University of Venda

UNIVERSITY OF VENDA

SCHOOL OF MATHEMATICAL AND NATURAL SCIENCES

DEPARTMENT OF CHEMISTRY

MSC THESIS

Title: **STUDY OF THE FRONTIER ORBITALS AND CLOSE-TO-HOMO ORBITALS OF ACYLPHLOROGLUCINOLS**

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ABSTRACT

A thorough study of the frontier Molecular Orbitals (MO) – the Highest Occupied MO (HOMO) and the Lowest Unoccupied MO (LUMO) – and of the close-to-HOMO molecular orbitals (HOMO-1, HOMO-2 and HOMO-3) was conducted on a representative number of acylphloroglucinols' molecules (84 monomeric compounds), considering all the conformers for each molecule. The study aimed at identifying patterns for the LUMO, HOMO, HOMO-1, HOMO-2, HOMO-3 energies, and the HOMO-LUMO, HOMO-HOMO-1, HOMO-HOMO-2, and HOMO-HOMO-3 energy gaps across the molecules considered and across different media (in vacuo and in three solvents with different polarities – chloroform, acetonitrile, and water). For the smaller molecules – for which the use of more demanding computational methods were affordable – the study also compared the results of different calculations methods, namely HF/6-31G(d,p), HF/6-31+G(d,p), MP2/6-31G(d,p), MP2/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p), considering MP2 results as reference to evaluate the performance of the other methods. The results are reported in comparative tables for the energy values, and in figures comparing all the aspects of interest for the shapes of the MO considered (comparisons for corresponding conformers across structures; comparison for the same conformer across different media; and comparison of the results of the same conformer with different calculation methods). The final outcome is the provision of new information relevant for further research on acylphloroglucinols, including reactivity predictions and QSAR (Quantitative Structure Activity Relationships) studies, and the generation of a MO database which may be useful to other researchers.