

# MEDICINAL CHEMISTRY & BIOLOGY STRATEGY MEETING PRINCETON 2021

May, 18th 2021, Tuesday  Hyatt Regency Princeton, New Jersey



## SPONSORS

## AGENDA

## KEYNOTE PRESENTATION

**TRACK 1:** Artificial Intelligence /  
Machine Learning

**TRACK 2:** Integrated Drug Discovery

**TRACK 3:** Hit To Lead Identification,  
Target Discovery &  
Validation

**TRACK 4:** Chemical Biology &  
Cheminformatics

**TRACK 5:** In Vivo & In Vitro  
Pharmacology

**TRACK 6:** Strategic Partnerships,  
Collaborations & Alliance  
Management

Click here to find out what  
our clients think about our  
**STRATEGY MEETINGS**



## 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.

## LEADING INSIGHTS FROM

### Guna Rajagopal

VP, Global Head,  
Computational Sciences,  
Discovery Sciences,  
Janssen



### Mark Tebbe

Co-Founder & CTO  
Quench Bio



### Jennifer Petter

Founder & CSO  
Arrakis  
Therapeutics



### Deepak Kumar Rajpal

Head, Translational  
Sciences US  
Sanofi



### Ivan Cornella- Taracido

VP, Proteomics &  
Chemical Biology,  
Cedilla Therapeutics



### Frank Leu

Co-Founder and  
CEO  
Novapeutics



### Monica Schenone

Head of Chemical  
Biology  
Pfizer



### Markus Haeberlein

Head of Research  
Alkermes





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MEDICINAL CHEMISTRY & BIOLOGY  
STRATEGY MEETING PRINCETON 2021



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# AGENDA

## MEDICINAL CHEMISTRY & BIOLOGY STRATEGY MEETING PRINCETON 2021



MEDICINAL CHEMISTRY



BIOLOGY

TRACK & ROOM (TIME)	1 ARTIFICIAL INTELLIGENCE / MACHINE LEARNING	2 INTEGRATED DRUG DISCOVERY	3 HIT TO LEAD IDENTIFICATION, TARGET DISCOVERY & VALIDATION	4 CHEMICAL BIOLOGY & CHEMINFORMATICS	5 IN VIVO & IN VITRO PHARMACOLOGY	6 STRATEGIC PARTNERSHIPS, COLLABORATIONS & ALLIANCE MANAGEMENT
08:00 - 08:30	REGISTRATION AND WELCOME					
08:30 - 09:00	<p>OPENING KEYNOTE PANEL SESSION</p> <p><b>NEW! — Assessing COVID-19 Impact On Drug Discovery and Medicinal Chemistry: What Are The Industry Priorities For 2021?</b></p> <ul style="list-style-type: none"> <li>• Weighing the considerations of rapid global vaccine development: Have time and efficiency affected the area of drug discovery and is so, by how much?</li> <li>• Exploring novel therapeutic options: Will there be a significant shift in R&amp;D priorities in 2021?</li> <li>• Evaluating the costs &amp; benefits of emerging technologies</li> <li>• Explore new opportunities for research and funding in 2021</li> </ul> <p><b>Jennifer Petter</b> — Founder &amp; CSO, Arrakis Therapeutics   <b>Ivan Cornella-Taracido</b> — VP, Proteomics &amp; Chemical Biology, Cedilla Therapeutics   <b>Guna Rajagopal</b> — VP, Global Head, Computational Sciences, Discovery Sciences, Janssen</p>					
09:00 - 10:00	Leveraging AI and ML to extract value from large, disparate, internal/external data sets to aid drug discovery <b>Guna Rajagopal</b> — VP, Global Head, Computational Sciences, Discovery Sciences, Janssen	<b>NEW! — Beyond small molecule ligands for RNA: Which RNAs and how? Novel concepts and techniques for identifying and validating therapeutically important RNA targets</b> <b>Jennifer Petter</b> — Founder & CSO, Arrakis Therapeutics	What are the Best ML and AI Applications Today and in Development to Enhance Collaborative Database Sharing to Achieve Rapid and Effective Drug Target Discovery? <b>Frank Leu</b> — Co-Founder and CEO, Novapeutics	<b>NEW! — Chemical Biology in Drug Discovery</b> <b>Monica Schenone</b> — Head of Chemical Biology, Pfizer	Future Challenges and Solutions with Advanced In-Vitro Assay Systems – A Look at Phenotypic and Biomarker Assays <b>Mark Tebbe</b> — Co-Founder & CTO, Quench Bio	Strategies for Monitoring the Quality of Outsourced Work – The Vulnerabilities Involved and How to Identify New Strategic Partnerships <b>Bill Farley</b> — VP, Business and Corporate Development, Sorrento Therapeutics
