

OP-01. A novel top-down approach to assess the antimicrobial activity of 121 essential oils against 8 diverse pathogenic bacteria and fungi

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In this exploratory study 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 highly volatile and poorly water-soluble. Therefore classical standardised assays such as the disk diffusion assay and the minimal inhibitory concentration assay were first adapted and optimised before screening. In addition, as several microorganisms are capable of growing as a biofilm, where they are often less sensitive to drugs, the AMA against fungi biofilm was also evaluated (Hood et al, 2003; Hyldgaard et al, 2012).

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. In a novel top-down approach, we assembled a library of 121 EOs whose compositions are fully known, to investigate their AMA in a comparable way. *In silico* data mining techniques, such as clustering and principal component analysis, were applied to chemical composition of the EOs and their corresponding biological activity. 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 applications of this method are diverse: (1) for an industrial application, three dissimilar EOs were selected from various natural products after an *in vitro* evaluation to replace some harmful synthetic compounds, (2) combining the chemical and biological data with data mining makes it possible to predict the AMA of an EO with a known composition.

Finally, the method is not limited to AMA data but can be applied to other bioactivity data.

Keywords: essential oil, antimicrobial activity, clustering analysis, principal component analysis, biofilm.

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ABSTRACTS

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