



[COVER](#)
[AGENDA-AT-A-GLANCE](#)
[SPEAKERS](#)
[VENUE](#)

Celebrating 25 years of innovation in drug discovery

 Wednesday, 4TH October 2023
 Artists For Humanity EpiCenter,
 100 W, 2nd Street, Boston

UGM Boston
 Oct. 4th 23




SUMMARY

Join ChemAxon's 25th-anniversary User Group Meeting in downtown Boston, October 4, 2023. We are excited to bring you expert presentations about the hottest topics shaping the industry today. Let us celebrate our shared history in drug discovery innovation.

Understanding the evolving needs of early drug discovery

Over the years, we have been dedicated to empowering scientists in their research efforts. We value the trust of the scientific community, and are proud to host a day filled with thought-provoking discussions about our shared passion.

AGENDA-AT-A-GLANCE

9:30AM EST → Registration

10:00AM – 10:50AM EST → CXN Session

10:50AM – 2:00PM EST → Morning Session

2:00PM – 5:30PM EST → Afternoon Session

5:30PM EST → Evening Session

[View the detailed agenda here](#)

MEET OUR GUEST SPEAKERS:



Patrick Walters
 Chief Data Officer
 Relay Therapeutics



David Klatte
 Senior Director, Scientific
 Solution Engineering
 Pfizer



Joe Michel
 Director of Informatics
 Cytokinetics



Dr. Arun Subramaniyan
 Vice President Cloud & AI,
 Strategy & Execution
 Intel



John McNeil
 Life Science R&D
 Informatics Strategist



Gerd Blanke
 Technical Director
 StructurePendium
 Technologies GmbH



Zofia Jordan
 Compound Compliance
 Consultant
 formerly of GSK

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BLOCK	TITLE	PRESENTER
REGISTRATION 9:30 EST		
CXN SESSION 10:00–10:50 EST	Opening Remarks	 Richard Jones, <i>CEO, Chemaxon</i>
	Chemaxon Roadmap	 Adrian Stevens, <i>CPO, Chemaxon</i>
MORNING SESSION 10:50–14:00 EST	Generative AI Begins to Dominate the AI Conversation in Early Drug Discovery	 Joe Michel, <i>Director of Informatics, Cytokinetics</i>
	COFFEE BREAK + DEMO CORNER	
	ChemistryView: how Pfizer simplifies its legacy desktop chemistry systems	 David Klatte, <i>Senior Director of Scientific Solution Engineering, Pfizer</i>
	Challenges and Opportunities for AI in drug discovery	 Pat Walters, <i>Chief Data Officer, Relay Therapeutics</i>
	LUNCH + NETWORKING + DEMO CORNER	
AFTERNOON SESSION 14:00–17:30 EST	Panel discussion on the use of AI in drug discovery - moderated by Jan Christopherson, <i>Application Scientist, Chemaxon</i>	 Joe Michel, <i>Director of Informatics, Cytokinetics</i>
	Advocating Change: One Synthetic Cannabinoid at a Time	 Zofia Jordan, <i>Compound Compliance Consultant, formerly of GSK</i>
	COFFEE BREAK + DEMO CORNER	
	Project team data visualization and decision support solutions: core requirements and must-have features	 John McNeil, <i>Life Sciences R&D Informatics Strategist</i>
	Are reaction data FAIR ... and what can we do with that?	 Gerd Blanke, <i>Chem- and bioinformatics Consultant</i>
	The World's Largest Protein-Ligand Complex and Binding Affinity Dataset for Data Driven Methods in Drug Design	 Dr. Arun Subramaniyan, <i>VP Cloud & AI Strategy and Execution, Intel</i>
	Closing Remarks	 Richard Jones, <i>CEO, Chemaxon</i>
EVENING SESSION 17:30 EST –	EVENING SOCIAL	
	GALA DINNER	

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MEET OUR SPEAKERS



Patrick Walters
Chief Data Officer
Relay Therapeutics

Pat will explore the application of machine learning and artificial intelligence in various drug discovery areas, highlighting emerging opportunities, and addressing open issues in the field.



Joe Michel
Director of Informatics
Cytokinetics

Joe will focus on how deep neural networks and generative AI are transforming molecular design, improving predictions, and enhancing the drug discovery process.



John McNeil
Life Science R&D
Informatics Strategist

John will talk about the core requirements and must-have features of collaborative data visualization and decision support solutions in the DMTA cycle.



Zofia Jordan
Compound Compliance
Consultant
formerly of GSK

Zofia will talk about how compliance aspects associated with sample management are becoming more critical due to the collaborative and globally distributed nature of research. She will showcase it through her experience working with the industry and authorities to modify the Third Generation Synthetic Cannabinoids amendment.



David Klatte
Senior Director, Scientific
Solution Engineering
Pfizer

David will introduce ChemistryView, Pfizer's custom developed Java component designed to simplify their legacy chemistry software systems. ChemistryView stemmed from a strong desire for the company's often 20-years old applications to be user customizable and to have consistent tools for managing advanced stereochemistry.



Dr. Arun Subramaniyan
Vice President Cloud & AI, Strategy & Execution
Intel

Arun will uncover a collaborative, multi-phase research project involving Intel, AWS, Insilico Medicine and IITR with the ultimate aim of creating the world's largest protein-ligand complex and binding affinity dataset that significantly accelerates drug research and discovery timelines.



Gerd Blanke
Technical Director
StructurePendium
Technologies GmbH

Gerd will talk about how chemical reaction data needs to comply with FAIR principles in order to be reliable, reproducible, and be used for accurate AI/ML predictions. He will address the specific challenges related to in-house chemical reaction data capturing and discuss what steps should be taken to make these databases more consistent for precise predictions.



Richard Jones
CEO
Chemaxon

Biography TBA



Adrian Stevens
CPO
Chemaxon

Biography TBA



Jan Christopherson
Application Scientist
Chemaxon

Biography TBA


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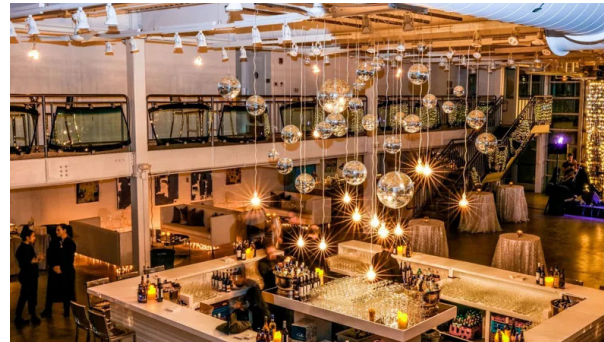
**artists for
humanity**
CREATIVE JOBS FOR CREATIVE TEENS

Artists For Humanity EpiCenter

100 W, 2nd street, Boston,
MA 02127

MAP & DIRECTIONS 

Artists For Humanity (AFH) offers an environmentally friendly and uniquely innovative space for special events. From meetings for 40 to cocktail receptions for 800, The EpiCenter is a blank canvas that can be transformed to realize your vision. Common events become extraordinary events when produced in an uncommon setting.



Hosting your event at
Artists For Humanity
directly supports our
mission!



We believe in giving back and are proud to host you at a venue dedicated to providing paid work opportunities for underprivileged youth in Boston.




REGISTER NOW!

Contact Kath De Vela

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 www.proventainternational.com