CompBioMed

A Centre of Excellence in Computational Biomedicine

Webinar Series

Webinar #11: Next Generation Ultra High-Throughput Protein-Ligand Docking with Deep Learning

31 March 2020

5pm CET / 4pm GMT (1h duration)

Register for free here: https://attendee.gotowebinar.com/register/5024116533915851788

Recent studies have shown extending virtual screening libraries beyond hundreds of millions of compounds offers insights into new chemotypes, scaffolds, and binding motifs. In order to utilize the massive compute power available to research today, new techniques for analysis and screening are required. Standard techniques such as rigid structural docking are CPU bound and slow, and the analysis techniques are not designed to handle discrimination at the scale of billions of compounds. This webinar will cover new machine learning-based techniques for ultra high-throughput docking, with an emphasis on how to interpret results for actionable research when dealing with an unwieldy scale of data. This webinar is targeted towards researchers working in the field of drug discovery, and/or individuals with a general interest in the practical development and application of machine learning techniques for high-throughput screening.

This is the 11th of a series of webinars organised by CompBioMed.
Watch the full series on www.compbiomed.eu/training!

Austin Clyde is a computer science research assistant at Argonne National Laboratory and a Ph.D. student at The University of Chicago. He holds a mathematics degree and a Master's degree in Computer Science from The University of Chicago. His research focuses on high-throughput bioinformatics applications in deep learning with collaborators ranging across medicinal chemistry to high performance computing.

Moderated by **Dr. Apostolos Evangelopoulos,** University College London

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