

March 18-20, 2026 | Boston, MA

www.ai-convergence-small-molecule-discovery.com

RESERVE YOUR
PLACE BY FRIDAY,
DECEMBER 12 TO
SAVE UP TO \$900



AI Convergence: Small Molecule Discovery Summit

Leveraging AI/ML x Med Chem x Computational Innovation

**Rapidly Design Multiparametrically
Optimized Small Molecules with Novel
Chemistry Against Hard Targets, Enhance
Preclinical Target Product Profiles &
Expedite Timelines from Concept to IND**

Expert Speakers Include:



Henry van den Bedem
Chief Technology
Officer
Expedition
Medicines



Shivam Patel
Head, Data Sciences
& ML
Psivant
Therapeutics



Petrina Kamya
Vice President &
Global Head, AI
Platforms
Insilico Medicine



Jonathan Gilbert
Senior Director,
Ecosystem Growth
& Contributor
Partnerships
Eli Lilly's TuneLab



Pat Walters
Chief Scientist
OpenADMET



Ajay Yekkirala
Co-Founder, Senior
Vice President &
Head, Discovery &
Development
Superluminal
Medicines

Data is an essential component for any AI effort. This program brings together several efforts around the most critical components of AI and ML workflows

Pat Walters, Chief Scientist, **OpenADMET**, 2026 Speaker

+1 617 455 4188 @ info@hansonwade.com

www.ai-convergence-small-molecule-discovery.com



ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

Your Opportunity to Leverage the Confluence of AI, Computational & Medicinal Chemistry Insights for Accelerated Small Molecule Discovery

AI Convergence: Small Molecule Discovery Summit

March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

Eli Lilly's recent launch of their AI platform **TuneLab**, alongside **Pfizer's** extended venture with **XtalPi**, **Monte Rosa Therapeutics'** progress in molecular glues and **Insilico Medicine's** rentosertib Phase II advancements, are fueling accelerated small molecule innovation. Coupled with growing pressure from patent cliffs and compressed development timelines, biopharma sit poised to industrialize AI/ML tools for small molecule discovery.

Arriving in Boston, the inaugural **AI Convergence: Small Molecule Discovery Summit** is your definitive forum leveraging the intersection of AI/ML, medicinal chemistry and computational data into experimentally validated, actionable insights that support, and keep the human-in-the-loop, in a re-architected, AI-integrated discovery paradigm.

Convening computational chemists, medicinal chemists, AI/ML experts and discovery leaders, across **techbio torchbearers**, **pharma adopters** and **biotech innovators**, this is your opportunity to engage in this industry-defining moment.

Acquire **actionable learnings** and **strategic collaborations** for your team through a hyper-focused, one-track agenda. Addressing the AI methods deployed, use cases, and confidence in tools and insights gained, this is your guide to AI-driven small molecule design, to target undruggable proteins, with optimized target product profiles, through faster iterative DMTA cycles.

As AI continues to accelerate decision-making velocity on hit-to-lead progression, and revives interest in chemical modality design, unite with us to catalyze the next wave of AI-powered small molecule innovation from concept to IND.

What Our Experts Have to Say

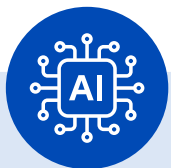
Through ML approaches we demonstrate that omics level data can be used as common language to connect disease biology to chemistry, leading to more efficient drug discovery

Mauricio Cortes, Senior Director & Head, Discovery Science, **Cellarity**, 2026 Speaker

It's always great to learn more about how different people are solving challenges in drug discovery with state-of-the-art AI technologies, given how fast this field is evolving

Hok Hei Tam, Co-Founder & Chief Technology Officer, **Montai Therapeutics**, Senior Principal, **Flagship Pioneering**, 2026 Speaker

What Sets This Meeting Apart?



