

PRECISION CONTROL OF EXCITED-STATE CHARGE TRANSFER IN A (E)-2-METHOXY-4-(((2-(NAPHTHALENYLAMINO) ETHYL) IMINO) METHYL)PHENOL BY SOLVENT AND MOLECULAR ENVIRONMENT

Ahalya Selvaraj ^a, Santhi Radhakrishnan ^a, Natarajan Elangovan ^{b*}

^a PG & Research Department of Chemistry, Seethalakshmi Ramaswami College, Affiliated to Bharathidasan University, Tiruchirapalli- 620 002, India

^b Department of Community Medicine, Saveetha Medical College and Hospital, Saveetha Institute of Medical and Technical Sciences, Chennai, Tamil Nadu, India

*e-mail: drelangovanchem@gmail.com

Abstract: The solution-phase photophysical behaviour and molecular interactions of a newly synthesised naphthalene-based Schiff base, (E)-2-methoxy-4-(((2-(naphthalenylamino) ethyl) imino) methyl)phenol (AH2) is studied. Quantum chemical calculations based on DFT at the B3LYP/cc-pVDZ level in the gas and explicit/implicit solvent phases were carried out to support these results, which allowed for the mapping of the PES, unveiling a marked solvent-dependent modulation of the HOMO-LUMO energy gaps (2.895 eV in DMSO to 3.585 eV in chloroform). The transition from pure liquid environments to biomolecular solutions was made to investigate the localised molecular interactions of the compound. Finally, these solution-state dynamics translate efficiently to liquid-phase biological assays where the compound showed promising selective antimicrobial efficacy against *Staphylococcus aureus* (MIC of 3.12 g/mL). These combined insights give a holistic fundamental understanding of the influence of fluid media on the charge transfer and biological recognition pathways of naphthalene derived Schiff bases.

Keywords: solvation effect, DFT, fluorescence, molecular docking, antimicrobial activity.