CompBioMed

A Centre of Excellence in Computational Biomedicine

e-Seminar Series

e-Seminar #16
PlayMolecule for Drug Discovery

25 May 2021 1pm CEST / 12pm BST (1h duration)

Register for free here: https://register.gotowebinar.com/register/8357997426947489037

In 2017, Acellera launched the platform PlayMolecule with the aim to democratize the use of molecular dynamics and machine learning applications in the drug discovery field. Today, PlayMolecule is freely available to researchers worldwide, helping them to get more clear insights on their targets and in exploring the vastness of the chemical space available. Counting more than 80.000 jobs launched to present day, PlayMolecule strives toward the achievement of a full-suite of applications based on top-notch artificial intelligence and machine learning for accelerating the discovery of new drugs in the fight against existing and emerging diseases.

This e-Seminar is intended for scientists and researchers in the field of pharmaceutical sciences that are interested in learning new methods and technologies to improve high-throughput virtual screening, computational hit finding, and molecular dynamics simulations applied to biologic systems.

In this e-Seminar, you will learn how to launch jobs on PlayMolecule, how to retrieve the results and create workflows connecting the different applications available on the PlayMolecule.org platform.

This is the 15th of a series of online e-Seminars organised by CompBioMed.

Watch the full series on www.compbiomed.eu/training!

Roberto Fino is a computational medicinal chemist at Acellera Labs SL.

Graduated from the University of Bari in Organic Chemistry in 2014, then a Research Fellow at Stefano Piotto's Lab, University of Salerno, working on improving docking and scoring of compounds in HTVS. In 2016, selected as MSCA fellow for the AEGIS ITN consortium and received Ph.D. from Technical University Munich at Helmholtz Center for Environmental Sciences and Health, with a thesis on Combining NMR fragment-based screening, Computer-Aided Drug Design and Multi-Component reactions in early-stage drug design. He was then visiting researcher at the ETH Modlab group at the UMCG of Royal University Groningen, where he contributed to the development of machine learning-based analysis for chemical-shift perturbation (CSP-Analyzer). Chemist, programmer, storyteller; he also plays the bass and guitar.

In July 2020 he joined Acellera Labs SL and he works on the delivery of cutting-edge computational tools to accelerate computational drug discovery.

Moderated by Tim Weaving, **UCL**

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