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# Evaluation of antimicrobial activity and retention behavior of newly synthesized vanilidene derivatives of Meldrum's acids using QSRR approach

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Highlights

- Lipophilicity and antimicrobial activity of 13 vanilidene derivatives of Meldrum´s acid has been evaluated.
- Clustering of the compounds according to their lipophilicity was performed with the help of principal component analysis (PCA) and hierarchical cluster analysis (HCA).
- ADME properties of newly synthetized derivatives were analyzed by applying sum of ranking differences (SRD) method.
- Statistically significant predictive models of antimicrobial activity were obtained using multiple linear regression (MLR) analysis.

## Abstract

Increased antimicrobial resistance together with the lack of new antimicrobial drugs suggest on an urgent need for new therapeutics in this field. Vanilidene derivatives of Meldrum´s acid present one of the possible approaches. In this work lipophilicity of 13 vanilidene derivatives of Meldrum´s acid as well as their predicted antimicrobial activity towards several characteristic species has been evaluated.

10 vanilidene derivatives have been previously synthesized and 3 new compounds are synthetized afterwards following the same procedure. These selected 13 candidates were examined using thin layer chromatography in two different solvent systems. Gained retention parameters were a starting point for further Quantitative Structure Property Relationships (QSRR) studies in which minimum inhibitory concentration (MIC) for *Candida albicans, Trichoderma viride, Penicillium italicum, Fuscarium oxysporum, Pseudomonas aeruginosa*