

Course program

AI- & data-driven drug design – An introduction

Format

- One-week course with a focus topic each of the five days. November 9-13, 2026
- Lectures 9-12, lunch 12-13 and hands-on workshop 13-17.

Day 1 (Nov 9) – Databases

	Content	Teacher	Affiliation
Lecture 1	Course introduction Information and participant presentation	David Gloriam	ILF, UCPH
Lecture 2	Drug, target and disease databases ClinicalTrials.gov, ChEMBL, DrugBank, DrugCentral, OpenTargets, Pharos, PubChem, Therapeutic targets database, (GPCRdb, GtoPdb, KLIFS), GTEX?	Javier Lorente	ILF, UCPH
Lecture 3	Industrial talk TBD	TBD	TBD
Workshop 1	Hunt for drug, target and disease data Find drug, target and disease data – either following a workshop material or related to your own project.	Javier Lorente, Søren Norge Andreassen, Aidan Flynn, David Gloriam	ILF, UCPH

Day 2 (Nov 10) – Structure-based drug design (small molecules)

	Content	Teacher	Affiliation
Lecture 4	The structure-based drug design toolbox Docking, LigPlot, SiteMap etc.	David Gloriam	ILF, UCPH
Lecture 5	Computational hit identification & hit-to-lead optimization Compounds properties being optimized and case story.	Henrik Daver	Lundbeck A/S
Lecture 6	Drug-target molecular interactions Molecular interactions (H-bonds etc.), shape fit and its role in selectivity etc.	David Gloriam	ILF, UCPH
Workshop 2	Structure-based ligand optimization Competition to build the best drug	Kasper Harpsøe, Icaro Simon, Pablo Macho, Jody Pacalon, David Gloriam	ILF, UCPH

Day 3 (Nov 11) – AI/ML tools for drug design (peptides & proteins)

	Content	Teacher	Affiliation
Lecture 7	Software for protein modeling & peptide drug design AlphaFold, Rosetta, ProteinMPNN, BindCraft ...	Albert Kooistra	ILF, UCPH
Lecture 8	Industry's toolbox and case story Commercially used methods and case stories	Rodrigo Alonso Ochoa	Novo Nordisk A/S
Lecture 9	AI-/ML-based peptide design at Gubra	Kasper Einarson	Gubra
Workshop 3	Protein modeling and peptide design Build a protein model and design peptide/mini-protein binders. Use of AlphaFold, Boltz etc. and maybe Colab notebook.	Albert Kooistra, Jody Pacalon, Jonas Verhellen, David Gloriam	ILF, UCPH

Day 4 (Nov 12) – Data visualization

	Content	Teacher	Affiliation
Lecture 10	Data visualization theory How the brain sees patterns: shape, position, color and size. Which graph for which data?	Sarah Mittenentzwei	TBD
Lecture 11	Title TBD	TBD	Illustreret videnskab
Lecture 12	Scripting tools for data visualization Tool tips to get started	Alexander Hauser	ILF, UCPH
Workshop 4	Data visualization workshop Using Claude	Sarah Mittenentzwei, Javier Lorente, David Gloriam, Jascha Henseler, Jacob Fredegaard Hansen	ILF, UCPH

Day 5 (Nov 13) – Data analysis using AI/ML

	Content	Teacher	Affiliation
Lecture 13	Data processing / preparation Features for small molecule and peptides, descriptors, data formats, transformation, normalization	Wouter Boomsma	DIKU, UCPH
Lecture 14	Predictive ML	Jakob Madsen	ILF, UCPH
Lecture 15	Industrial data analysis and case story	Lars Juhl Jensen	ZS discovery
Workshop 5	Data analysis workshop Using Claude	Arnault-Quentin Vermillet, Jascha Henseler, Jacob Fredegaard Hansen, Lykke Pedersen, David Gloriam	ILF, UCPH
Wrap-up	Wrapping up the course Tips of next-level courses and course evaluation.	David Gloriam	ILF, UCPH