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	Beyond the AI hype: Reviewing the last 10 years and forecasting the next 10 years <b>Topic TBC for Sponsor</b>	Reinstating phenotypic screening in your drug discovery workflow: discover novel phenotypes brought by innovative screening tools <b>Topic TBC for Sponsor</b>	Delineating the pros and cons of molecular dynamics simulations in fragment-based drug design <b>Topic TBC for Sponsor</b>	Computational and cheminformatics methods for chemical synthesis and hit discovery for difficult targets and emerging therapeutic modalities <b>Topic TBC for Sponsor</b>	In Vitro "Mode of Action" and In Vivo Outcome Measures and Toxicological Studies - What Can Be Farmed Out to Specialist Companies? <b>Topic TBC for Sponsor</b>	How to improve current alliances and gain more effective collaborations: lessons learned from effective IND-FIH ventures <b>Topic TBC for Sponsor</b>
12:00 - 13:00	NETWORKING LUNCH					
13:00 - 13:30	KEYNOTE PRESENTATION					
13:30 - 14:30	Opportunities and challenges for AI in emerging modalities <b>Michael Luzzio</b> — VP, Director, Molecular Therapeutics, Skyhawk Therapeutics	Recent progress in TPD: solving challenges and issues facing targeted protein degradation <b>Zhihua Sui</b> — VP, Head of Chemistry & Discovery Outsourcing, Agios Pharmaceuticals	Target Validation - How Do We Get Closer to Human Disease? <b>Joseph Mancini</b> — Head of Biology; Senior Director, adMare BioInnovations	<b>NEW! — Best practices in target druggability assessment and prioritization</b> <b>Ivan Cornella-Taracido</b> — VP, Proteomics & Chemical Biology, Cedilla Therapeutics	<b>NEW! — New Tools and Technologies - Can 3D Culture, HiPSC and Organ-on-chip Technologies Help to Bridge the Translational Medicine Gap?</b> <b>Marcie Glicksman</b> — Head of Biology, EnClear Therapies	Beginning with the end in mind: outlining the essential and critical decisions towards better collaboration <b>Markus Haerberlein</b> — Head of Research, Alkermes
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	Expediting the drug discovery process through leverage of generative modeling: discussion and case studies <b>Topic TBC for Sponsor</b>	Advancing cycle time, analysis and purification efficiency through novel technologies and innovative approaches <b>Topic TBC for Sponsor</b>	Adopting AI and ML in Target Validation - How to Ensure we Generate Suitable High-Quality, Consistent and Well-Structured Data <b>Topic TBC for Sponsor</b>	Evolution of physical and virtual screening libraries <b>Topic TBC for Sponsor</b>	Using Disease Models in Safety Pharmacology - Strategies to Swiftly Progress Compounds through Preclinical Development <b>Topic TBC for Sponsor</b>	Diamonds in the rough in contract research: learning outcomes from failed research reinforcing current partnerships & collaborations <b>Topic TBC for Sponsor</b>
16:30 - 17:00	16:30 - 16:50: NETWORKING / 1-1 MEETINGS			16:50 - 17:00: BREAK		
17:00 - 18:00	Harnessing the technology of noisy intermediate-scale quantum (NISQ) in drug discovery <b>Bertrand Le Bourdonnec</b> — VP Chemistry, Pharmaceutical & Pre-Clinical Sciences, Deciphera Pharmaceuticals	<b>NEW! — Evolution of Integrated Drug Discovery</b> <b>Richard Heidebrecht</b> — VP, R&D, Glycologix	<b>NEW! — Innovative approaches to early drug discovery through novel chemical modalities</b> <b>Adam Gilbert</b> — Senior Scientific Director, Design & Synthesis Sciences, Pfizer	State-of-the-art predictive and experimental methods for chemical matter selectivity and tox liability mapping	<b>NEW! — Translatability – from in vitro to in vivo, preclinical to clinic, bench to bedside</b> <b>Jing Li</b> — Executive Director, PTC Therapeutics	<b>NEW! — Building Strong Collaborations with Therapeutic Area Partners</b> <b>Deepak Kumar Rajpal</b> — Head, Translational Sciences US, Sanofi
18:00 - 19:00	DRINKS & CANAPES RECEPTION					







