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RESEARCH

Synthesis, Computational, DFT Calculations, Photophysical and Docking Studies of Novel Fluorescent Pyrimidine-Chlorothymol Hybrid as Potent Antimicrobial Agent

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Abstract

Molecular fluorescent probes have found numerous applications in material science and biology. Fluorescently labelled heterocyclic compounds are found usage in light-emitting diodes, high throughput screening, bioanalytical applications, and diagnostics. Hence, this study focuses on the synthesis of a novel functionalized 4-((6-chloro-2-(trifluoromethyl) pyrimidin-4-yl)amino)-2-isopropyl-5-methyl phenol (CTPP) molecule using molecular hybridization approach as an antimicrobial agent and fluorescent probe. The synthesized CTPP molecule was characterized utilizing various spectroscopic techniques. The synthesized CTPP molecule was validated for their antimicrobial studies. With MIC values of 11.8 ± 0.26 and 14.6 ± 0.35 µM against *S. aureus* and *C. albicans* strains, respectively, the CTPP molecule significantly surpassed the reference medications streptomycin and fluconazole. The molecular docking results revealed that CTPP molecules has shown favourable binding interactions with good binding site energies against the target 3VO8 and 7PJC proteins. Computational studies were performed using the DFT method with a B3LYP/6–311G basis set used to explore the molecular geometry, global reactive descriptors, MEP, absorption, emission, ELF, LOL, RDG and NLO characteristics. It was discovered that the CTPP molecule's calculated NLO values were superior to reference molecule urea in both the gas and solvent phases. Moreover, the first and second hyperpolarizability values for CTPP molecule in gas and DMSO phase indicate that they could be employed as good nonlinear optical materials. The results of both theoretical and experimental research demonstrate that the CTPP molecule is a promising one that can be applied to NLO-based products in the optoelectronic industry.

Keywords Pyrimidine · Chlorothymol · Photophysical · NLO properties · Molecular docking

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