



# -Biologically-Active Heterocyclic Molecules with Aggregation Induced BlueShifted Emission and Efficient Luminescence both in Solution and Solid States

Osama Younis, Mahmoud S. Tolba, Esam A. Orabi, Adel M. Kamal, Reda Hassanien, Osamu Tsutsumi, Mostafa Ahmed

## Abstract:

Biocompatible materials with aggregation-induced emission (AIE) have potential biological applications in bioimaging and bioprobes. Although many heterocyclic compounds have bio-applications, strong  $\pi$ - $\pi$  stacking usually causes aggregation-caused quenching (ACQ) of their luminescence. The design of AIE-active heterocyclic systems is thus highly needed. In this work, new chalcones and their thienopyrimidine derivatives have been synthesized and their molecular structures were affirmed by elemental and spectral analyses. The compounds displayed high thermal stability, and the luminescence of selected chalcones was studied in the solution and solid states at different temperatures. Moreover, density functional theory (DFT) calculations were done to study the molecular geometry of the ground and first excited states and the intermolecular interactions of these compounds. The studied dyes exhibited AIE behavior with two unusual phenomena, where one derivative gave blue-shifted emission after aggregation, and another derivative emitted efficiently both in the solid and solution states to fill the gap between AIE and ACQ materials. The DFT calculations revealed that changing the electronic structure of a terminal group can drastically alter the aggregation mode of the interacting molecules and hence change the optical properties of AIE luminogens. The new compounds may have potential bio-applications as some of them showed effective antibacterial and antifungal activities.

## Published In:

Journal of Photochemistry & Photobiology A: Chemistry , 400 , 112642