**Jennifer Petter**  
Founder & CSO  
Arrakis Therapeutics



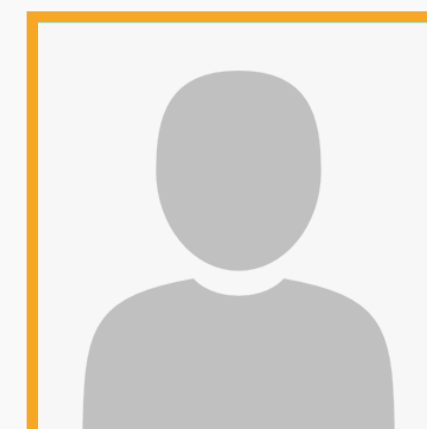
**Ivan Cornella-Taracido**  
VP, Proteomics & Chemical Biology  
Cedilla Therapeutics

OPENING KEYNOTE PANEL SESSION

08:30 - 09:00

### Assessing COVID-19 Impact On Drug Discovery and Medicinal Chemistry: What Are The Industry Priorities For 2021?

- Weighing the considerations of rapid global vaccine demand & development: Have time and efficiency affected the area of drug discovery and is so, by how much?
- Exploring novel therapeutic options: Will there be a significant shift in R&D priorities in 2021?
- Evaluating the cost & benefit of emerging technologies
- Explore new opportunities for research and funding in 2021



Speaker  
TBC

AFTERNOON KEYNOTE PRESENTATION

13:00 - 13:30

Topic TBC



# TRACK 1

## Artificial Intelligence / Machine Learning

# MEDICINAL CHEMISTRY & BIOLOGY STRATEGY MEETING PRINCETON 2021



**Guna Rajagopal**  
VP, Global Head,  
Computational Sciences,  
Discovery Sciences  
**Janssen**

🕒 09:00 - 10:00

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



**Speaker  
TBC**

🕒 11:00 - 12:00

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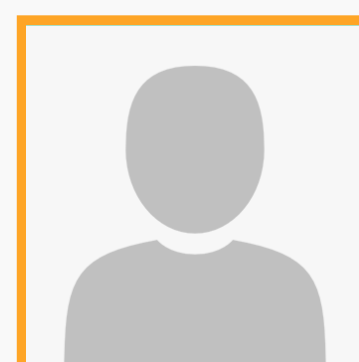
**Beyond the AI hype: Reviewing the last 10 years and forecasting the next 10 years**



**Michael Luzzio**  
VP, Director, Molecular  
Therapeutics  
**Skyhawk  
Therapeutics**

🕒 13:30 - 14:30

**Opportunities and challenges for AI in emerging modalities**



**Speaker  
TBC**

🕒 15:30 - 16:30

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**Expediting the drug discovery process through leverage of generative modeling: discussion and case studies**



