

# NIBR @ ISMC2021

September 1<sup>st</sup>, 2021

|              | Subject   | Location                  |
|--------------|---|---------------------------|
| <b>15:45</b> | Get Together  | Basel Campus<br>Main Gate |
| <b>16:00</b> | Introduction to the Event   | Fabrikstrasse16           |
| <b>16:10</b> | Reimagine Medicine at Novartis  | Fabrikstrasse16           |
| <b>16:30</b> | Science Encounters<br>Interact with NIBR scientists and collaborators to<br>learn about and discuss: <ul style="list-style-type: none"><li>○ The discovery of alpelisib</li><li>○ Fast lab open access screening facility</li><li>○ Chemical biology</li><li>○ Encoded chemistry technologies</li><li>○ Data science and AI in drug discovery</li><li>○ Synthetic technologies</li><li>○ NIBR postdoc program</li></ul> | Fabrikstrasse16           |
| <b>18:15</b> | Optional: Tour of Research Buildings  | Fabrikstrasse 16          |
| <b>19:00</b> | End of Event  | Fabrikstrasse 16          |

## Detailed Program

### **The discovery of alpelisib**

Learn how medicinal chemistry has impacted the discovery of alpelisib, a potent and selective PI3K $\alpha$  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.

### **Encoded chemistry technologies**

Discover what encoded chemistry technologies are and how it is applied to discover ligands to 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.

### **NIBR postdoc program**

Learn about the Post-Doc program 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 program experience.

### **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

### **Synthetic 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.

### **Fast lab/academic collaborators**

Get an introduction to NIBR's FAST lab (Facilitated Access to Screening) where you'll 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's involved in planning such a collaboration, what needs to be considered, as well as the available screening technologies and non-proprietary small molecule libraries