Learn to apply AI/ML methods in concert with computational tools to predict target protein folding and binding surfaces for target enablement with **Cellarity** and the **AI Small Molecule Drug Discovery Center**, **Icahn School of Medicine at Mount Sinai**



Supercharge structure-based and ligand-based drug design with AI/ML technologies to confront hard targets with **UCB**, **Rapafusyn Pharmaceuticals**, **Montai Therapeutics**, **GSK** and **Congruence Therapeutics**



Leverage generative models to spotlight novel opportunities in small molecule chemistry and structure with **Expedition Medicines**, **Psivant Therapeutics**, **Insilico Medicine** and **Johnson & Johnson**



Tap into unexplored chemical space beyond traditional datasets by utilizing virtual screening platforms powered using AI/ML with **Pro-Phet**, **Novo Nordisk**, **Model Medicines** and **Variational AI**



Investigate AI/ML methods and federated learning platforms that optimize small molecules for enhanced ADME-T and drug-like properties to derisk pipeline progression efforts with **Sanofi** and **Eli Lilly's TuneLab**



Hear Why Your Peers are Eager to Participate



“I see this meeting as an invaluable forum to exchange ideas and critically evaluate emerging computational methods and their application to real-life problems. It poses the perfect opportunity to connect with peers who are shaping how AI is applied and to build collaborations that will help translate our early-stage discoveries in academic settings towards clinical impact”

Avner Schlessinger, Professor & Director,
AI Small Molecule Drug Discovery Center,
Icahn School of Medicine at Mount Sinai,
2026 Speaker



“This meeting uniquely unites experts at the intersection of AI/ML, physics-based modeling and medicinal chemistry, which is where the next breakthroughs in small molecule design are happening. The agenda is perfectly aligned with how we are building our platform Revenir to accelerate drug discovery”

Maximilian Ebert, Executive Director,
Computational Chemistry, **Congruence**
Therapeutics, 2026 Speaker



“This conference is not only for AI/ML subject matter experts. In fact, as a non-expert in AI, I am attracted to this meeting for the possibility of bringing together top *in silico*, *in vitro*, and *in vivo* drug discovery experts to explore how data-driven modeling, predictive analytics, and laboratory-based innovation can reinforce each other. I look forward to discussing integrative workflows, and synergistic strategies to accelerate drug discovery”

Ivan Cornella-Taracido, Chief
Scientific Officer & Co-Founder, **Covant**
Therapeutics, 2026 Speaker



“Hanson Wade conferences offer excellent speakers and presentations on the latest science topics in a stimulating environment. I invite you to join this pivotal discussion”

Alexander Hillisch, Head, Digital
Molecule Discovery & Executive
Director, **UCB**, 2026 Speaker

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

Pioneering Academics & Open Community



Avner Schlessinger
Professor & Director
AI Small Molecule Drug
Discovery Center,
Icahn School of Medicine
at Mount Sinai



Pat Walters
Chief Scientist
Open ADMET

Techbio Torchbearers & Biotech Innovators



Hariprasad Vankayalapati
Co-Founder & Chief
Scientific Officer
Biolexis Therapeutics



Mauricio Cortes
Senior Director & Head,
Discovery Science
Cellarity



Maximilian Ebert
Executive Director,
Computational Molecular
Sciences
Congruence
Therapeutics



Ivan Cornella-Taracido
Chief Scientific Officer &
Co-Founder
Covant Therapeutics



Henry van den Bedem
Chief Technology Officer
Expedition Medicines



Petrina Kamya
Vice President & Global
Head, AI Platforms
Insilico Medicine



Daniel Haders
Chief Executive Officer
Model Medicines



Hok Hei Tam
Co-Founder & Chief
Technology Officer
Montai Therapeutics
Senior Principal
Flagship Pioneering



Tom Shani
Co-Founder & Chief
Executive Officer
Pro-Phet



Shivam Patel
Head, Data Sciences & ML
Psivant Therapeutics



Rick Ewing
Vice President & Head,
Chemistry
Rapafusyn
Pharmaceuticals



Ajay Yekkiralu
Co-Founder, Senior
Vice President &
Head, Discovery &
Development
Superluminal
Medicines



Jacob Berlin
Chief Executive Officer
Terry Therapeutics



Handol Kim
Chief Executive Officer
Variational AI

Leading Pharma Adopters



Jonathan Gilbert
Senior Director,
Ecosystem Growth &
Contributor Partnerships
Eli Lilly's TuneLab



Carol Mulrooney
Senior Principal Scientist,
Cheminformatics
GSK



Xinhao Li
Senior Scientist II, *In Silico*
Discovery
Johnson & Johnson



Vinicius Oliveira
Senior Scientist,
Computational Chemistry
Novo Nordisk



David Kombo
Principal Scientist II
Sanofi



Alexander Hillisch
Head, Digital Molecule
Discovery & Executive
Director
UCB

Pre-Conference Workshop Day

Wednesday, March 18

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

Check-In & Morning Coffee

8.00

Workshop A

9.00 - 12.00

Overcoming Data Access & Integration Barriers to Enable AI/ML-Driven Small Molecule Drug Discovery with Open Data & Federated Learning Platforms

