

The design, synthesis, spectral and electrochemical characterization of a series of novel pyrrolidine derivatives have been described. The synthesis was achieved by 1,3-dipolar cycloaddition of azomethine ylides and ferrocene-substituted chalcones, while detailed characterization of the compounds was performed by IR, NMR and elemental analyses, followed by X-ray diffraction experiment for one representative. The electrochemical properties of obtained ferrocene-containing heterocycles were examined by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). These techniques revealed the quasi-reversible one-electron oxidation process. DNA-binding capacity of all products was studied using CV and DPV, highlighting a derivative with five times better binding affinity than the others. DFT calculations and molecular docking studies were carried out to gain more exhaustive insight into the type of interactions of the distinguished compound and the nucleic acid.