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Synthesis and Investigation of Photophysical Behaviour and Antioxidant Activities of Sulfamic acid Catalyzed dimethyl-4-(4-hydroxy-2-oxo-2H-chromen-3-yl)-1H-pyrrole-2,3-dicarboxylate Series

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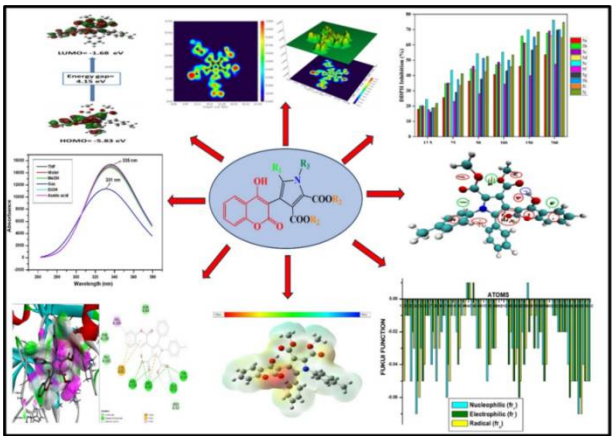
ABSTRACT

This study reports the synthesis of dimethyl-4-(4-hydroxy-2-oxo-2H-chromen-3-yl)-1H-pyrrole-2,3-dicarboxylate derivatives. The structural aspects of the newly synthesized compounds were accomplished by several physio-chemical techniques like ^{1}H-NMR, ^{13}C-NMR, and HRMS. The synthesized compound was photo-physically characterized by UV-Vis studies. The spectroscopic characteristics of the synthesized substances were studied using time-dependent density functional theory (TD-DFT). The integral equation formalism polarisable continuum model (IEFPCM) was used to simulate different solvent environments, such as the gas phase, ethanol, tetrahydrofuran (THF), methanol, water, and acetic acid. To validate the computational model, theoretical UV-Visible spectra for each solvent condition were created and compared to experimental spectroscopic data. Antioxidant activity was evaluated at different concentrations. In-silico ADMET predictions were performed, confirming adherence to Lipinski's rule of five.

Graphical abstract:



Keywords: Sulfamic acid, NBO, Docking, Population analysis, ELF, UV-Vis spectra, Biological evaluation and RDG.