**Bertrand Le Bourdonnec**  
VP Chemistry,  
Pharmaceutical &  
Pre-Clinical Sciences  
**Deciphera  
Pharmaceuticals**

🕒 17:00 - 18:00

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





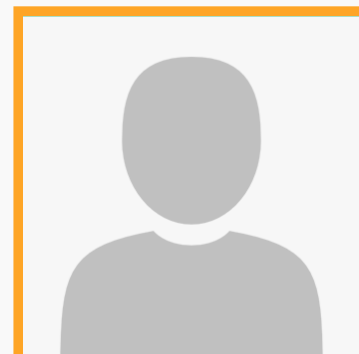


**Jennifer Petter**  
Founder & CSO  
**Arrakis  
Therapeutics**

🕒 09:00 - 10:00

### Beyond small molecule ligands for RNA: Which RNAs and how? Novel concepts and techniques for identifying and validating therapeutically important RNA targets

- Identifying small molecules, even drug-like small molecules, that bind folded RNA targets selectively is largely a solved problem. True?
- Identifying folded RNA domains in mRNAs or pre-mRNAs that impact RNA function with clear mechanisms remains a largely unsolved problem. True? And if true, what should be done?
- What lessons should be learned from extant small-molecule ligands reported to bind their RNA targets and yield cognate biology?
- What drug discovery tools or platforms are best suited to identifying small-molecule leads against RNAs?

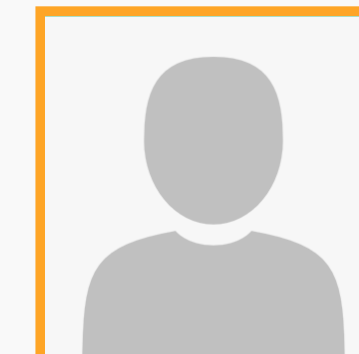


**Speaker  
TBC**

🕒 11:00 - 12:00

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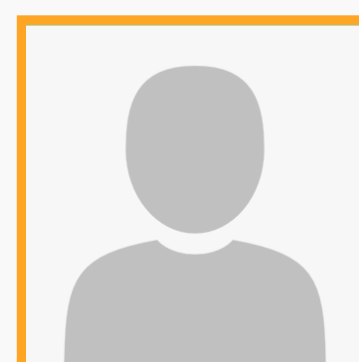
### Reinstating phenotypic screening in your drug discovery workflow: discover novel phenotypes brought by innovative screening tools



**Zhihua Sui**  
VP, Head of Chemistry &  
Discovery Outsourcing  
**Agios  
Pharmaceuticals**

🕒 13:30 - 14:30

### Recent progress in TPD: solving challenges and issues facing targeted protein degradation



**Speaker  
TBC**

🕒 15:30 - 16:30

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



**Richard  
Heidebrecht**  
VP, R&D  
**Glycologix**

🕒 17:00 - 18:00

### Evolution of Integrated Drug Discovery

- Best practices managing internal and external assets
- Balance between killer gold standard assays and normal screening activities
- Useful in silico tools (databases to AI)



# TRACK 3

Hit To Lead Identification,  
Target Discovery &  
Validation

# MEDICINAL CHEMISTRY & BIOLOGY STRATEGY MEETING PRINCETON 2021



**Frank Leu**  
Co-Founder and CEO  
Novapeutics

🕒 09:00 - 10:00

**What are the Best ML and AI Applications Today and in Development to Enhance Collaborative Database Sharing to Achieve Rapid and Effective Drug Target Discovery?**



**Speaker**  
TBC

🕒 11:00 - 12:00

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

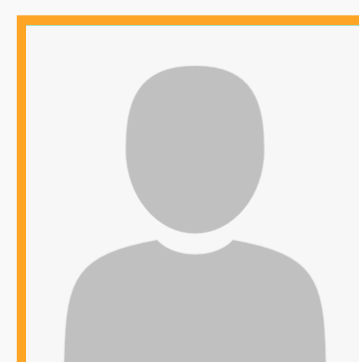


**Joseph Mancini**  
Head of Biology;  
Senior Director  
adMare  
BioInnovations

🕒 13:30 - 14:30

**Target Validation - How Do We Get Closer to Human Disease?**

- Genetics as a driver of Target Validation
- Are mouse models useful for success in the clinic
- Do iPSC primary cells which are differentiated replicate human cells
- Are Organoids the closest to human tissue
- Do organs on a chip provide the future for target id and validation



