursion



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 KEYNOTE OPENING ADDRESS

Kick starting ML Projects with minimal data & evolving models for embedded DMTA support

- How to kick start an ML project with minimal data
 - Continuous monitoring of data and model drift to improve models
 - Success stories of Active Learning & alternate methods in model evolution
 - Combining ML with Physics based methods
- James Lumley,** Head of Cheminformatics, **GSK**



THE IMPACT OF AI ON SPEED AND INNOVATION WITHIN DRUG R&D

09.30 Leveraging AI in drug discovery - the art of balancing exploration and exploitation

- The exploration-exploitation dilemma in drug discovery (e.g. discovering novel chemical space v.s. screening through existing compound libraries) also manifest itself when it comes to leveraging the power of AI for accelerating innovation and reducing cost.
- Supporting exploratory v.s. exploitative activities in the AI/ML space in pharma research requires different technologies and different skillset from people – yet we would need to make sure both types of activities work cohesively to maximize the value
- Our journey of establishing and growing a MLOps service in Roche pRED in the past 4 years is likely to help to shed some lights on balancing exploration and exploitation in a big pharma research organisation
- Closing reflections on key factors that drive a successful AI strategy in drug discovery, with a focus on mastering the balance between exploration and exploitation across different organizational environments

Le Mu, Product Line Manager for End-to-End AI/ML, Product Owner and Tech Lead for Roche pRED-MLOps service, **Roche**

10.00 Augmenting DMTA using predictive AI modelling at AstraZeneca

- Building data products are key to fully exploit AI in drug discovery
 - We built data and AI solutions to expedite small molecule and antibody discovery at AZ
 - The impact on projects and consequently number of users are growing
- Prakash Rathi,** Augmented Drug Design Engineering Lead, **AstraZeneca**

10.30 Morning Coffee

11.00 Session reserved for Schrödinger

Sathesh Bhat, Executive Director, **Schrödinger Therapeutics Group**



AI/ML FOR TARGET IDENTIFICATION

11.30 Augmenting target discovery and early drug discovery with AI

- Criteria for AI-enabled workflows for early drug discovery
 - Levelling up the basic data package for any target, at scale
 - Combining cutting edge AI methods with wet-lab follow-up
- Florian Nigsch,** Director Data Science, **Novartis**

12.00 Mapping Cardiovascular Health through Multimodal Analysis of UK Biobank Data

- Combining phenotypes from the UK Biobank's multimodal dataset including cardiac MRI, ECG, and ventricular point cloud data
 - Harnessing unsupervised deep learning models for unbiased extraction and characterization of modality-specific phenotypes
 - Integration of phenotypic information from multiple modalities through contrastive learning
 - Development of a strategy to uncover novel genetic determinants of heart disease leveraging these holistic phenotypes
- Lisa Schneider,** Machine Learning Scientist, **Bayer** and **Vlad Kim,** Research Scientist, **Bayer**

12.30 Networking Lunch

13.30 Session reserved for Cresset



14.00 Transforming Target and Drug Discovery with Visual Biology derived AI disease models

- Leveraging Anima's Lightning.AI platform to run millions of visualizations in high throughput, imaging hundreds of cellular pathways in both healthy and diseased cells
 - Using this data to train neural networks that visually learn the difference between healthy and diseased cells
 - Identifying novel targets backed by experimental validation using visual biology knowledge graphs
 - Discovery of small molecule drugs that visually reverse disease phenotypes by modulating their mRNA biology
- Generoso Iannicello,** Chief Business Officer, **Anima Biotech**

14.30 Practical Machine Learning applications for fragment-based drug discovery

- Using ML for auto-templated docking in a structure-rich environment
 - Using LLMs for characterisation and clustering of protein-ligand binding sites
 - Discuss integration of the above in Astex's fragment-based drug discovery platform
- Marcel Verdonk,** Senior Director, **Astex Pharmaceuticals**

15.00 Afternoon Tea

15.30 Design Principles for Balancing Lipophilicity and Permeability in beyond Rule of 5 Space

- Principals of the beyond the rule of 5 space and applications for PROTAC design
- Combining computation and measurement to create computationally consistent datasets.