A pressing challenge in applying AI to drug discovery is limited access to high-quality, appropriately sized datasets, particularly for early-stage biotech firms. Without robust, diverse, and validated data, AI/ML models struggle to deliver reliable predictions or actionable wet lab outcomes. Open-source and federated learning platforms aim to bridge this gap by providing access to proprietary AI models trained on extensive preclinical, safety, and target product profile data. This workshop explores data-centric challenges and collaborative platforms that democratize AI for small molecule discovery.

Participants will explore:

- The opportunities of open data and federated learning platforms, as well as privacy-preserving data sharing in collaborative drug discovery environments
- Strategies for integrating proprietary and shared datasets to improve model generalizability and predictive power
- Approaches for validating AI-generated hypotheses in wet lab settings, including alignment of experimental design with model outputs
- Techniques for ensuring data quality, chemical diversity, and reproducibility in training datasets
- Examples of how access to large-scale datasets has accelerated small molecule lead optimization and candidate selection

Workshop Leaders



Pat Walters
Chief Scientist
Open ADMET

Lunch Break & Networking

12.00

Workshop B

1.00 - 4.00

Evaluating AI Tools for Target Identification in Small Molecule Discovery: Strengths, Limitations & Strategic Fit

The application of AI to target protein folding and identification is rapidly evolving, with tools like AlphaFold, and emerging hybrid models offering unprecedented insights into protein structure and function. Yet, the diversity of available technologies, each with distinct strengths and limitations, presents a challenge for teams seeking to integrate these tools into their discovery workflows. This workshop offers a foundational and critical evaluation of the current AI landscape for target enablement, helping attendees navigate the complex trade-offs between accuracy, scalability, interpretability, and experimental validation.

Participants will explore:

- The comparative strengths and weaknesses of leading AI tools for predicting protein folding, binding surfaces, and post-translational modifications
- Tool performance for hard-to-drug targets such as GPCRs, transcription factors, and RNA-binding proteins
- Strategies for integrating AI predictions with experimental methods (e.g. cross-linking, cryo-EM, FRET) to validate cryptic binding pockets and dynamic conformations
- Case studies on the use of AI in target identification and the role of pharmacophore modeling
- Practical considerations for selecting the right AI tool based on target class, data availability, and downstream application in small molecule design

Workshop Leaders



Avner Schlessinger
Professor & Director
AI Small Molecule Drug Discovery Center,
Icahn School of Medicine at Mount Sinai

End of Pre-Conference Workshop Day

4.00



+1 617 455 4188 @ info@hansonwade.com

www.ai-convergence-small-molecule-discovery.com



Conference Day One

Thursday, March 19

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE



8.00 Check-In & Morning Coffee



Ivan Cornella-Taracido
Chief Scientific Officer
& Co-Founder
Covant Therapeutics

8.50 Chair's Opening Remarks

Reflecting on the State of Play of AI/ML-Derived Small Molecules

9.00 Panel Discussion: Is 2026 the Year for Demonstrating the Practical ROI of AI/ML-Integrated Discovery for Small Molecules?

This industry leaders panel will discuss the small molecule industry collaborations and advancements shaping the space, key challenges to overcome, and where the biggest opportunities remain.

- Taking stock of the strengths, weaknesses, opportunities and threats (SWOT) of AI/ML-derived small molecules
- What advancements in AI/ML x med chem x computational convergence should we be most excited about?
- How do you perceive the AI/ML-derived small molecule space? How has industry sentiment changed in the last 12 months?
- What are the technical or scientific bottlenecks that are slowing AI/ML-derived small molecule discovery?
- What are the most reliable and experimentally validated use cases for AI/ML-methods that are being integrated into the small molecule discovery funnel? And which use cases for small molecule discovery remain challenging to get right?



