

MEDICINAL CHEMISTRY STRATEGY MEETING SAN DIEGO 2021

May, 25th Tuesday, 2021 Hard Rock Hotel San Diego



SPONSORS

AGENDA

KEYNOTE PRESENTATION

TRACK 1:
Artificial Intelligence / Machine Learning

TRACK 2:
Chemical Biology & Cheminformatics

TRACK 3:
Design & Custom Synthesis

TRACK 4:
Hit to Lead Identification

TRACK 5:
Integrated Drug Discovery

OUR VISION

To be a platform for creating life-saving therapies and to facilitate the creation of a completely patient centric pharmaceutical industry.

OUR MISSION

By encouraging key leaders and their companies to put the patient at the very heart beat of every innovation. Sharing valuable insights and strategies to assist in the discovery, development and commercialisation of life saving therapies.

OUR UNIQUE MEETING FORMAT



Roundtable Discussions

These interactive and informal discussion groups are the hallmark of the meeting. The brightest minds in the industry are brought together in 60-minute sessions that enable participants from all over the world to share ideas, challenges and lessons learned.



Personalised Agenda

Each delegate receives a personalised agenda with the roundtable discussions that you choose. You only attend sessions and meetings that fit your challenges and interests, ensuring your time spent on the online platform is focused and well-utilised.



One-to-one Meetings

The most effective and time efficient way to assess potential partners at a strategic level. Identify key solution providers that can take your business to the next level and we will help arrange private meetings so you can connect.



Strategic Networking

Strategic networking opportunities form a key benefit of the meeting. Our new online format for building and strengthening alliances to make lasting connections that benefit you.

CONTRIBUTORS TO THE AGENDA

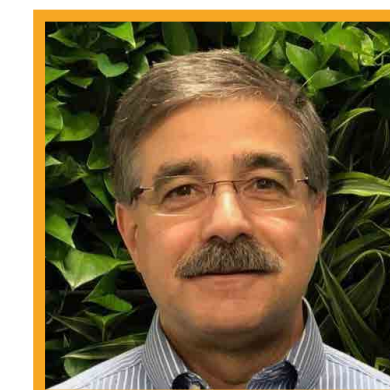
Uli Schmitz

Executive Director,
Structural Chemistry
Gilead Sciences



Paul Galatsis

VP, Chemistry
Vibliome
Therapeutics



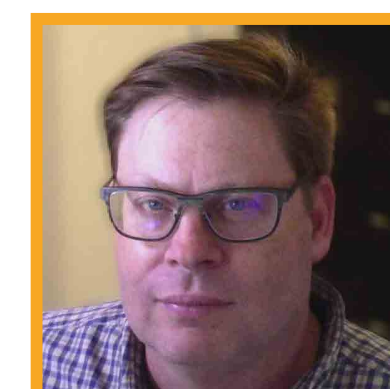
Mike Petrassi

VP, Medicinal Chemistry
Calibr/Scripps
Research



Prasun Mishra

CEO
Agility
Pharmaceuticals



Bill Shirley

Senior Director,
Structural Chemistry
Gilead Sciences



Tudor Oprea

Professor of Medicine and
Chief, Translational
Informatics Division,
Department of Internal
Medicine
Univeristy of New
Mexico



Syed Askari

CEO and Founder
Maculus
Therapeutics



Robert Hilgraf

Senior Director,
Medicinal Chemistry
REVOLUTION
Medicines

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WuXi AppTec provides a broad portfolio of R&D and manufacturing services that enable companies in the pharmaceutical, biotech and medical device industries worldwide to advance discoveries and deliver groundbreaking treatments to patients. As an innovation-driven and customer-focused company, WuXi AppTec helps our partners improve the productivity of advancing healthcare products through cost-effective and efficient solutions. With industry-leading capabilities such as R&D and manufacturing for small molecule drugs, cell and gene therapies, and testing for medical devices, WuXi AppTec's open-access platform is enabling more than 3,700 collaborators from over 30 countries to improve the health of those in need – and to realize our vision that “every drug can be made and every disease can be treated.”

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Collaborative Drug Discovery (CDD) provides an intuitive software suite extensively used by creative biologists and chemists working in academic, biotechnology and pharmaceutical settings. Their flagship product, CDD Vault, enables researchers to intuitively organize and analyze both biological study data and chemical structures, and to collaborate with partners through a straightforward web interface.



