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Abstract

Synthesis, Characterization and Antimicrobial Activities of Some Schiff Bases with Non-Linear Optical Applications †

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Introduction: Schiff bases or imine compounds are considered a very remarkable category of organic compounds because of their π-delocalized structure and because of their pharmacological properties. Thus, the delocalization of the π-electrons defines the classic structures with an optical response due to the large hyperpolarizabilities which result from a "push–pull" system. Furthermore, imine compounds have been revealed to be promising leads for the design of more competent antimicrobial agents [1–3]. **Materials and methods:** Organic commercial and synthetic materials were used for the synthesis of the heterocyclic compounds. All compounds were characterized with physicochemical techniques (elemental analysis, ^{1}H, ^{13}C, FTIR and UV-Vis spectroscopy) [4]. The SHG capability of samples was measured by using an experimental set-up [1,5]. **Results:** A series of Schiff bases containing heterocyclic compounds (pyrazoles, pyrimidines, benzimidazoles, benzothiazole, etc.) was synthesized and characterized. The nonlinear optical (NLO) response of some Schiff bases is investigated by the static hyperpolarizability coefficients (β), calculated using the semi-empirical quantum chemistry algorithms (MOPAC software). All compounds were evaluated by qualitative and quantitative methods against a panel of selected bacterial and fungal strains [6,7]. **Conclusions:** It was found that relationship between donor/acceptor moieties, the dihedral angles around the azo bridge (-N=N-) transmitter group, the pass length as well as the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), strongly influenced the NLO response.

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