Alexander Hillisch
Head, Digital Molecule
Discovery & Executive Director
UCB



Hok Hei Tam
Co-Founder & Chief Technology
Officer
Montai Therapeutics
Senior Principal
Flagship Pioneering



Petrina Kamya
Vice President & Global
Head, AI Platforms
Insilico Medicine

Applying AI/ML Methods to Predict Target Protein Folding & Binding Surfaces for Target Enablement



Avner Schlessinger
Professor & Director
AI Small Molecule
Drug Discovery
Center,
Icahn School of
Medicine at Mount
Sinai

9.30 Integration of AI Approaches in Preclinical Academic Settings to Target a Challenging Solute Carrier (SLC) Target

- Combine patient-derived, multi-omic data with AI modeling to enable the discovery of underexplored transporter targets linked to neurological disease
- Identify new chemical probes that modulate transporter activity using structure-based virtual screening, molecular modeling, and rational design
- Share how integrative computational and experimental workflows provide a roadmap for expanding the druggable target landscape beyond enzymes and receptors



Mauricio Cortes
Senior Director & Head,
Discovery Science
Cellarity

10.00 Enabling Drug Discovery Through High Dimensional Data: Elucidating Novel Druggable Nodes by Connecting Disease Biology to Chemistry Through Transcriptomics

- Discuss how ML models can make omics data actionable for drug discovery
- Recognize that experimental benchmarking is essential to guide implementation
- Exploit lab-in-the-loop to improve outcomes



10.30 Structured Speed Networking

This informal session provides the perfect opportunity to connect with industry frontrunners and key opinion leaders in the AI/ML-enabled discovery for small molecules space. Establish meaningful connections to build upon at the rest of the conference.



11.00 Morning Break & Refreshments

Conference Day One

Thursday, March 19

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

Harnessing AI/ML Models to Supercharge Structure-Based Drug Design



Alexander Hillisch
Head, Digital Molecule
Discovery & Executive
Director
UCB

11.30 Holistic *De Novo* Drug Design at UCB

- Change the ways of working in NCE drug discovery, by combining human design, AI and physics-based approaches
- Move towards a predict-first culture
- Establish a collaborative ideation platform that makes the difference



Rick Ewing
Vice President & Head,
Chemistry
**Rapafusyn
Pharmaceuticals**

12.00 Application of AI Processes to Non-Grading Molecular Glues: Case studies on GSTP1 & TRAFF2

- Discuss the application of a developed AI process for predicting target vulnerability towards non-degrading molecular glue platforms
- Highlight the ternary crystal structures of molecules bound to GSTP1 where a novel mode of binding is uncovered
- Address the ternary crystal structures of molecules disrupting the PPI of TRAF2, showing a mechanism of PPI inhibition only possible through ternary complex formation

Investigating Generative Molecular Design Models to Define Novelty in Small Molecule Chemistry & Structure



Henry van den Bedem
Chief Technology
Officer
Expedition Medicines

12.30 Learning the Rules of Covalency: Proteome-Scale Data & Quantum-Enabled AI Unlocks Programmable Chemistry

- An overview of how EXM created a built-for-purpose data platform integrating covalent reaction design and high-throughput hardware/software innovations, to provide proteome-scale target engagement datasets with atomic-level resolution
- Understand how the data platform drives next-generation predictive and generative quantum-enabled AI for chemistry
- Showcase how EXM's reactive chemistry generative designs go beyond human intuition and hit classically difficult-to-drug targets like transcription factors



1.00 Lunch Break & Networking



Shivam Patel
Head, Data Sciences
& ML
Psivant Therapeutics

2.00 Understanding Reward Function in Reinforcement Learning

- Explore whether generative AI has the capability to generate desired molecules
- Learn how to assess quality of reward function
- Investigate what impact quality of reward function has on generation



Xinhao Li
Senior Scientist II, *In Silico* Discovery
Johnson & Johnson

2.30 DELTA (Decompose, Enumerate, Library, Transform, Atlas): The Computational Toolkit for Targeted Protein Degradation

- Showcase DELTA as an integrated, modular platform that accelerates targeted protein degradation (TPD) research
- Address how DELTA streamlines PROTAC design and optimization through systematic decomposition, enumeration, library curation, and computational profiling
- Share how DELTA integrates medicinal chemistry expertise with advanced computational analysis to deliver comprehensive, data-driven insights that support confident decision-making

Conference Day One

Thursday, March 19

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA



Petrina Kamy
Vice President & Global
Head, AI Platforms
Insilico Medicine

3.00

Harnessing Pharmaceutical Superintelligence & Generative Molecular Design Across the End-to-End Discovery Funnel to Derisk Small Molecule Programs



