CURSO: NMR FOR DRUG DISCOVERY
ESSE CURSO SERÁ MINISTRADO EM INGLÊS!!!!

PROFESSOR: Julien Orts (ETH)

LIMITE DE VAGAS: 20

PRE-REQUISITES: Basic NMR knowledge, proficient with your own computer.

OBJECTIVES: The objective of the course is to provide the participant an overview of the available methods used in drug discovery, from ligand based screening to structure calculations of ligand-protein complexes. We will review classical protocols as well as exotic methods to characterize protein-ligand interactions. Theory and practical aspects will be covered. Participants are expected to actively participate to the course by solving exercises and/or reviewing papers.

Participants are encouraged to bring their personal computers.
If time permits, we will have practical session on protein-ligand structure calculations (further information about software will be communicated).

PROGRAM

Fundamentals of NMR
Fundamentals of Physical Chemistry
Characterizing the sample composition and the NMR relevant properties of the sample
Types of available NMR experiments
Examples of typical data set
Overview of non-standard protocols for protein-ligand structure determination

As examples, the course will cover:
Basic product operator applied to NMR pulse sequences for drug discovery,
NOE theory and applications,
Full matrix formalism and applications,
INPHARMA, NMR Molecular replacement, Inter-ligand NOE…
Filtered experiments,
Structure calculations,
Automated assignment concepts,
Chemical shift perturbations,
Ligand based screening strategies,
etc.