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Nanome, the first virtual reality (VR) software company to launch an immersive real-time collaboration platform for scientific discovery, is changing the way we understand and interact with science at the molecular level. The software environment allows users to visualize, modify, and simulate proteins, chemical compounds, and nucleic acids to accelerate scientific decision making. The platform facilitates effective communication of data and integrates with existing computational chemistry workflows—features that have led to the adoption of the San Diego-based company's enterprise solution by several pharmaceutical and biotech companies worldwide. For more information, visit nanome.ai

KEY OPINION LEADER



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AGENDA

MEDICINAL CHEMISTRY STRATEGY MEETING SAN DIEGO 2021



TRACK & ROOM (TIME)	01 - ARTIFICIAL INTELLIGENCE / MACHINE LEARNING	02 - CHEMICAL BIOLOGY & CHEMINFORMATICS	03 - DESIGN & CUSTOM SYNTHESIS	04 - HIT TO LEAD IDENTIFICATION	05 - INTEGRATED DRUG DISCOVERY
08:00 - 08:30	REGISTRATION AND WELCOME				
08:30 - 09:00	OPENING KEYNOTE PANEL SESSION Assessing the COVID-19 Impact on Drug Discovery in Medicinal Chemistry: The Industry Priorities for 2021? <ul style="list-style-type: none"> • Weighing the pros and cons of rapid global therapy development to strategize for lost time and improve efficiency in 2021 and beyond • How we utilize data integration from multiple sources to accelerate progress • Evaluating the costs & benefits of emerging technologies • Explore new opportunities for research and funding in 2021 				
09:00 - 10:00	Evaluating the impact of AI generative methods and ML models in drug discovery Uli Schmitz — Executive Director, Structural Chemistry, Gilead Sciences	Shifting away from the single-target paradigm: linking pharmacological data with biological pathways via high-throughput computational methods Mike Petrassi — VP, Medicinal Chemistry, Calibr/Script Research	Optimizing autonomy in synthesis: discussing the current state and outlook towards better efficiency Syed Askari — President & CEO, Maculus Therapeutix	Novel strategies to balancing high-throughput capabilities with multi-parametric studies	Partnering and Licensing with an Academic Medical Center Peter Kotsonis & Ellen Kats, Ph.D (Co-host) — Executive Director, Office of Strategic Alliances, UCSF & Assistant Director, Business Development & Licensing, UCSF
10:00 - 11:00	10:00 - 10:20: NETWORKING / 1-1 MEETINGS		10:20 - 10:40: NETWORKING / 1-1 MEETINGS		10:40 - 11:00: NETWORKING / 1-1 MEETINGS
11:00 - 12:00			Furthering the new paradigm: the marriage of robotics and advanced analytics in drug design Topic TBC for Sponsor		Advancing cycle time, analysis and purification efficiency through novel technologies and innovative approaches Topic TBC for Sponsor
12:00 - 13:00	NETWORKING LUNCH				
13:00 - 13:30	KEYNOTE PRESENTATION				
13:30 - 14:30	Beyond the AI hype: What has worked, and what will be improved in the future? Bill Shirley — Senior Director, Structural Chemistry, Gilead Sciences	Leveraging DNA-encoded libraries and cheminformatics to discover novel reactions and chemistries	How does the target integrate with the clinical side? What can we do to ensure success in the clinic? Paul Galatsis — VP, Chemistry, Vibliome Therapeutics	Computational Methods for Hit to Lead Optimization - how do we prioritize good from bad? David Wustrow — Vice President, Discovery, RAPT Therapeutics	Effective Integration of Multidisciplinary Teams to Ensure Seamless Drug Discovery Processes Yuhua Ji — Head of Medicinal Chemistry, Zai Lab US
14:30 - 15:30	14:30 - 14:50: NETWORKING / 1-1 MEETINGS		14:50 - 15:10: NETWORKING / 1-1 MEETINGS		15:10 - 15:30: NETWORKING / 1-1 MEETINGS
15:30 - 16:30	Leveraging AI and ML to extract value from large, disparate, internal/external data sets to aid drug discovery Topic TBC for Sponsor	Improving CADD capacities: moving past classical AI and ML towards the quantum age Topic TBC for Sponsor	Innovative design & development steps to optimise outsourcing speed, reliability and cost Topic TBC for Sponsor	Delineating the pros and cons of molecular dynamics simulations in fragment-based drug design Topic TBC for Sponsor	Optimising early drug discovery through harmonised DDI testing, genetic heterogeneity and PK data analysis Topic TBC for Sponsor
16:30 - 17:00	16:30 - 16:50: NETWORKING / 1-1 MEETINGS			16:50 - 17:00: BREAK	
17:00 - 18:00	Beyond the Hype of New Machine Learning Technology and Onto Delivery Tudor Oprea — Professor of Medicine and Chief, Translational Informatics Division, Department of Internal Medicine, University of New Mexico	Evaluating the challenges surrounding obtaining and structuring the right data sets Katherine Matsumoto — Director, Product Management, Recursion Pharmaceuticals	Novel computational approaches to design next gen drugs keeping optimized scale up and yield in mind	Targeting Protein-Protein Interactions (PPIs) - Challenges and Technologies Robert Hilgraf — Senior Director, Medicinal Chemistry, REVOLUTION Medicines	Reinstating phenotypic screening in your drug discovery workflow: discover novel phenotypes brought by innovative screening tools Prasun Mishra — CEO, Agility Pharmaceuticals
18:00 - 19:00	DRINKS & CANAPES RECEPTION				