3.30

Afternoon Break & Networking



Jacob Berlin
Chief Executive Officer
Terry Therapeutics

4.00

Built at the Intersection: Chemistry First, AI-Native *De Novo* Small Molecule Discovery & Development

- Highlight EMMI as Terry Therapeutics' full stack AI and experimental platform that brings together proprietary, ultra-high throughput hardware and lab automation with generative, predictive and selection AI models to aid expert scientists in developing novel solutions to some of medicine's toughest problems
- Create your own specific and precise data and establish an integrated process and team structure that successfully deploys AI for small molecule drug discovery
- Highlight the platform and a use case



Breakout Roundtable Discussions

Digging Into the Challenges & Opportunities of Deploying AI/ML Methods to Facilitate Small Molecule Discovery Using Agents, Large Language Models (LLMs) & Shared Goals Across Cross-Functional Teams

4.30

Uncover the stories behind leaps and setbacks in AI/ML-guided small molecule discovery. Each roundtable will be hosted by a moderator who will share an AI/ML technology use case for small molecule discovery, its applications, technology convergence, advantages, limitations and future directions.

Building Agents & Exploring Emerging LLM Use Cases for Small Molecule Discovery Funnel Applications



Daniel Haders
Chief Executive Officer
Model Medicines

Forming Cross-Functional AI Systems in Biopharma: Aligning Chemists, Biologists & Data Scientists Through Shared Language, Unified Objectives & Scalable Integration Frameworks



Ivan Cornella-Taracido
Chief Scientific Officer &
Co-Founder
Covant Therapeutics



Ivan Cornella-Taracido
Chief Scientific Officer
& Co-Founder
Covant Therapeutics

5.00

Chair's Closing Remarks & End of Conference Day One

Conference Day Two

Friday, March 20

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE



8.00 Check-In & Morning Coffee



Ivan Cornella-Taracido
Chief Scientific Officer
& Co-Founder
Covant Therapeutics

8.50 Chair's Opening Remarks

Leveraging Virtual Screening Platforms Powered Using AI/ML & Tapping into Vast Unexplored Chemical Spaces Beyond Traditional Datasets to Generate New Small Molecules

9.00 The Data Problem in AI Drug Discovery: From Biased Inputs to Biological Truth

- Highlight the data, not algorithm bottlenecks in AI-driven drug discovery. Humans and models train on narrow chemical and biological spaces, shaped by convenience or funding. Pro-Phet designs efficient libraries for popular proteins and reuses biased datasets
- Build models that reflect biology, not bias, by starting with sequence, not pre-structure data. Learn from biological language to normalize inputs across diverse sources, creating a shared information standard. Embrace negative data, failures, non-binders and weak affinities so that AI learns boundaries and contexts
- Create confidence through cleaner, broader, more representative data. Couple sequence-level modeling, normalization, and large-scale screening. Apply the law of large numbers to biology and operate across billions of protein-molecule interactions, with stabilized patterns and clear outliers. Build reproducibility so AI solves biology, instead of mirroring it



Tom Shani
Co-Founder & Chief
Executive Officer
Pro-Phet

9.30 AI-Physics Convergence for Early Discovery: From Tractability & Large-Scale Screening to Candidate Prioritization

- Demonstrate a reproducible workflow that integrates tractability/pocket mapping, large-scale ligand-based and structure-based virtual screening, potency ML using interaction fingerprints, and physics-based scoring (MM-PBSA, RBFEP+, dissociation FE)
- Share applications across two target studies. The first being, 8M-scale screening, pharmacophore/LBVS+SBVS funnel to 496 candidates. The second being, ensemble docking, ML selection, physics-based rescoring
- Demonstrate the translation of computational signals into ranked, purchase-ready lists and model-informed designs in LiveDesign
- Highlight the advantages and caveats in speed and accuracy (e.g., HMR for throughput, cycle-closure curation to remove high-uncertainty RBFEP transformations, off-target filters like hERG). Experimental validation is still ongoing



Vinicius Oliveira
Senior Scientist,
Computational
Chemistry
Novo Nordisk

10.00 Quality Over Quantity: Rethinking AI-Driven Drug Discovery

- Highlight the data fallacy in AI drug discovery and why the common belief that "more data means better models" can actually mislead R&D efforts in pharmaceutical AI
- Elevate how the power of model design and well-designed AI architectures can efficiently learn from smaller, high-quality datasets to enable meaningful insights without massive data volumes
- Demonstrate a path towards smarter discovery and how shifting focus from data quantity to data quality and model integrity leads to more reliable predictions, faster iterations, and ultimately better drug candidates



