



# Screening for *Streptococcus pyogenes* antibacterial and *Candida albicans* antifungal bioactivities of organic compounds in natural essential oils of *Piper betle* L., *Cleistocalyx operculatus* L. and *Ageratum conyzoides* L.

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## Abstract

Chemical composition and bioactivities including bacterial and fungal resistance of the essential oils extracted from leaves of *Piper betle* L. (**T**) and *Cleistocalyx operculatus* L. (**V**) and aerial parts of *Ageratum conyzoides* L. (**H**) were investigated. The components presenting in the essential oils of the natural sources were analyzed by a gas chromatography–mass spectrometry. Molecular docking simulation was utilized to support an antimicrobial mechanism of the essential oil compounds on *Candida albicans* fungus and *Streptococcus pyogenes* bacteria. This was based on the inhibition of the extracted compounds onto the microbial proteins, i.e. 4ESW and P0C0C7, respectively. There are 32 compounds identified in total in the three essential oils. The most effective inhibitors are the following: (i) chavicol acetate (**T3**), eugenol acetate (**T11**) and eugenol (**T4**) found in *Piper betle* L.; (ii) precocene II (**H10**) and precocene I (**H6**) found in *Ageratum conyzoides* L.; and (iii) caryophyllene oxide (**V15**) and *cis*-Lanceol (**V19**) found in *Cleistocalyx operculatus* L.. The overall antifungal and antibacterial capability of the investigated essential oils given indirect justification via their average inhabitability towards the two proteins accords with the order *Piper betle* L. *Ageratum conyzoides* L. *Cleistocalyx operculatus* L.. The results suggest these as promising natural sources for antimicrobial remedies.

**Keywords** *Piper betle* L. · *Ageratum conyzoides* L. · *Cleistocalyx operculatus* L. · Antibacterial · Antifungal · Molecular docking

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