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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 synthesized 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 synthesized 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*, *Fusarium oxysporum*, *Pseudomonas aeruginosa*

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