

Essential oil components can be tested as drug candidates

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A research team at the VIB-KU Leuven Center for Microbiology and the KU Leuven Department of Biology showed that, contrary to generally

held belief, most components of essential oils could meet the criteria set for drug candidates. Essential oil components are the constituents of essential oils, which are complex mixtures of plant metabolites obtained by dry or steam distillation, or by citrus peel pressing.

The research project, supervised by prof. Patrick Van Dijck (VIB-KU Leuven Center for Microbiology) and prof. Walter Luyten (KU Leuven Department of Biology), is rooted in the observation that in the past decades, [drug](#) discovery has mainly shifted to [high-throughput screening](#) of large, synthetically produced chemical libraries, while natural product drug research has diminished.

Prof. Van Dijck: "Natural products such as [essential oils](#) and their components are often avoided in drug discovery, for example, because they are relatively hydrophobic and volatile. This can cause interference during (high throughput) screening."

However, recent technical developments combined with restrictions on the use of chemicals led to a renewed interest in natural product drug discovery. Some of the new methods to study essential oils and their components were developed in the laboratory of prof. Van Dijck under the coordination of Dr. Adam Feyaerts, mainly with the aim of finding new antimicrobials, for example antifungal drugs.

Dr. Adam Feyaerts: "Nowadays, a relatively large number of essential oils and their components are already available as dietary supplements, but only a few have made the transition to drugs. As most technical barriers were removed, I wondered whether avoiding essential oils and their components in drug discovery was still justified. So, we evaluated certain parameters used in conventional drug discovery for more than 600 essential oil components to assess their potential as [drug candidates](#)."

Prof. Walter Luyten: "The discovery and development of a new drug

takes a long time and is very expensive, not in the least because so many initial candidates turn out not to be suitable. In other words, the earlier in the drug discovery process non-promising molecules can be eliminated, the better. Many candidate drug molecules fail when they are tested in animals."

A treasure trove of potential drugs?

Fortunately, in silico [drug discovery](#) filters have been developed that can predict drug disposition based on combinations of specific calculated parameters, which reduced the rate at which potential drugs failed later in the drug development pipeline. This study shows that essential oil components can be assessed using the filters implemented by the pharmaceutical industry.

Dr. Adam Feyaerts: "Our findings suggest that essential oil components can be promising sources of new drugs and deserve more attention, especially if they originate from essential oils that have already shown clinical benefits. Essential oil components also have unique properties that might be useful for some therapeutic applications, such as for lung or airway diseases, for transdermal administration, and for diseases of the central nervous system."

More information: Adam F. Feyaerts et al. Striking essential oil: tapping into a largely unexplored source for drug discovery, *Scientific Reports* (2020). [DOI: 10.1038/s41598-020-59332-5](https://doi.org/10.1038/s41598-020-59332-5)

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