Novartis Institutes for BioMedical Research

# NIBR@EFMC-ISMC2020

**September 9th, 2020**

| | Subject | Location |
|---|---|---|
| **15:45** | Get Together | Basel Campus<br>Main Gate |
| **16:00** | Introduction to the Event | Fabrikstrasse 16 |
| **16:10** | Reimagining Medicine at Novartis | Fabrikstrasse 16 |
| **16:30** | Science Encounters<br>Interact with NIBR scientists and collaborators to learn about and discuss:<br>○ The discovery of alpelisib<br>○ Tackling challenging protein-protein interactions<br>○ Encoded chemistry technologies<br>○ Chemical biology<br>○ Digital and data science in drug discovery<br>○ Synthesis technologies<br>○ NIBR postdoc programme<br>○ Fast lab open access screening facility | Fabrikstrasse 16 |
| **18:15** | Optional: Tour of NIBR Research Buildings | Fabrikstrasse 16 |
| **19:00** | End of Event | Fabrikstrasse 16 |

**Novartis Institutes for BioMedical Research**
Campus Basel
Fabrikstrasse 16, Ground Floor

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# Detailed Programme

**The discovery of alpelisib**
Learn how medicinal chemistry has impacted the discovery of alpelisib, a potent and selective PI3Kα inhibitor for the treatment of breast cancer. The session will cover aspects from NIBR's early discovery to late stage clinical trials, detailing the phases from hit generation to clinical candidate, and illustrating the key design steps using live modelling sessions with co-crystal structures.

**Tackling challenging protein-protein interactions**
The discovery of a clinical candidate is rarely a long calm river! It is punctuated by pitfalls, breakthroughs and unexpected results. Join the session to get a glimpse of the exciting work of a medicinal chemist through the example of inhibitors of p53/mdm2, a highly challenging protein/protein interaction. The session will cover several aspects, from hit generation to the delivery of a clinical candidate for the treatment of solid tumors. We will show you how structural technologies (crystallography, modeling) were key to turn a challenging approach into a successful story.

**Encoded chemistry technologies**
Discover what encoded chemistry technologies are and how they are applied to discover ligands for biological targets of pharmaceutical interest. This session will give you first-hand insight into the synthesis of ultra-large combinatorial compound libraries. Participants will have live demonstrations of reagent dispensing robots, automation enabling the parallelization of affinity selection experiments using magnetic beads, as well as illustrative screening outcomes in the form of a 3D model of a DNA-encoded small molecule bound to a biological target.

**Chemical biology**
Deepen your understanding on how small molecules produced via synthetic chemistry are applied to study and modulate biological systems. Participants will be shown examples of a) use of proteomic readouts to study function of small molecules, b) chemical synthesis on proteins: introducing tags and linkers with small molecules attached, c) photo affinity linking tool box – which tools to use?, and d) methods for assessing protein localization and function as a consequence of small molecule treatment.

**Digital and data science in drug discovery**
Artificial intelligence (AI) sounds cool – will computers just develop drugs on their own in the future? Come and learn how AI and data science transforms the way we do drug discovery in the future. Get insights into topics such as generative chemistry or machine learning and understand where those systems excel or fail in the lead optimization process.

**Synthesis technologies**
Learn how synthetic methods and chemical technologies can be used to impact drug discovery. Harnessing the power of enzymes allows us exquisite access to specific chirality in molecules, in a green and sustainable way. Combining this with a range of chemical synthetic methods and technologies enables fast access to a wide chemical space of pharmaceutical relevant molecules. A range of equipment, videos and posters will be presented.

**NIBR postdoc programme**
Learn about the postdoc programme at NIBR and what it has to offer you. Participants will have the possibility to discuss with NIBR postdoctoral fellows the science currently ongoing in their labs (posters, live demos) and hear about their overall programme experience.

**Fast lab/academic collaborators**
Get an introduction to NIBR's FAST lab (Facilitated Access to Screening) where you will be presented with case stories on how this is facilitating academic collaborators to explore their biology of interest using compound screening at Novartis? Learn what is involved in planning such a collaboration, what needs to be considered, as well as the available screening technologies and non-proprietary small molecule libraries.