Handol Kim
Chief Executive Officer
Variational AI

Conference Day Two

Friday, March 20

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE



10.30 Morning Break & Networking



Daniel Haders
Chief Executive Officer
Model Medicines

11.00 Breaking the Throughput Barrier: Ultra-Large Virtual Screening as a Precision Amplifier for AI-Driven Drug Discovery

- Move towards out-of-domain chemistry by using models that generalize beyond the data we already have, enabling discovery in unexplored regions of biology and chemistry
- Generate novel chemistry and move beyond rediscovery of known scaffolds by investing in platforms that can generate truly new chemical matter
- Expand throughput and explore the full depth of chemical diversity where transformative, next generation drugs reside

Tackling Hard Targets with Enhanced Insights from AI/ML Technologies Used in Combination with Ligand-Based Drug Design Approaches



Ajay Yekkiral
Co-Founder, Senior
Vice President &
Head, Discovery &
Development
Superluminal
Medicines

11.30 Session Reserved for Superluminal Medicines



Hok Hei Tam
Co-Founder & Chief
Technology Officer
Montai Therapeutics
Senior Principal
Flagship Pioneering

12.00 The CONECTA™ Platform: Integrating Multimodal Foundation Models with Nature's Chemical Intelligence to Find Solutions for Hard-To-Drug Targets

- Advanced AI is making it possible to discover new oral therapeutics for chronic disease and address significant unmet patient needs
- Montai Therapeutics' CONECTA™ platform integrates proprietary bioassay data from a diverse chemical space and multimodal foundation models built on billions of chemical and biological datapoints
- This platform enables us to find diverse compounds inspired by nature's chemical intelligence that can solve previously undruggable targets with the highest probability of becoming successful drugs



Carol Mulrooney
Senior Principal
Scientist,
Cheminformatics
GSK

12.30 Applying ML to Analyze DNA Encoded Library Data in 3D

- Highlight that current methods to identify structural similarities among hits from DEL screens focus on 2D methods
- Analyze pharmacophore and shape similarity is valuable although computationally expensive
- Learn how to approximate expensive steps with ML and apply to historical and test data sets



1.00 Lunch Break & Networking



Maximilian Ebert
Executive Director,
Computational
Molecular Sciences
Congruence
Therapeutics

2.00 Multi-Parameter Optimization Guided by Explainable AI (Xai), Generative Chemistry & Physics-Based Ensemble Modeling: Shortening the Path from Hit-to-Lead Using Revenir

- Uncover how the Revenir drug discovery platform integrates molecular dynamics, ensemble pocket discovery, and collects AI-driven analytics to accelerate structure function understanding
- Using two case studies to demonstrate how an explainable ML framework identifies atomic drivers of potency and liabilities to guide medicinal chemistry optimization
- Explore how generative design powered by Revenir data enables the rapid discovery of novel, experimentally validated small molecules

Conference Day Two

Friday, March 20

AI Convergence: Small
Molecule Discovery Summit
March 18-20, 2026 | Boston, MA

ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE

2.30 MolecuLern: AI-Driven Precision in Small-Molecule Glue Degraders Through a Data-First Approach to De-Risk & Accelerate Drug Discovery



Hariprasad Vankayalapati
Co-Founder & Chief Scientific Officer
Biolexis Therapeutics

- Demonstrate how data-first AI frameworks in discovery reduce attrition by sharing practical, validated examples of how they are being used to design real, experimentally confirmed small-molecule degraders, showing what works (and what doesn't) in moving from prediction to proof
- Gain insight into emerging strategies for precision molecular glue design and highlight novel approaches to rationally engineer glue degraders by integrating structural biology, cheminformatics, and predictive modeling offering valuable lessons for anyone working on targeted protein degradation, GLUES or PROTACs, or complex modality discovery
- Discover frameworks to de-risk R&D pipelines and learn how data-centric model validation and feedback loops can reduce late-stage attrition, accelerate candidate selection, and improve return on discovery investment. Ideas that can be applied across therapeutic areas to accelerate the path from concept to candidate

