Abstract

This thesis work is part of the spectroscopic and structural characterisation by X-ray diffraction as well as the non-linear optical and biological properties of Schiff bases containg triazole-moities, as well as molecular docking.

The promising biological results previously obtained in our team, prompted us to study the effect of substitution on biological activity, in order to determine the group(s) responsible and influencing these activities, on the one hand, and to proceed with the investigation and optimisation by molecular docking, on the other hand.

The study of the biological properties of the five Schiff bases revealed good antifungal activity against a plant pathogen. While the results of the antibacterial activity showed that our compounds are inactive against some tested strains and moderately active against others.

Investigation of the non-linear optical properties, on the three Schiff bases (L1), (L2) and (L3), shows a good response to the second (SHG) and third harmonic (TH) even exceeding the LiNbO3 reference.

Molecular docking allowed us to predict the affinity and interaction modes between the different ligands and the protein responsible for the activation of the four microorganisms previously tested *in vitro*.

This approach by molecular docking allowed us to correlate the biological study carried out experimentally *in vitro* and the theoretical simulation approach *in silico*.

Key words : Halogeneted Schiff bases, 1,2,4-Triazole, X-ray diffraction, Molecular docking, Biological properties, Non-linear optics.