CompBioMed

A Centre of Excellence in Computational Biomedicine

Webinar series

Webinar #5: High Throughput Molecular Dynamics for Drug Discovery

25 October 2018

12pm CEST (1 hour duration)

Register here: https://attendee.gotowebinar.com/register/6310037151741503235

Molecular dynamics (MD) simulations are used to capture dynamic processes of proteins across different timescales, with atomistic detail. The recent software and hardware innovations have decreased the computational cost of classical MD simulations, which can now be performed in a high-throughput manner. This has allowed MD simulations to play a relevant role in drug discovery.

In this webinar we will talk about the advances and methodologies behind high-throughput simulations, and we will show how to easily prepare and set up a system to study protein-ligand binding and compute its binding properties.

This is the 5th of a series of webinars that the CompBioMed Centre of Excellence organises in collaboration with the VPH Institute.

Watch the full series on www.compbiomed.eu!

Adrià Pérez is a Research Fellow at the Computational Science group, GRIB, at **Universitat Pompeu Fabra (UPF)**. He holds a Biochemistry degree from Universitat Autònoma de Barcelona and a Master's degree in Bioinformatics from UPF. The Computational science research group led by Gianni de Fabritiis is dedicated to computational science in biomedicine and machine learning. The group research interests are rooted in application of computation to solve real world problems. Specifically, we develop new methods and algorithms and we apply them to computational chemistry, drug design, protein folding, etc. The group and the spin-off company Acellera, founded in 2006, has collaborated with major industries worldwide like Sony, Nvidia, HTC mobile, UCB, Pfizer.

Moderated by Ben Czaja, University of Amsterdam

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