Abstract

Elaboration and characterization of organic products of biological interest substituted by methylsand halogens.

This work is a systematic study on organic products of biological interest substituted by methyls and halogens.

In this thesis it is presented some theoretical reminders relating to the determination of crystalline structures from X-rays as well as theoretical notions on optical spectroscopy.

Also a bibliography is presented concerning the density functional theory (DFT) that we used during our work as well as on the different representations of Hirshfeld surfaces which made it possible to identify all the intermolecular contacts taking place at within these crystals.

Finally, we cited some methods of biological characterization such as in-vitro experiments and the calculation of molecular dynamics of the docking.

In our work, it is presented respectively the synthesis and the experimental crystallographic results of the X-ray diffraction relating to the resolution of the structure of the two products: N - ((4-Chlorophenyl) (2-Hydroxynaphtalen-1-YL) Methyl) Acetamide and (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol- 5 (4H) -one at room temperature as well as an IR and Raman spectroscopy study. All of the intermolecular interactions present in these compounds have been elucidated and studied by establishing Hirshfeld surfaces.

Along with the experimental study, we did a simulation study using Gaussian 09 codes and VASP to perform the DFT calculations.

The results obtained from quantum chemistry calculations using the theory of functional have been compared with experience. This comparison concerns structural parameters extracted from X-ray diffraction and infrared (IR) and Raman spectroscopy.

The applications of our structures in the medical field have led to investigations to name only oxidation by experimental and theoretical methods.

In this thesis, it is presented the synthesis and structural analysis by X-ray diffraction of N - ((4-Chlorophenyl) (2-Hydroxynaphtalen-1-YL) Methyl) A Methyl) Acetamide (C19H16NClO2) and (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol- 5 (4H) -one ($C_{11}H_9ON_3$) at room temperature which crystallize respectively in space groups P 21 / n with four molecules per mesh and C2 / c with Z = 8.

Thanks to the Crystal Explorer program, we analyzed the Hirshfeld surface, and we were able to understand crystal stacking and identify the intermolecular interactions that provide cohesion in the crystals studied.

Calculations of molecular conformations on N - ((4-Chlorophenyl) (2-Hydroxynaphtalen-1-YL) Methyl) Acetamide (CHMA), were made from the functional hybrid B3LYP with the set of two bases 6-311G and DGDZVP, which led to C1 symmetry conformations with similar minimal formation energies. We have retained in our calculations, the B3LYP functional with the DGDZVP base, where the formation energy is minimal (-38071.881731 eV) and the R^2 confidence chords (geometric parameters) are better in the angles and lengths. link.

Concerning (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol-5 (4H) -one, molecular conformation calculations are also made from the B3LYP functional with the set of bases 6-311G and DGTZVP, which led to C1 and Cs symmetry conformations with similar minimal formation energies. Based on the results of the formation energies provided, it was deduced that the most stable conformation of (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol-5 (4H) -one and that which gave a minimum energy value equal to -19185.027675 eV, a weak polarity equal to 8.4928 Debye, a Cs symmetry and a very good R^2 agreement (of angles and connections) with the experimental one corresponds to the DGTZVP base with the B3LYP functional.

The molecular conformation of CHMA and (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol-5 (4H) -one was also determined by the theoretical calculation code VASP (Vienna Ab initio Simulation Package), where this time the periodicity of the crystal is taken into account. After geometric optimization, the results found give bond lengths and angles very close to the experiment.

The theoretical frequency calculation results obtained from quantum chemistry (DFT) are compared with infrared and Raman spectroscopic experimental results.

Theoretical spectroscopic calculations helped identify the different modes of vibration of the molecule.

Investigations on the applications of N - ((4-Chlorophenyl) (2-Hydroxynaphtalen-1-YL) Methyl) Acetamide and (Z) -4- (4-hydroxybenzylidene) -3-methylisoxazol- 5 (4H) -one guided us to carry out in-vitro experiments concerning the antioxidant property followed by the calculation of the molecular docking