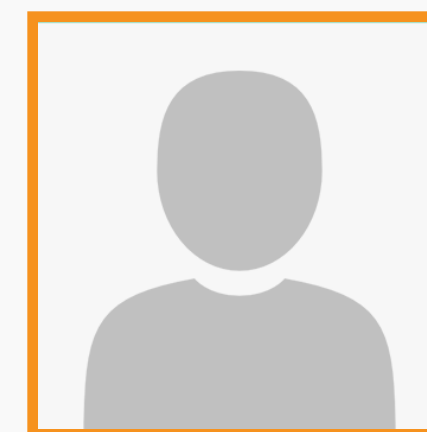
Speaker
TBC

OPENING KEYNOTE PANEL SESSION

🕒 08:30 - 09:00

Assessing the COVID-19 Impact on Drug Discovery in Medicinal Chemistry: The Industry Priorities for 2021?

- Weighing the pros and cons of rapid global therapy development to strategize for lost time and improve efficiency in 2021 and beyond
- How we utilize data integration from multiple sources to accelerate progress
- Evaluating the costs & benefits of emerging technologies
- Explore new opportunities for research and funding in 2021



Speaker
TBC

2ND KEYNOTE PRESENTATION

🕒 13:00 - 13:30

Topic TBC



TRACK 1

Artificial Intelligence / Machine Learning

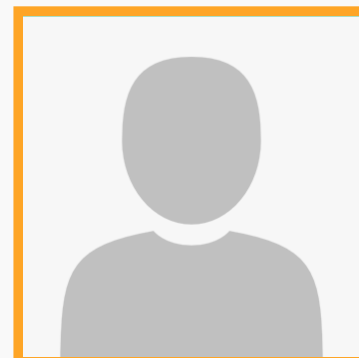
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Uli Schmitz
Executive Director,
Structural Chemistry
Gilead Sciences

🕒 09:00 - 10:00

Evaluating the impact of AI generative methods and ML models in drug discovery



WuXi AppTec

🕒 11:00 - 12:00

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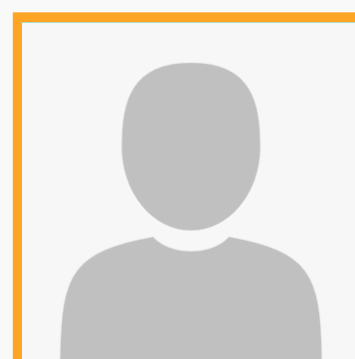
Harnessing the technology of noisy intermediate-scale quantum (NISQ) in drug discovery - Title TBC



Bill Shirley
Senior Director,
Structural Chemistry
Gilead Sciences

🕒 13:30 - 14:30

Beyond the AI hype: What has worked, and what will be improved in the future?

