QUANTUM CHEMICAL AND EXPERIMENTAL STUDIES, ANTI-MICROBIAL, ANTI-MUTAGENIC, DNA BINDING AND ANION SENSORS PROPERTIES OF A SCHIFF BASE DERIVED FROM 3,5-BIS(TRIFLOUROMETHYL)ANILINE WITH 3,5-DICHLOROSALICYLALDEHYDE

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Abstract- Schiff base was synthesized from the reaction of 3,5-bis(triflouromethyl)aniline with 3,5-dichlorosalicylaldehyde. The structure of Schiff base has been investigated by FT-IR, UV-VIS, ^{1}H-NMR, ^{13}C-NMR and X-ray data. Moreover, the antimicrobial activity of the compound was investigated for its minimum inhibitory concentration (MIC) to bacteria and yeast cultures. UV-Vis spectroscopy studies of the interactions between the Schiff base and calf thymus DNA (CT-DNA) showed that the compound interacts with CT-DNA via intercalative binding. A DNA cleavage study showed that the Schiff base cleaved DNA without any external agents. Characterization of the Schiff base was carried out using theoretical quantum-mechanical calculations and experimental spectroscopic methods. The molecular structure of the compound was confirmed using X-ray single-crystal data, NMR, FTIR and UV-VIS, which was in good agreement with the structure predicted by the theoretical calculations using density functional theory (DFT). The colorimetric response of the Schiff base receptors was investigated before and after the addition of an equivalent amount of each anion to evaluate the anion recognition properties. In this regard, while the addition of CN^- anion into the solution containing the compound resulted in a significant color change, the addition of F^-, Br^-, I^-, SCN^-, ClO_4^-, HSO_4^-, AcO^-, $H_2PO_4^-$, N_3^- and OH^- anions resulted in no color change. This study is supported by a grant (Project Number: TÜBİTAK 115F253) from the Scientific and Technical Research Council of Turkey.

Keywords- Quantum Chemical Studies, MIC, DNA-Binding, Anion Sensors.