

## EXCELLENCE IN MOLECULAR DESIGN

📅 14<sup>th</sup> Mar. 2023

📍 Institut Pasteur, Paris, France  
Amphitheater Duclaux



### PROGRAM

**8:40 am** Welcome at Amphitheater Duclaux

**9:10 am** Welcome address

**Dr Jean-Yves Ortholand** - President of the French Society for Medicinal Chemistry

**Dr Gilbert Lassalle** - SVP Head of Medicinal Chemistry France, Evotec

**Dr Olivier Sperandio** - Group Leader & Head of the iPPI-DB initiative, Institut Pasteur

**9:30 am** **Dr Christoph Grebner** - Sanofi, Frankfurt, Germany

“Artificial intelligence and explainability in molecular design”

**10:00 am** **Dr Gilles Labesse** - University of Montpellier, Montpellier, France

“Structure-Based and Integrative Design of B-Raf Inhibitors Devoid of Deleterious PXR Binding”

**10:30 am** Coffee break and meet the partners/ participants at Centre François Jacob

**11:15 am** **Dr Fredrik Zetterberg** – Galecto, Inc., Göteborg, Sweden

“Discovery of GB1211, the first orally available galectin-3 inhibitor to advance into clinical development as a potential treatment for cancer and fibrosis indications”

**11:45 am** **Andreas Lutten** - 2022 winner of Evotec Prize - University of Uppsala, Uppsala, Sweden

“Discovery of Enzyme Inhibitors through Virtual Screening of Vast Chemical Space”

**12:15 pm** Lunch and meet the partners/ participants at Centre François Jacob

1:45 pm **Dr Quentin Perron, Co-founder & CSO** - Iktos, Paris, France  
“DockAI: Efficient Exploration of ultra-large chemical spaces using Active Learning.”

2:00 pm **Dr Raquel Rodriguez Perez** - Novartis, Basel, Switzerland  
“Machine learning-based predictions of ADME properties in pharmaceutical industry”

2:30 pm **Dr Stefania Monteleone** - Evotec, Abingdon, United Kingdom  
“FMO-guided Identification of PPI Hotspots and Modulators”

3:00 pm **Coffee break and meet the partners/ participants at Centre François Jacob**

3:45 pm **Dr Christophe Zimmer / Dr Olivier Sperandio** - Institut Pasteur, Paris, France  
**Dr Christophe Zimmer** – “Deep learning and imaging for antibiotic drug discovery”  
**Dr Olivier Sperandio** – “Prediction of functional binding sites using 3D fully convolutional neural networks »

4:30 pm **Dr Merveille Eguida** - University of Strasbourg, Strasbourg, France  
“Automated target-focused library design using subpocket similarity combined with generative chemistry”

5:00 pm **Closing remarks**

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