Practical Drug Discovery in Chemical Space Using TransCure Online Tools at www.gdb.unibe.ch

Description	Over 12 million "drug-like" small molecules are available today from commercial providers. We will show how to use open-access online tools available at www.gdb.unibe.ch, developed over the last four years within the NCCR TransCure, to select small series of compounds from this large chemical space for purchase and experimental evaluation, and how to perform follow-up studies to optimize activities, identify a drug target, and predict off-target effects. Bring your own laptop for the workshop.
Eligibility	Participants must have a Master's Degree in life sciences or similar background.
Course Structure	One-day course (see agenda below).
Assessment	Presence check.
Date & Time	Friday, September 22nd, 2017, 08:45 – 16:00.
Credits	N/a
Facilitators	Jean-Louis Reymond (University of Bern, Dept. of Chemistry & Biochemistry) and collaborators (see program)
Location	University of Bern, Department of Chemistry and Biochemistry, Freiestrasse 3, 3012 Bern, Club room on 5th floor.
Registration	Please send an email to valentina.rossetti@transcure.unibe.ch by August 31st, 2017.
No. of spots	The maximum capacity of the course is 15 students. Priority will be given to members (PhD students & postdoctoral fellows) from the NCCR TransCure.

Program

08h45-09h15 Welcome coffee and get together

09h15-10h00 **Introduction**: Cheminformatics and exploration of chemical space for drug discovery. *Jean-Louis Reymond*

10h15-11h00 **Workshop 1:** Interactive visualization of >12 million patented compounds from the SureChEMBL database. *Daniel Probst*

11h15-12h00 **Workshop 2:** Similarity searching browsers for virtual screening: How to select analogs of one or more known compounds for purchase and biological evaluation in drug discovery projects. *Josep Arus*

12h00-13h15 Lunch

13h15-14h00 **Workshop 3:** webMolCS: How to select the compounds after virtual screening, how to explore the biological active compounds. *Mahendra Awale*

14h15-15h00 **Workshop 4:** The Polypharmacology Browser: How to identify a drug target and predict off-target effects and toxicity. A case study with the TRPV6 inhibitor. *Mahendra Awale*

15h15-16h00 **Workshop 5:** Grimoire: How to store and share compound related data within the NCCR TransCure network. *Daniel Probst*

16h00 End