Harnessing AI/ML Methods to Predict & Optimize Small Molecules for Drug-Like Properties to Increase Probability of Success & Derisk Pipeline Progression Efforts

3.00 Generating AI Strategies for the Enhancement of Hit Finding & Optimization



David Kombo
Principal Scientist II
Sanofi

- Virtual screening strategies for ultra-large databases
- Predictive AI/ML models for potency at the target and ADME-Tox profiling
- Property-based drug design coupled with AI/ML models, chemical space network analysis and composite metrics important in lead optimization

3.30 Accelerating Drug Discovery with Eli Lilly's TuneLab



Jonathon Gilbert
Senior Director,
Ecosystem Growth
& Contributor
Partnerships
Eli Lilly's TuneLab

- TuneLab provides access to Eli Lilly-trained AI models to help accelerate breakthrough medicines to patients
- The platform employs federated learning, a privacy-preserving approach that enables biotechs to tap into Eli Lilly's AI models without directly exposing their proprietary data
- Learn how to become a participant in this first-of-its-kind, collaborative AI/ML drug discovery platform



Ivan Cornella-Taracido
Chief Scientific Officer
& Co-Founder
Covant Therapeutics

4.00 Chair's Closing Remarks & End of Conference

Companies in Attendance Include



Forge New, Strategic & Existing Partnerships in the Fast-Evolving AI/ML Small Molecule Discovery Space

Designed to aid AI/ML-driven small molecule discovery, the **AI Convergence: Small Molecule Discovery Summit** is your unique platform to engage directly with top biopharma experts across the field.

Our audience of industry professionals are actively seeking collaborators with **innovative AI/ML models** for generative molecular design, **novel computational services** with predictive and simulation capabilities, and **advanced chemistry lab automation solutions** to streamline wet lab experimental validation, creating the ideal opportunity to identify market gaps and position your services as the solution.

Following **Eli Lilly's** collaboration with **Superluminal Medicines**, **Pfizer's** extended venture with **XtalPi** and **Merck's** expanded deal with **Variational AI** to advance small molecule therapeutics, investment and partnerships in AI-driven small molecule discovery have surged. Now is the critical moment to establish strategic partnerships and thought leadership as the field reaches a pivotal tipping point in embedding AI/ML tools into the small molecule discovery paradigm.



Your Premier Platform for Networking & Knowledge Exchange

As the only event dedicated to the convergence of AI with computational and medicinal chemistry for small molecule discovery, look forward to connecting with the very decision-makers reimagining every aspect of the small molecule discovery funnel.



Generate Tangible Commercial Opportunities

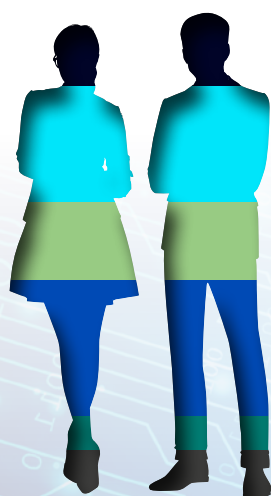
Position your organization alongside a targeted audience of small molecule discovery professionals, that have a direct need for your services. Foster new and existing relationships, drive collaborations, explore commercial partnerships and rub shoulders with the industry's leaders.



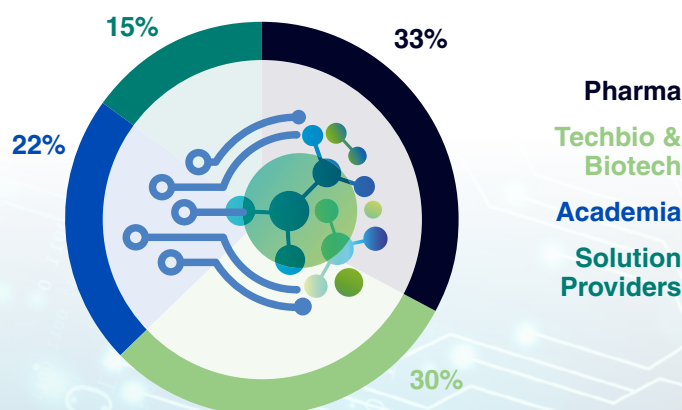
Confront Key Discovery Challenges

Key hurdles include predicting target protein folding, designing differentiated structures, and automating processes. The field is highly receptive to innovative approaches that address these obstacles, presenting the perfect opportunity for you to showcase the tangible use cases and wet lab validation of your generative AI/ML models, predictive computational services and lab automation capabilities.