**Speaker**  
TBC

🕒 15:30 - 16:30

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**Adopting AI and ML in Target Validation – How to Ensure we Generate Suitable High-Quality, Consistent and Well-Structured Data**



**Adam Gilbert**  
Senior Scientific  
Director, Design &  
Synthesis Sciences  
Pfizer

🕒 17:00 - 18:00

**Innovative approaches to early drug discovery through novel chemical modalities**

- Selecting the correct modality for the target of interest i.e. small molecule inhibitor, chimeric compounds, protein degraders, covalent inhibitors, vaccines
- Pros/cons as well as challenges/opportunities of different chemical modalities
- Screening paradigms and hit validation strategies for each modality





# TRACK 4

## Chemical Biology & Cheminformatics

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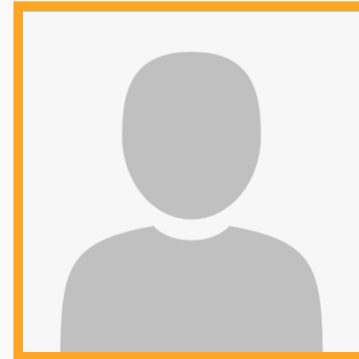
**Monica Schenone**

Head of Chemical  
Biology  
**Pfizer**

🕒 09:00 - 10:00

### Chemical Biology in Drug Discovery

- Covalent strategies
- Transcription Factors
- What is the next “big thing”



**Speaker  
TBC**

🕒 11:00 - 12:00

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Computational and cheminformatics methods for chemical synthesis and hit discovery for difficult targets and emerging therapeutic modalities



**Ivan Cornella-Taracido**

VP, Proteomics &  
Chemical Biology  
**Cedilla  
Therapeutics**

🕒 13:30 - 14:30

Best practices in target druggability assessment and prioritization

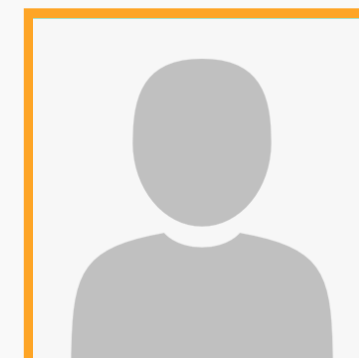


**Speaker  
TBC**

🕒 15:30 - 16:30

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Evolution of physical and virtual screening libraries



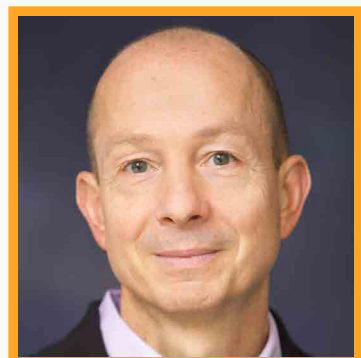
**Speaker  
TBC**

🕒 17:00 - 18:00

State-of-the-art predictive and experimental methods for chemical matter selectivity and tox liability mapping





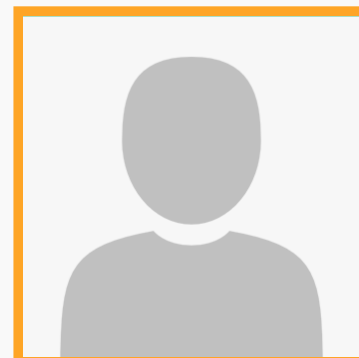


**Mark Tebbe**  
Co-Founder & CTO  
Quench Bio

🕒 09:00 - 10:00

### Future Challenges and Solutions with Advanced In-Vitro Assay Systems – A Look at Phenotypic and Biomarker Assays

- What are the current best practices for phenotypic and biomarker assays, what needs to be addressed in the future?
- What other advanced in vitro systems are being used and what are the future directions (organs on a chip, etc.)?
- Where is this technology going? What is the next gen for each assay type?



