## O.78. A computational approach to finding new drug targets for pathogenic *Candida* species

Romeu Viana[1,2]*, Diogo Couceiro[1,2], Tiago Carreiro[1,2], Caio Souza [4], Oscar Dias [3], Isabel Rocha [4], Cláudio M. Soares [4], Miguel Cacho Teixeira[1,2]

[1] *Department of Bioengineering, Instituto Superior Técnico, University of Lisbon, Lisboa, Portugal*

[2] *iBB - Institute for Bioengineering and Biosciences, Biological Sciences Research Group, Lisboa, Portugal*

[3] *CEB - Centre of Biological Engineering, Universidade do Minho, Braga, Portugal*

[4] *ITQB Nova - Instituto de Tecnologia Química e Biológica António Xavier, Lisboa, Portugal*

**romeuviana@tecnico.ulisboa.pt*

Candida species are among the most impactful fungal pathogens, normally associated with very high mortality rates. With the rise in frequency of multidrug-resistant clinical isolates, the identification of new drug targets and new drugs is crucial to overcome the increase in therapeutic failure.

In this study, we present the first validated genome-scale metabolic models for three pathogenic Candida species, Candida albicans, Candida auris and Candida parapsilosis. These models were reconstructed using the open-source software tool merlin 4.0.2 and are provided in the well-established systems biology markup language (SBML) format, thus, being usable in most metabolic engineering platforms, such as OptFlux or COBRA. These models were used as a platform for the discovery of new drug targets, through the determination of gene essentiality in conditions mimicking the human host. Using predictive computational techniques, Homology Modelling and Molecular Docking, we were able to identify potential inhibitory compounds for the identified drug targets, whose experimental validation is underway. This computational approach provides a promising platform for the identification of new drug targets and new antifungal drugs to tackle human candidiasis.