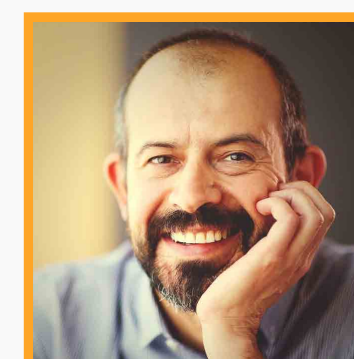


**Speaker
TBC**

🕒 15:30 - 16:30

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Leveraging AI and ML to extract value from large, disparate, internal/external data sets to aid drug discovery



Tudor Oprea
Professor of Medicine
and Chief, Translational
Informatics Division,
Department of Internal
Medicine
**University of
New Mexico**

🕒 17:00 - 18:00

Beyond the Hype of New Machine Learning Technology and Onto Delivery



TRACK 2

Chemical Biology & Cheminformatics

MEDICINAL CHEMISTRY

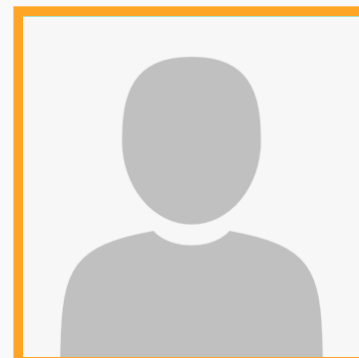
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Mike Petrassi
VP, Medicinal
Chemistry
Calibr/Scripps
Research

🕒 09:00 - 10:00

Shifting away from the single-target paradigm: linking pharmacological data with biological pathways via high-throughput computational methods

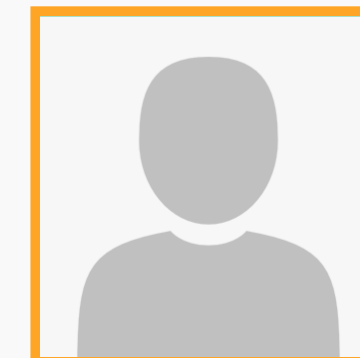


**Collaborative
Drug Discovery
(CDD)**

🕒 11:00 - 12:00

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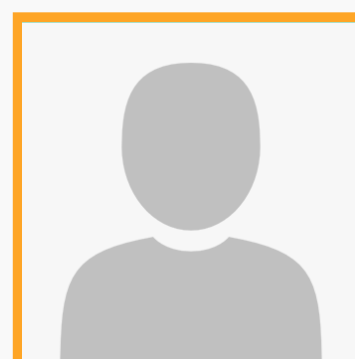
Discussing strategies in modeling of chemical reactions at larger scales - Title TBC



**Speaker
TBC**

🕒 13:30 - 14:30

Leveraging DNA-encoded libraries and cheminformatics to discover novel reactions and chemistries



**Speaker
TBC**

🕒 15:30 - 16:30

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Improving CADD capacities: moving past classical AI and ML towards the quantum age



**Katherine
Matsumoto**
Director, Product
Management
**Recursion
Pharmaceuticals**

🕒 17:00 - 18:00

Evaluating the challenges surrounding obtaining and structuring the right data sets



TRACK 3

Design & Custom Synthesis

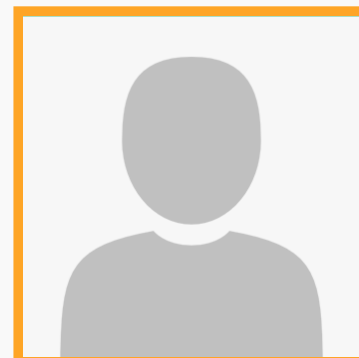
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Syed Askari
President & CEO
**Maculus
Therapeutix**

🕒 09:00 - 10:00

**Optimizing autonomy in synthesis:
discussing the current state and
outlook towards better efficiency**



**Speaker
TBC**

🕒 11:00 - 12:00

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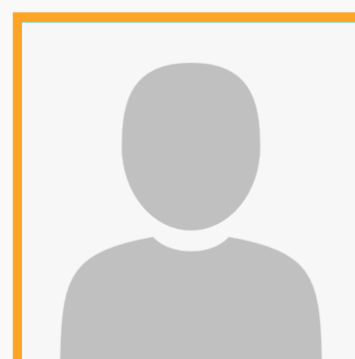
**Furthering the new paradigm: the
marriage of robotics and advanced
analytics in drug design**



Paul Galatsis
VP, Chemistry
**Vibriome
Therapeutics**

🕒 13:30 - 14:30

**How does the target integrate with
the clinical side? What can we do to
ensure success in the clinic?**

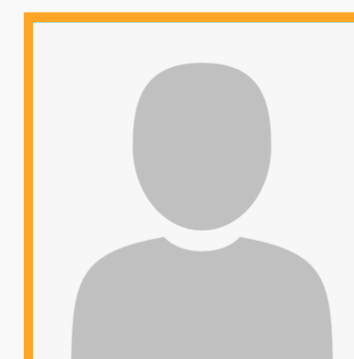


**Speaker
TBC**

🕒 15:30 - 16:30

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**Innovative design & development
steps to optimise outsourcing speed,
reliability and cost**