**Speaker**  
TBC

🕒 11:00 - 12:00

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### In Vitro “Mode of Action” and In Vivo Outcome Measures and Toxicological Studies - What Can Be Farmed Out to Specialist Companies?

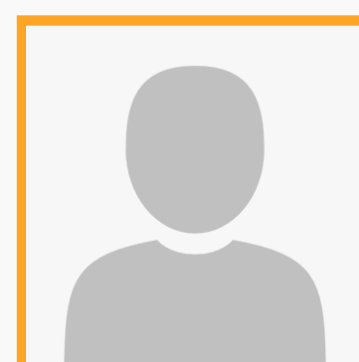


**Marcie Glicksman**  
Head of Biology  
EnClear Therapies

🕒 13:30 - 14:30

### New Tools and Technologies - Can 3D Culture, HiPSC and Organ-on-chip Technologies Help to Bridge the Translational Medicine Gap?

- Where do the use of stem cells fit into the drug discovery process?
- What do more complex cell models offer?
- When can cell models replace animal models?



**Speaker**  
TBC

🕒 15:30 - 16:30

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### Using Disease Models in Safety Pharmacology - Strategies to Swiftly Progress Compounds through Preclinical Development



**Jing Li**  
Executive Director  
PTC  
Therapeutics

🕒 17:00 - 18:00

### Translatability – from in vitro to in vivo, preclinic to clinic, bench to bedside

- How comprehensive is our understanding of human biology that feeds into preclinical discovery work?
- How can we improve the lack of efficacy and reduce clinical failure?
- Discussing current efforts and challenges that improve clinical success rates in industry



# TRACK 6

Strategic Partnerships,  
Collaborations & Alliance  
Management

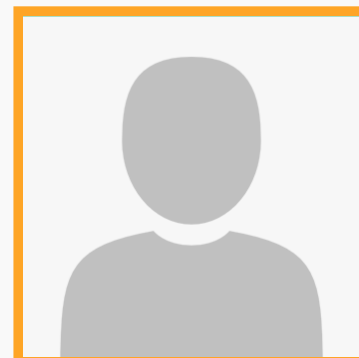
# MEDICINAL CHEMISTRY & BIOLOGY STRATEGY MEETING PRINCETON 2021



**Bill Farley**  
VP, Business and  
Corporate Development  
**Sorrento  
Therapeutics**

🕒 09:00 - 10:00

**Strategies for Monitoring the  
Quality of Outsourced Work – The  
Vulnerabilities Involved and How to  
Identify New Strategic Partnerships**



**Speaker  
TBC**

🕒 11:00 - 12:00

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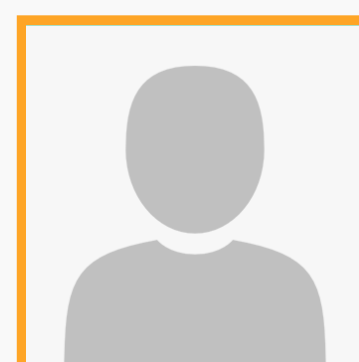
**How to improve current alliances and  
gain more effective collaborations:  
lessons learned from effective IND-  
FIH ventures**



**Markus  
Haerberlein**  
Head of Research  
**Alkermes**

🕒 13:30 - 14:30

**Beginning with the end in mind:  
outlining the essential and critical  
decisions towards better  
collaboration**



**Speaker  
TBC**

🕒 15:30 - 16:30

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**Diamonds in the rough in contract  
research: learning outcomes from  
failed research reinforcing current  
partnerships & collaborations**



**Deepak Kumar  
Rajpal**  
Head, Translational  
Sciences US  
**Sanofi**

🕒 17:00 - 18:00

**Building Strong Collaborations with  
Therapeutic Area Partners**

- What worked in your experience in building strong partnerships with Therapeutic Area partners to be impactful?
- What are the models of collaboration that seem to produce impactful results for Therapeutic Area partners?
- What kind of scientific engagement resulted in building partnerships with Therapeutic Areas that resulted in efficiency and decision making?
- Has upskilling been part of building strong collaborations with Therapeutic Area partners?

