

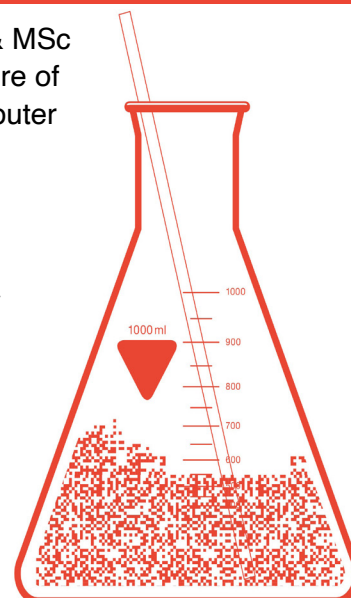
# Digitalization in Chemistry

## “Predicting structure, reactivity & properties in modern drug discovery”

The one-week summer school should give interested chemists & students (BSc & MSc Level) an insight on how digitalization is currently applied or will influence the future of Chemistry, chemical engineering and process development. In recent years computer assisted techniques find their ways into chemical processes, they are especially beneficial in fields of drug discovery but also for toxicology. The simulation of ligand molecules in receptors with molecular modelling software is already well established in industry. But digitalization offers a lot more, structural databases, computer-assisted retro-synthesis, artificial intelligence in drug development, fully automated synthesis and more will change the way how we work in near future.

During the 5 day summer school every day will focus on one topic; molecular modelling, databases, drug discovery and robotics/lab automatization. Besides the profound theory part given by presentations, case studies and workshops of invited specialists, company visits will give a hint on applied digitalization.

Lecture language will be English.



### Summerschool Schedule:

Day & Topic	Mo 20.7 Molecular Modelling	Tue 21.7. Molecular Modelling	Wed 22.7 Drug Discovery	Thu 23.7. Drug discovery	Friday 24.7. Automatisation
8:30 - 9:15	<b>General Introduction,</b> S. Wendeborn/S.Saxer	<b>Maestro Workshop 2</b> <b>Katia Dekimeche/David Rinaldo,</b> Computer room 11.M.06	<b>Christoph Boss,</b> 20 Years of Medicinal Chemistry - Always Look at the Bright Side (of Life!), Kleiner Hörsaal 01.N.07	<b>Marco Stenta,</b> Basic Principles of Modelling, Concept of modeling, Design of Models, Reaction modeling, Kleiner Hörsaal 01.N.07	<b>Company visit Chemspeed Technologies AG</b> <b>Christian Dittrich/M.Schneider,</b> <b>WHERE:</b> Chemspeed Technologies AG, Wölferstrasse 8, 4414 Füllinsdorf <b>START! 09:00 – 09:10:</b> Welcome at Chemspeed Headquarters <b>09:10 - 09:30:</b> Company Tour <b>09:30 – 10:45:</b> Presentation: "Standardized, Digitalized and Accelerated Solutions for Organic Chemistry" <b>10:45 – 12:00:</b> Laboratory Demos
9:30-10:15	<b>Schödinger Company</b> (Open Session) <b>Presenter: Katia Dekimeche/David Rinaldo,</b> Grosser Hörsaal 02.W.18		<b>Christoph Boss,</b> The Screening Compound Collection - A Key Asset in Drug Discovery, Kleiner Hörsaal 01.N.07		
10:30-11:15			<b>Julien Hazemann;</b> Machine Learning in Drug Discovery, Kleiner Hörsaal 01.N.07		
11:30-12:15			<b>Alexander Metz,</b> Structure-based Virtual Screening against SARS-CoV-2 Main Protease, Kleiner Hörsaal 01.N.07		
Lunch Break 12:30-13:30	<b>Databases</b>			<b>Data Sciences elsewhere</b>	
13:30-14:15	<b>Maestro Workshop 1: Katia Dekimeche/David Rinaldo</b> Schödingers Maestro Software introduction / Hands-on Workshop, Computer room 11.M.06	<b>Simon Walter</b> ETL (Extract, Transform, Load – "Work with" and "Learn from" databases such as Protein, small molecules, conformational diversity etc. databases, Kleiner Hörsaal 01.N.07		<b>Case study, Organizer: Marco Stenta</b> Application of Modelling, such as Reactions and Molecular properties, Computer aided molecular design & modelling, Kleiner Hörsaal 01.N.07	<b>Christian Korneder,</b> Autonomus Driving, Kleiner Hörsaal 01.N.01
14:30-15:15					
15:30-16:15					
16:30-17:15					

## The summerschool is following the official Corona - Rules!

**Date:** 20.-24.7.2020

**Location:** FHNW Campus Muttenz, Switzerland (<https://www.fhnw.ch/en/about-fhnw/locations/muttenz>)



**More information on:**

<https://www.fhnw.ch/de/die-fhnw/hochschulen/lifesciences/events/digitalization-in-chemistry>

**Organizer:** [FHNW School of Life Sciences](#)