Henrik Moebitz, Director, CADD, Global Discovery Chemistry, **Novartis**



16.00 How to make better informed decisions in small molecule drug design

- One of the most significant changes in drug discovery today is the accelerated adoption of digital technologies that is transforming the pharma industry
 - As this digital revolution gains momentum, one of our strategic priorities at UCB is to fully harness these technologies to boost effectiveness and efficiency of drug discovery
 - Our ability to bring further innovation to the fingertips of researchers will allow new ways to discover and make medicines in a much shorter time frame than is currently possible. I will share how we have built this framework to help us become better decision makers
- Yogesh Sabnis,** Director of Lead Design, **UCB Pharma**

COMPUTATIONAL CHEMISTRY AND AI-DRIVEN DRUG DESIGN

16.30 AI based technologies for mining chemical space in drug design

- Discussing key challenges in AI-based drug design: exploring chemical space, interpretability, data analysis
 - (Large) Language Models in searching and exploring virtual chemical spaces
 - New technologies for interpretation of structure-activity-relationships
- Christoph Grebner,** Senior Principal Scientist, **Sanofi**

17.00 Panel Discussion: The future of AI-driven drug design

- Reviewing recent advancements in AI-powered computational chemistry and drug design
- Discussing how to overcome current challenges in adoption and trust in AI-based design methods
- Where are we heading? What does the future of AI-designed drugs look like?

Moderator:

Darren Green, Director, **ChemPlus Cheminformatics Consultants** and Honorary Professor of Chemistry, **UCL**

Panellists:

Yogesh Sabnis, Director of Lead Design, **UCB Pharma**
Marcel Verdonk, Senior Director, **Astex Pharmaceuticals**
Henrik Moebitz, Director, CADD, Global Discovery Chemistry, **Novartis**



17.30 Chair's Closing Remarks and Close of Day One

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

SPONSORSHIP AND EXHIBITION OPPORTUNITIES

SAE Media Group offer sponsorship, exhibition, advertising and branding packages, uniquely tailored to complement your company's marketing strategy. Prime networking opportunities exist to entertain, enhance and expand your client base within the context of an independent discussion specific to your industry.

Should you wish to join the increasing number of companies benefiting from sponsoring our conferences please call:
Ash Khan | +44 207 827 6110 | ash.khan@saemediagroup.com

SPONSORED BY:



Chemists in the world's leading research organizations use **Cresset** solutions to discover, design, optimize, synthesize and track the best small molecules. By integrating their in silico CADD and design-make-test-analyze discovery solutions with Cresset's first-class discovery research resources, researchers will have access to patented CADD Software, collaborative Torx® DMTA platform and expert Discovery CRO scientists. In helping organizations reach better design and synthesis decisions faster and more efficiently, we enable them to win the race to success in industries including: pharmaceuticals, agrochemicals, flavors and fragrances. www.cresset-group.com



Schrödinger is transforming the way therapeutics and materials are discovered. Schrödinger has pioneered a physics based computational platform that enables discovery of high-quality, novel molecules for drug development and materials applications more rapidly and at lower cost compared to traditional methods. The software platform is licensed by biopharmaceutical and industrial companies, academic institutions, and government laboratories around the world. Schrödinger's multidisciplinary drug discovery team also leverages the software platform to advance a portfolio of collaborative and proprietary programs to address unmet medical needs. www.schrodinger.com

08.30 Registration & Coffee

09.00 Chair's Opening Remarks
Maureen Makes, VP Engineering, Recursion

KEYNOTE OPENING ADDRESS

09.10 Industrialized Data Generation to Drive Discovery

- What fit for purpose drug discovery data looks like and why it is key to innovation
- Systems that make data available and usable for discovery
- Overview of scaling models with the combination of compute and data

Maureen Makes, VP Engineering, Recursion



KEYNOTE ADDRESS

09.40 Advances in Computational Approaches to Accelerate Therapeutic Discovery & Development

- Molecular design & optimization in the age of AI
- Strategies and impact on for integrating AI into the drug discovery process- updates and advancements from Novo Nordisk
- Reviewing the current state of the industry - challenges and future perspectives

Peter Clark, VP Computational Drug Design, Novo Nordisk



ENHANCING DATA GENERATION, QUALITY AND AUTOMATION

10.10 Transcending data scarcity in AI-driven drug discovery

- Iambic's AI-driven experimental platform
- Issues associated with developing AI-models with a lack of appropriate data
- Clinical updates from Iambic's lead program

Fred Manby, Co-Founder and CTO, Iambic Therapeutics

10.40 Morning Coffee

11.10 The Increasing Role of Lab Automation Beyond Screening: Maximizing Machine Learning Utility in Drug Discovery with Enhanced Data Generation

- Recently, the rise of AI/ ML for drug discovery has put a clear and increasing focus on the need for improved data depth and data quality as key factors for successful AI/ ML applications
- On the other hand, laboratory automation for the longest time has primarily been associated with high-throughput screening applications for hit identification
- This is changing rapidly, as the talk will show: based on a brief introduction into the evolution of the AI/ ML and lab automation space over the past 10 years, the focus will be on the unique synergy between the two technologies, including the rationale, case studies, and the latest trends in utilizing lab automation as a key enabling technology for AI drug discovery