Seniority of Attendees



Type of Companies Attending



*Statistics Taken from the 10th Computational Drug Design for Biologics Summit

Get Involved



Tazeen Kapadia
Partnerships Director
Tel: +1 617 455 4188
Email: sponsor@hansonwade.com

Ready to Register?

3 Easy Ways to Book



www.ai-convergence-small-molecule-discovery.com/register/



Tel: +1 617 455 4188



Email: info@hansonwade.com



UNPACK how techbio, pharma and biotech companies are harnessing the power of AI/ML methods, alongside computational and medicinal chemistry approaches, to accelerate small molecule pipeline progression



EXPAND your understanding of novel AI/ML methods and applications, and confidence levels in platforms that are transforming the small molecule discovery paradigm



CONVENE with industry peers, to build lasting connections and complementary collaborations that advance small molecule hit-to-lead progression

Pharma, Biotech & Techbio Pricing*	Register By Friday, December 12	On the Door Price
Conference + 2 Workshops	\$3,397 (Save \$900)	\$4,297
Conference + 1 Workshop	\$2,998 (Save \$700)	\$3,698
Conference Only	\$2,599 (Save \$500)	\$3,099
Academic Pricing**	Register By Friday, December 12	On the Door Price
Conference + 2 Workshops	\$2,797 (Save \$900)	\$3,697
Conference + 1 Workshop	\$2,498 (Save \$700)	\$3,198
Conference Only	\$2,199 (Save \$500)	\$2,699
Service & Solution Provider Pricing***	Register By Friday, December 12	On the Door Price
Conference + 2 Workshops	\$4,297 (Save \$900)	\$5,197
Conference + 1 Workshop	\$3,798 (Save \$700)	\$4,498
Conference Only	\$3,299 (Save \$500)	\$3,799

* To be eligible for this price, the group or individual must be from a pharma, biotech or techbio company that has a publicly disclosed pipeline. They must not be outsourcing their pipeline or offer paid for products and/or partnering services.

** To be eligible for this price, the group or individual must be full-time academic(s).

*** If you offer paid for products and/or partnering services, have you considered sponsoring this event? Sponsorship includes multiple passes at a discounted rate. Inquire to learn more.

Team Discounts****

- 10% discount – 2 Attendees
- 15% discount – 3 Attendees
- 20% discount – 4+ Attendees

****Please note that discounts are only valid when two or more delegates from one company book and pay at the same time.

Discounts cannot be used in conjunction with any other offer or discount. Only one discount offer may be applied to the current pricing rate.

Contact: register@hansonwade.com



Venue

Hampton by Hilton & Homewood Suites Boston Seaport District
670 Summer Street, Boston, MA 02210
www.hilton.com/en/hotels/bosshw-homewood-suites-boston-seaport-district/

TERMS & CONDITIONS

Full payment is due on registration. Cancellation and Substitution Policy: Cancellations must be received in writing. If the cancellation is received more than 14 days before the conference attendees will receive a full credit to a future conference. Cancellations received 14 days or less (including the fourteenth day) prior to the conference will be liable for the full fee. A substitution from the same organization can be made at any time.

Changes to Conference & Agenda: Every reasonable effort will be made to adhere to the event programme as advertised. However, it may be necessary to alter the advertised content, speakers, date, timing, format and/or location of the event. We reserve the right to amend or cancel any event at any time. Hanson Wade is not responsible for any loss or damage or costs incurred as a result of substitution, alteration, postponement or cancellation of an event for any reason and including causes beyond its control including without limitation, acts of God, natural disasters, sabotage, accident, trade or industrial disputes, terrorism or hostilities.

Data Protection: The personal information shown and/or provided by you will be held in a database. It may be used to keep you up to date with developments in your industry. Sometimes your details may be obtained or made available to third parties for marketing purposes. If you do not wish your details to be used for this purpose, please write to: Hanson Wade Ltd, Eastcastle House, 27/28 Eastcastle Street, London, W1W 8DH, United Kingdom



+1 617 455 4188

@ info@hansonwade.com

www.ai-convergence-small-molecule-discovery.com



ABOUT

EXPERT SPEAKERS

AGENDA

PARTNER WITH US

RESERVE YOUR PLACE