Inserm

La science pour la santé
From science to health

Inserm Workshop 271

Utiliser l'apprentissage automatique pour prédire les structures de protéine dans vos recherches

Using machine learning for protein structure prediction in your research

24-26 Mai 2023 / May 24-26, 2023 ◘ Bordeaux, France

Mercredi 24 Mai 2023 ◘ Wednesday May, 24 2023

15:30 - 16:00	**Reception of participants**
16:00 - 16:15	Welcome and presentation by the organizers
SESSION I	**Overview and history of ML in structural biology**
16:15 - 17:00	History of structure prediction - outline of challenges and approaches **Jessica Andreani (CEA, Paris, France)**
17:00 - 17:30	**Coffee break**
17:30 - 18:15	Development and description of RoseTTAFold/ Protein design **David Juergens (Baker lab, University of Washington, USA)**
18:15 - 19:00	AlphaFold two years on: application, impact, and future development **Oleg Kovalevskiy (DeepMind, London, United Kingdom)**
19:30	**Dinner**

Jeudi 25 Mai 2023 ◘ Thursday May, 25 2023

06:30 - 08:30	**Breakfast**
SESSION II	**ML applications in structure determination**
08:30 - 09:15	Applications to connect ML with X-ray/Cryo-EM structure determination/ bottom up structure biology **Tom Terwilliger (New Mexico Consortium, Los Alamos, USA)**
09:15 - 10:00	ML with high-throughput workflow **Panagiotis Kastritis (Martin Luther University Halle-Wittenberg, Germany)**
10:00 - 10:30	**Coffee break**
10:30 - 11:15	AI to help with NMR, predict intrinsic disorder and folding upon binding **Malene Ringkjøbing Jensen (IBS Grenoble, France)**
11:15 - 12:00	DeepEMhancer: a deep learning solution for cryo-EM volume post-processing **Carlos Sorzano (Centro Nacional de Biotecnología-CSIC, Madrid, Spain)**
12:00 - 14:00	**Lunch**

SESSION III	ML for complexes and drug design
14:00- 14:45	Prediction of complexes **Christian Cambillau (University College Cork, Ireland)**
14:45 - 15:30	ML and mass spectroscopy protein-nucleic acid interactions **Richard Scheltema (Utrecht University, Netherlands)**
15:30 - 16:00	**Coffee Break**
16:00 - 16:55	Modeling large complexes **Jan Kosinski (EMBL Hamburg, Germany)**
16:45 - 17:30	An Industry perspective to using AI in drug design **Matthias Haffke (Novartis, Basel, Switzerland)**
17:30 - 18:30	**Round Table Discussion**
19:30 - 20:15	**Cocktail**
20:15	**Dinner**

Vendredi 26 Mai 2023 ◘ Friday May, 26 2023

06:30 - 08:30	**Breakfast**
SESSION IV	Future of ML in structural biology
08:30 - 09:15	General overview of applications and limitations **Alex Bateman (EMBL-EBI, Cambridge, United Kingdom)**
09:15 - 10:00	AI to generate ligands/protein design through prediction of function **Joseph Rogers (University of Copenhagen, Denmark)**
10:00 - 10:30	**Coffee Break**
10:30 - 11:15	Available resources and recommended practices for working with predicted models **Preeti Choudhary/Deborah Harrus (PDBe-EBI, Cambridge, United Kingdom)**
11:15 - 12:00	Publishing work that uses AI predictions **Sarah Osman (Nature Publishing, United Kingdom)**
12:00 - 14:00	**Lunch**
14:00	**Departure**