ML and AI in structural biology
Looking beyond AlphaFold2 for remaining blindspots

Monday 14/11
Introduction: 9:30-10:00
session #1 (10:00-12:00) Use in experimental pipelines
Amelie Stein (Copenhagen, via zoom)
Marc Graille (CNRS/Polytechnique) “Impact of AlphaFold2/RosettaFold models to solve the phase problem in X-ray crystallography”

session #2 (13:30-15:30) Oligomers
Jessica Andreani (CEA) “AI for the prediction of protein complex structures: overview, examples and perspectives”
Thibault Tubiana (I2BC) “Get to know your protein better with AlphaFold, example with HEV's ORF1.”

Visualisation Workshop #1 (15:45-17:45) NOX #1 (focus on intrinsically disordered segments)
NOX #1 : Experimentalists: Marie Erard, Oliver Nüsse, Accompanying modeling expert: Burcu Aykac Fas

Tuesday 15/11
session #3 (9:00-10:45) Intrinsically disordered proteins/domains:
Isabelle Callebaut (CNRS/SU) "Low confidence predictions of AlphaFold : disorder and beyond"
Tatiana Galochkina (U. Paris Cité)

session #4 (11:15-12:00) Membrane proteins:
Zoe Cournia (Athens) "Predicting protein-membrane interfaces using ensemble machine learning and molecular simulations"

Visualisation Workshop #2 (14:00-16:00) NOX #2 (focus on comparison with structures and ligands/PTM)
Experimentalist: Sana-zineb Aimeur, Tania Bizouarn, Accompanying modeling expert: Hubert Santuz

Visualisation Workshop #3 (16:15-18:15) MCTP (focus on MD exploration of models)
Experimentalists: Emmanuelle Bayer, Marie-Cécile Caillaud, Accompanying modeling expert: Sujith Sritharan

Wednesday 16/11
Visualisation Workshop #4 (10:00-12:00) - Fzo1 (focus on contact maps/oligomers)
Experimentalists: Julien henry, Mohammad Ozeir, Accompanying modeling expert: Raphaelle Versini

Session #5:
Presentation of workshop sessions’ outputs (14:00-15:00)
Roundtable (15:00-16:00)

Registration for zoom access: https://tinyurl.com/2wzm5vp4