**Speaker
TBC**

🕒 17:00 - 18:00

**Novel computational approaches
to design next gen drugs keeping
optimized scale up and yield in mind**



TRACK 4

Hit to Lead Identification

MEDICINAL CHEMISTRY

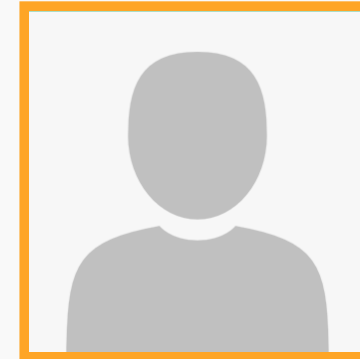
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Speaker
TBC

🕒 09:00 - 10:00

Novel strategies to balancing high-throughput capabilities with multi-parametric studies



Nanome

🕒 11:00 - 12:00

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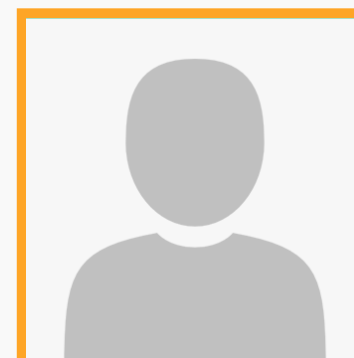
Innovative approaches to early drug discovery through novel chemical modalities



David Wustrow
Vice President,
Discovery
RAPT
Therapeutics

🕒 13:30 - 14:30

Computational Methods for Hit to Lead Optimization - how do we prioritize good from bad?



Speaker
TBC

🕒 15:30 - 16:30

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Delineating the pros and cons of molecular dynamics simulations in fragment-based drug design



Robert Hilgraf
Senior Director,
Medicinal Chemistry
REVOLUTION
Medicines

🕒 17:00 - 18:00

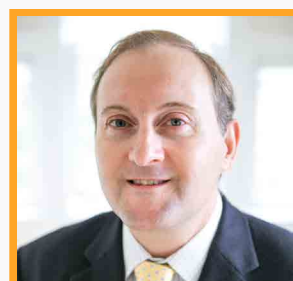
Targeting Protein-Protein Interactions (PPIs) – Challenges and Technologies



TRACK 5

Integrated Drug Discovery

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Peter Kotsonis
Executive Director,
Office of Strategic Alliances
UCSF

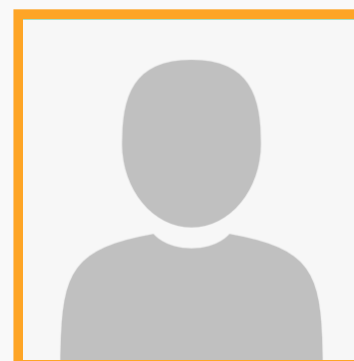
(CO-HOST)

🕒 13:30 - 14:30

**Partnering and Licensing with an
Academic Medical Center**



Ellen Kats, Ph.D
Assistant Director, Business
Development & Licensing
UCSF



**Speaker
TBC**

🕒 11:00 - 12:00

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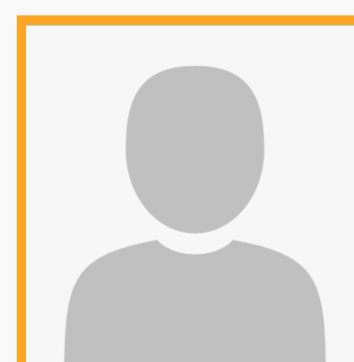
**Advancing cycle time, analysis and
purification efficiency through
novel technologies and innovative
approaches**



Yuhua Ji
Head of Medicinal
Chemistry
Zai Lab US

🕒 13:30 - 14:30

**Effective Integration of
Multidisciplinary Teams to Ensure
Seamless Drug Discovery Processes**



**Speaker
TBC**

🕒 15:30 - 16:30

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**Optimising early drug discovery
through harmonised DDI testing,
genetic heterogeneity and PK data
analysis**



Prasun Mishra
CEO
Agility
Pharmaceuticals

🕒 17:00 - 18:00

**Reinstating phenotypic screening
in your drug discovery workflow:
discover novel phenotypes brought by
innovative screening tools**

