

## Exploring for antimicrobial compounds in complex natural mixtures using similarity analysis

Adam Feyaerts<sup>1,2,\*</sup>, Helene Tournu<sup>1,2</sup>, Yves Briers<sup>3</sup>, Daniele Pepe<sup>4</sup>, Rob Lavigne<sup>3</sup>, Walter Luyten<sup>5</sup> and Patrick Van Dijck<sup>1,2</sup>

<sup>1</sup> VIB Department of Molecular Microbiology, KU Leuven, 3001, Leuven, Belgium

<sup>2</sup> Laboratory of Molecular Cell Biology, KU Leuven, 3001, Leuven, Belgium

<sup>3</sup> Department of Biosystems, KU Leuven, 3001, Leuven, Belgium

<sup>4</sup> Department of Chemistry, B6c, University of Liège, 4000 Liège, Belgium

<sup>5</sup> Department of Pharmaceutical and Pharmacological Sciences, KU Leuven, 3000, Leuven, Belgium

\*Corresponding author. E-mail: adam.feyaerts@mmbio.vib-kuleuven.be

### Abstract

The antimicrobial activity (AMA) of 121 essential oils (EOs) and 2 EO components (EOCs) were assessed against eight diverse human (multi-resistant) pathogenic bacteria and **fungi**. In general the bioactivity of EO(C)s is difficult to assess because they are intrinsically volatile and poorly water-soluble. Therefore classical standardized assays were first adapted and optimized before screening [1]. In addition, as several microorganisms are capable of growing as a biofilm the AMA against **fungal biofilm** was also evaluated.

Differences in the methods used to assess AMA of EOs and the choice of test organism(s) as well as the lack of detailed information about the composition of the EO(s) complicate the comparison between data from different publications [2]. In a novel approach, we assembled an EO collection whose compositions are fully known, to investigate their AMA in a comparable way. Data mining techniques were applied to the chemical composition of the EOs and their corresponding biological activity [3]. The outcome was consistent with previous findings, hence validating not only this new approach but also confirming these earlier findings with the stronger statistical power of this study.

As a direct result we could assign specific AMA to similar EOs and identify corresponding classes of EOCs. Moreover, we could identify at least one known EOC with an unknown interesting and specific AMA. However, we expect that the analysis of more complex patterns will uncover additional interesting bioactivities of EOCs. The method is not limited to AMA data but can be applied to other bioactivity data.

### References

[1] Hood JR, Wilkinson JM, Cavanagh HMA (2003) Evaluation of Common Antibacterial Screening Methods Utilized in Essential Oil Research. *Journal of Essential Oil Research*, 15(6):428-433

[2] Hyldgaard M, Mygind T, Meyer RL (2012). Essential oils in food preservation: mode of action, synergies, and interactions with food matrix components, *Front Microbiol.*, 3(12)

[3] Hastie, T., Tibshirani, R. & Friedman, J. The elements of statistical learning: data mining, inference, and prediction, New York Springer, New York, 2nd Ed., 2009