AGRICULTURAL UNIVERSITY OF ATHENS

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DEPARTMENT OF BIOTECHNOLOGY

REGULAR SEMINAR SERIES

1. Seminar Title

Molecular Modeling and Simulation of the Mycobacterial Cell Envelope

2. Presenter Information

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3. Date (Athens Timezone) & Location

Date: *20/11/26*

Time: *14.30-15.30 (EEST / EET)*

Timezone: *Athens, Greece (EET / EEST)*

Location: *Hassiotes Building, room B2, Department of Biotechnology, AUA*

Type: *Hybrid*

Link*:* **Microsoft Teams meeting**

Join: https://teams.microsoft.com/meet/3590006900584698?p=gAr0KlMhTbMp9ow3r4
Meeting ID: 359 000 690 058 469 8
Passcode: rh9Gj34w

4. Abstract

Mycobacteria are generally non-motile bacteria covered by an protective envelope consisting of a mycobacterial outer membrane (MOM), a peptidoglycan (PG) layer, and a mycobacterial inner membrane (MIM). This cell envelope provides the bacterial cell with structural integrity and protects the cell from hostile environments while allowing the transport of solutes and proteins. Despite its importance, our understanding on this cell envelope is rudimentary at best. Because of technical difficulties in deciphering these complex cell envelopes by experiments, all-atom and coarse-grained (CG) modeling and simulation should be able to provide an unprecedented understanding of the structure and dynamics of the mycobacterial cell envelope. As a first step, I will present our ongoing efforts to develop *Mycobacterial Lipid Modeler* in CHARMM-GUI, as well as an all-atom and CG simulation study of MOM and MIM membranes. This step is expected to open more opportunities to use all-atom and CG molecular modeling and simulation to obtain an in-depth and molecular-level understanding of how different lipid compositions modulate the MIM and MOM properties, how the PG layer is connected to the MIM and MOM, and thus the overall structure of the mycobacterial cell envelope, as well as how membrane proteins behave in and interact with the MIM or MOM.