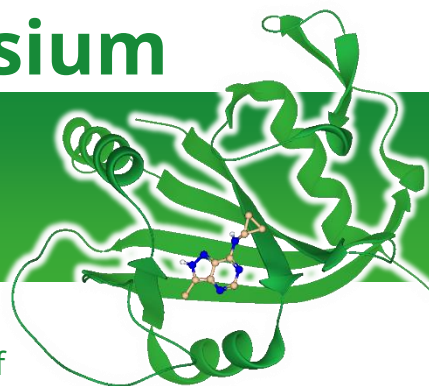




BioSolveIT
expect actives!

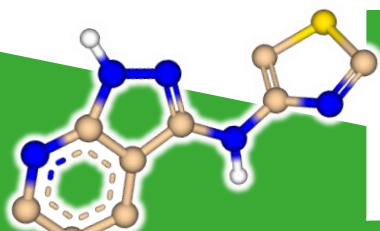
DrugSpace Symposium

It's a small world!
24-25th May 2022



The second virtual BioSolveIT DrugSpace Symposium revolves around the little gems of drug discovery; small molecules and fragments!

The symposium features interdisciplinary cross-talks between computational approaches, medicinal chemistry cases, crystallography, synthesis, small-compound evolution, and the handling of databases in reasonable time.



Time (CEST)

Wednesday 25th

3:00 – 4:30 pm

2nd Conference Day
Social Mixer and
Workshop: FBDD with BioSolveIT Applications
BioSolveIT
Join us in Gathertown with [this link!](#)

Time (CEST)

Tuesday 24th

Time (CEST)

Wednesday 25th

4:45 – 5:00 pm

Welcome Address - Christian Lemmen
BioSolveIT

4:45 – 5:00 pm

Welcome Address - Christian Lemmen
BioSolveIT

5:00 – 5:40 pm

Xavier Barril
University of Barcelona
"A Bottom-Up Approach to Screening
Massive Virtual Collections"

5:00 – 5:40 pm

Sven Brünschweiler
MAG-LAB
"A Step toward NRF2-DNA Interaction
Inhibitors by Fragment-Based NMR
Methods"

5:40 – 6:20 pm

Adam Bond
University of Dundee
"Amide-to-Ester Substitution as a Strategy
for Optimising PROTAC Permeability and
Cellular Activity"

5:40 – 6:20 pm

Laurent Maveyraud
University of Toulouse
"Crystallographic Screening in FBDD:
Application to the Phosphopantetheinyl
Transferase of Mycobacterium Abscessus"

6:20 – 7:00 pm

Marcus Gastreich
BioSolveIT
"Zetta-Sized Chemical Space Navigation"

6:20 – 7:00 pm

Paul Beroza
Genentech
"Chemical Space Docking: Large-Scale
Structure-Based Virtual Screening for
ROCK1 Inhibitors"

7:00 – 7:40 pm

Esther Kellenberger
University of Strasbourg
"Analysis of Fragment Libraries"

7:00 – 7:40 pm

Peter Ertl
Novartis
"Magic Rings: Navigation in the Ring
Chemical Space Guided by the Bioactive
Rings"

7:40 – 8:20 pm

Jeremy Edmunds
Abbvie
"Application of FastGrow to the Design
and Synthesis of Drug Like Compounds"

7:40 – 8:20 pm

Anna Hirsch
*Helmholtz Institute for Pharmaceutical
Research Saarland (HIPS)*
"Exploiting Fragment-Based Design in Anti-
Infective Drug Discovery"

Everyone is cordially invited to join and participate.

Registration is free but required:

<https://www.biosolveit.de/drugspace-symposium-spring-2022/>