Kinga Bercsenyi, Chief Business Officer, Arctoris

EXPLORING IMPACTS OF GENERATIVE AI

11.40 Custom AI applications for quantitative histopathology in pharmaceutical research

- AI to automate tasks, which were previously limited to pathologists. Examples will include
 - quantifying histopathological parameters of non-alcoholic steatohepatitis (NASH)
 - quantifying parameters of lung fibrosis
- Applications with unsupervised and generative methods.
 - an algorithm for anomaly detection in histopathological images will be presented which can support early tox assessment
 - approaches using generative adversarial networks to convert histological stains that generate virtual stains that can be indistinguishable for pathologists

Fabian Heinemann, Head Central Data Science EMEA, Boehringer Ingelheim



12.10 Evolving virtual assistants using Large Language Models

- Early efforts here involved using expert systems to deliver a virtual assistant like experience to users
- We were able to generate successful POC in medicinal chemistry
- The advent of LLMs has massively increased the opportunities for virtual agents to provide value to users
- The philosophy, historical work and current/future directions in this space will be described

Lewis Vidler, Senior Director - Structure Based Drug Design, Eli Lilly

12.40 Networking Lunch

13.40 AI-driven prediction of protein-ligand co-folding for discovery of transformational medicines

- DragonFold – an end-to-end deep learning algorithm for 3D protein-ligand co-folding prediction
- Validation of AI-targets in an integrative loop
- Updates on novel AI-derived drug candidates for cancers and previously undruggable targets

Hannah Macdonald, Associate Principal Scientist, Charm Therapeutics



AI-DRIVEN OPTIMIZATION OF CLINICAL TRIALS

14.10 Causal AI & Mechanostatics - Increasing Probability of R&D Success from Concept to Clinic

- Discovering, developing, and launching AI driven precision medicines for complex, chronic diseases
- Creating better diagnostic tools and more personalized treatment options for unmet medical needs
- Improving the discovery and selection of novel targets matched to patient biology
- Informing the design of clinical trials that are faster to readout and more likely to succeed
- Linking patients to effective treatments via their mechanism of disease

Steve Gardner, CEO, PrecisionLife

14.40 Afternoon Tea

15.10 An end-to-end AI platform for novel drug discovery

- Combining Insilico's AI platform with a fully automated, next-generation laboratory for maximal success
- Detailing the recent advances in Insilico's clinical pipeline – results from phase 2
- Challenges associated with progressing AI-designed molecules through the pipeline

Petrina Kamya, President Insilico Medicine Canada & VP, Global Head of Platforms, Insilico Medicine

15.40 Unlocking AI's Potential in Clinical Trial Data: Innovations and Use Cases

- Introduction: How AI revolutionizes clinical trials with enhanced insights, efficiency, and speed
- AI in Trials: Real-time analysis, streamlined processes, and faster drug development
- Use Cases: Predictive models, automated data management, and statistical support
- Challenges: Tackling data quality, integration, and ethical issues
- Future: The evolving role of AI in transforming clinical trials

Ravi Gupta, Advisor - Clinical Data Automation, Data & Analytics, Eli Lilly & Company

16.10 Closing keynote panel: Will AI live up to the current hype?

- How far have we come – what are the major breakthroughs in the past year?
- What challenges remain to fully integrate AI into drug discovery processes?
- Discussing the issues of ethical concerns, data privacy, and regulatory barriers
- How far do we have to go – future looking perspectives on where the industry is headed

Moderator:

Darren Green, Director, ChemPlus Cheminformatics Consultants and Honorary Professor of Chemistry, UCL

Panelists:

Petrina Kamya, President Insilico Medicine Canada & VP, Global Head of Platforms, Insilico Medicine
 Maureen Makes, VP Engineering, Recursion
 Peter Clark, VP Computational Drug Design, Novo Nordisk
 Fred Manby, Co-Founder and CTO, Iambic Therapeutics

16.40 Chair's Closing Remarks and Close of Day Two
Maureen Makes, VP Engineering, Recursion

MARKETING PARTNERSHIP OPPORTUNITIES

SAE Media Group is offering companies the opportunity to partner on our dedicated events in order to help raise your company profile, add value, create awareness of your products/services to our key audience within the pharmaceutical industry. Interested in partnering?

Contact Toni Akinyele | +44 207 827 6723 | toni.akinyele@saemediagroup.com

Official Media Partners



Key Media Partners



WHY YOU SHOULD ATTEND:

- **Hear** from the biotechs revolutionizing the industry: Recursion and updates on their surprise Exscientia merger, and Insilico, presenting insights on the first generative AI designed model entering phase II
- **Network** with senior leaders from Novartis, Eli Lilly and Novo Nordisk, to discuss the latest advancements in computational chemistry and applications of generative AI within early drug discovery.
- **Engage** in discussions with industry experts to discuss the role data quality and automation will play in driving forward the next phase of AI advancements.

