

## Practical Drug Discovery in Chemical Space Using TransCure Online Tools at [www.gdb.unibe.ch](http://www.gdb.unibe.ch)

<b>Description</b>	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 <a href="http://www.gdb.unibe.ch">www.gdb.unibe.ch</a> , 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.
<b>Eligibility</b>	Participants must have a Master’s Degree in life sciences or similar background.
<b>Course Structure</b>	One-day course (see agenda below).
<b>Assessment</b>	Presence check.
<b>Dates</b>	Wednesday, November 12, 2014
<b>Credits</b>	N/a
<b>Facilitators</b>	Jean-Louis Reymond (University of Bern, Dept. of Chemistry & Biochemistry)
<b>Location</b>	University of Bern, Department of Chemistry and Biochemistry, Freiestrasse 3, 3012 Bern, Club room on 5 <sup>th</sup> floor
<b>Registration</b>	Send an email to <a href="mailto:Johanna.Botthof@ibmm.unibe.ch">Johanna.Botthof@ibmm.unibe.ch</a> no later than October 31, 2014
<b>No. of spots</b>	The maximum capacity of the course is 20 students. Priority will be given to members (PhD students & postdoctoral fellows) from NCCR & IFP TransCure.

## Program

- 08h45-09h15 Welcome coffee and get together
- 09h15-10h00 The Learning Game: how to become an expert medicinal chemist by teaching yourself drug properties, targets and names. Xian Jin
- 10h15-11h00 The Chemical Space Mapper: looking into what's available among the 12 million commercial compounds in the ZINC database with a "google-maps" like application. Mahendra Awale
- 11h15-12h00 Keynote lecture: How much can be predicted? The art and practice of medicinal chemistry. Karl-Heinz Altmann
- 12h00-13h15 Lunch
- 13h15-14h00 The Multifingerprint Browser: How to select analogs of one or more known compounds for purchase and evaluation during initial discovery and optimization. Jean-Louis Reymond
- 13h15-14h00 The Polypharmacology Browser: How to identify a drug target and predict off-target effects and toxicity. Mahendra Awale
- 15h15-16h00 Switching from purchase to synthesis to reach nanomolar activities: examples from the NCCR TransCure. Céline Jeanneret
- 16h00 End