UNIVERSITÉ LIBRE DE BRUXELLES ULB VUB VRIJE UNIVERSITEIT BRUSSEL

The Research Group of

Industrial Microbiology and Food Biotechnology (IMDO, VUB)
and the **Unit of Theoretical Chronobiology (ULB)**

have the honour to invite you to the public PhD defence of

ir. Rudy Pelicaen

to obtain the degree of Doctor of Bioengineering Sciences (VUB)
and Doctor of Sciences (ULB)

Title of the PhD thesis:

Genome-scale metabolic modeling of candidate functional starter cultures for cocoa bean fermentation

Promotors:

Prof. Dr. Stefan WECKX (VUB)

Prof. Dr. Didier GONZE (ULB)

The defence will take place on

Monday, July 6, 2020, at 17 h

Given the COVID-19 regulations, the capacity to attend the defence on the Campus Humanities, Sciences and Engineering of the Vrije Universiteit Brussel, Pleinlaan 2, 1050 Elsene, is limited. The defence can also be followed through a live stream. Contact stefan.weckx@vub.be for more information.

Members of the jury

Prof. Dr. Dominique MAES (VUB, chair)
Prof. Dr. Tom LENAERTS (ULB, secretary)
Prof. Dr. Peter TOMPA (VUB)
Prof. Dr. Laurence VAN MELDEREN (ULB)
Prof. Dr. ir. Kristel BERNAERTS (KU Leuven)
Prof. Dr. Christoph WITTMANN (Saarland University, Germany)
Prof. Dr. Stefan WECKX (VUB, promotor)
Prof. Dr. Didier GONZE (ULB, promotor)

Curriculum vitae

Rudy Pelicaen was born on April 2, 1990, in Etterbeek, Belgium. In 2013, he graduated at the Vrije Universiteit Brussel (VUB), obtaining a Master degree in Bioengineering Sciences. He obtained a Master degree in Bioinformatics and Modeling at the Université libre de Bruxelles (ULB) in 2014. In November 2014, he started a joint PhD at the Research Group of Industrial Microbiology and Food Biotechnology of the VUB under the supervision of Prof. Dr. Stefan Weckx, and at the Unit of Theoretical Chronobiology of the ULB, under the supervision of Prof. Dr. Didier Gonze, at first with the financial support of the VUB in the framework of the Interuniversity Institute of Bioinformatics in Brussels and from January 2016 onward with a PhD fellowship strategic basic research from the Research Foundation – Flanders (FWO-Vlaanderen). Rudy Pelicaen is co-author of two peer-reviewed publications, among which one is a first-author publication. During his PhD, he gave in total four oral presentations at national and international conferences and symposia.

Abstract of the PhD research

Cocoa bean fermentation is an essential fermentation process to obtain the necessary raw material for the production of cocoa-derived products, among which chocolate. Despite its huge economic importance, cocoa bean fermentation is still a spontaneous fermentation process, relying on the variability of the environmental conditions and microbiota. To gain a better control over the latter, the use of functional starter cultures has been proposed. In this PhD study, genome-scale metabolic modeling of candidate functional starter culture strains was performed to gain more insight into their metabolic properties under cocoa fermentation conditions.

Genome-scale metabolic network reconstruction and modeling of *Acetobacter pasteurianus* 386B revealed the limitations that are currently encountered in describing its metabolism and the metabolic adaptations of this strain to cocoa fermentation conditions.

The reconstruction of a microorganism's metabolism based on its genome sequence is error-prone, thus manual curation by an expert is needed. Genome-scale metabolic network reconstruction of *Acetobacter ghanensis* LMG 23848^T and *Acetobacter senegalensis* 108B was performed using a semi-automated approach with experimental validation. Analysis and comparison of their metabolic networks revealed a wider metabolic diversity than previously thought and stressed the importance of incorporating genomic evidence when describing *Acetobacter* species.

Growth of bacterial cell populations under cocoa fermentation conditions is a dynamic process. Dynamic flux balance analysis allowed to gain insight into the possible intracellular metabolic flux distributions that could explain the population and metabolite dynamics found. This analysis highlighted different metabolic strategies for *A. pasteurianus* 386B and *A. ghanensis* LMG 23848^T to sustain their growth under cocoa fermentation conditions.

Finally, applying the genome-scale metabolic network reconstruction and modeling workflow to *Lactobacillus fermentum* 222 and *Lactobacillus plantarum* 80 revealed that possible consumption of unknown medium compounds may explain their population and metabolite dynamics found under cocoa fermentation conditions.

Overall, this PhD study demonstrated how *in silico* analysis of sequenced bacterial genomes and *in silico* experimentation using genome-scale metabolic models may provide biological insights related to the metabolism of those bacteria.