Alternatively fax your registration to +44 (0)870 9090 712 or call +44 (0)870 9090 711

AI IN DRUG DISCOVERY 2025

Conference: 10 - 11 March 2025, Hilton London Kensington, UK

SAE MEDIA
GROUP

3 WAYS TO REGISTER

Online at
www.ai-indrugdiscovery.com

Email your booking form to
marketingteam@saemediagroup.com

PHONE on
+44 (0) 870 9090 711

Our Reference P-443

DELEGATE DETAILS

Please complete fully and clearly in capital letters. Please photocopy for additional delegates.

Title: Forename:

Surname:

Job Title:

Department/Division:

Company/Organisation:

Email:

If you would like to continue to receive email updates about our events, please tick ☐

Company VAT Number:

Address:

Town/City:

Post/Zip Code: Country:

Direct Tel: Direct Fax:

Mobile:

Switchboard:

Signature: Date:

I agree to be bound by SAE Media Group Terms and Conditions of Booking

ACCOUNTS DEPT

Title: Forename:

Surname:

Email:

Address (if different from above):

Town/City:

Post/Zip Code: Country:

Direct Tel: Direct Fax:

VENUE Hilton London Kensington, UK

For any queries, call us on **+44 (0) 870 9090 711**,
email: events@saemediagroup.com

BOOKING SUMMARY

Terms and Conditions of Booking

Payment: Our payment terms are as follows: if booking 16 days or more before the conference, payment should be made within 14 days of date of invoice. If booking 15 days or less before the conference, payment is due on receipt of invoice and must be received no later than the last working day prior to the event start date. In the event, that the customer has not paid by the last working day before the event, we reserve the right to obtain card details for payment to be taken for the full invoice amount or as a guarantee of payment. Access to the Document Portal will not be given until payment is received.

Substitutions/Name Changes: If you are unable to attend you may nominate, in writing, another delegate to take your place at any time prior to the start of the event. Two or more delegates may not 'share' a place at an event. Please make separate bookings for each delegate.

Cancellation: If you wish to cancel your attendance at an event and you are unable to send a substitute, then we will refund/credit 50% of the due fee, providing that cancellation is made in writing and received 28 days prior to the start of the event. Regrettably cancellation after this time cannot be accepted. We will however provide the conferences documentation via the Document Portal to any delegate who has paid but is unable to attend for any reason. Due to the interactive nature of the Briefings, we are not normally able to provide documentation in these circumstances. We cannot accept cancellations of orders placed for Documentation or the Document Portal as these are reproduced specifically to order. If we have to cancel the event for any reason, then we will make a full refund of your payment but disclaim any further liability.

Alterations: It may become necessary for us to make alterations to the content, speakers, timing, venue or date of the event compared to the advertised programme. Privacy policy/Opt out For full details on our privacy policy please go to www.smgconferences.com/privacy-legals/privacy-policy. If you no longer wish to receive email updates you can opt out by going to the following webpage www.smgconferences.com/opt-out

EARLY BIRD DISCOUNT

- ☐ Book by 27 November to receive £400 off the conference price
- ☐ Book by 10 January to receive £200 off the conference price
- ☐ Book by 31 January to receive £100 off the conference price

CONFERENCE PRICES

I would like to attend: (Please tick as appropriate) Price VAT

IN-PERSON ATTENDANCE

☐ Conference only £2298.00 + VAT

PROMOTIONAL LITERATURE DISTRIBUTION

☐ Distribution of your company's promotional literature to all conference attendees £999.00 + VAT

As an added benefit of attending this conference, check here to receive a free subscription to Medical Design Briefs, the leading new technology magazine for bio-medical professionals. Choose either: ☐ Print (U.S. only) ☐ Digital

Please note that the above ticket price includes access to all approved distributable PDF presentations post-event, priced at £99. To opt out, please contact via email: delsalesuk@saemediagroup.com or call: +44 (0) 207 827 6000.

DOCUMENTATION

I cannot attend but would like to Purchase access to the following Document Portal Price

☐ Access to the conference documentation on the Document Portal £699.00 + VAT

VAT

VAT at 20% is charged on the attendance fees for all delegates. VAT is also charged on Document portal and literature distribution for all UK customers and for those EU Customers not supplying a registration number for their own country here

PAYMENT

Payment must be made to **SMi Group Ltd**, and received before the event, by one of the following methods **quoting reference P-443 and the delegate's name**. Bookings made within 7 days of the event require payment on booking, methods of payment:

- ☐ **UK BACS** Sort Code **300009**, Account **00936418**
- ☐ **Wire Transfer** Lloyds TSB Bank plc, 70-71 Cheapside, London, EC2V 6EN
Swift (BIC): **LOYDGB21013**, Account **00936418**
IBAN **GB48 LOYD 3000 0900 9364 18**
- ☐ **Credit Card** A payment link will be sent with your Invoice

If you have any further queries please call the Events Team on tel **+44 (0) 870 9090 711** or you can email them at events@saemediagroup.com