

The synthesis of a series of methyl 2-alkyl-5-aryl-4-ferrocenoylpyrrolidine-2-carboxylates has been achieved by [3 + 2] dipolar cycloaddition of azomethine ylides to acryloylferrocene. The electrochemical properties of novel products were examined by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). These techniques revealed the quasi-reversible one-electron oxidation process. The DNA-binding capacity of all the products was also studied using CV and DPV, and significant interactions between synthesized compounds and nucleic acid, mostly of the electrostatic type, were disclosed. DFT calculations and molecular docking tests were carried out to gain a more exhaustive insight into the interactions of the obtained products with nucleic acid. A detailed characterization of the new compounds was performed by IR, NMR and elemental analyses, followed by single-crystal X-ray diffraction experiments for two representatives.