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Title: Theoretical study of the molecular and electronic structures of β-carbolines and MAO substrates using the theory of density functional

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A theoretical spectroscopic study of the reversible inhibitory β-carbolines of monoamine oxidase (MAO) and the specific substrates of their enzymes, serotonin and noradrenaline, was carried out using the Functional Density Theory (FDT). The β-carbolines studied were: Harmina (7-methoxy-1-methyl-9H-pyrido [3,4-b] indole); Harmana, 1-Methyl-9H-pyrido [3,4-b] indole; Norharmana, 9H-pyrido [3,4-b] indole; Harmaline, 7-methoxy-1-methyl-4,9-dihydro-3H-pyrido [3,4-b] indole; Harmol, 1-methylethyl-2,9-dihydropyrido [3,4-b] indol-7-ol. Molecular structures were determined by optimizing the geometry of each molecule with the abinitio method and the 6-31G * base function, the $\Delta H_{formation}$ with semi-empirical methods PM3 and the excitation energies using TFD. The results showed that the calculations produced UV absorption spectra similar to the experimental spectra in both hydrophobic and hydrophilic media. In view of this, predictions were made of the photoactive region, photophysical properties and mode of action of each molecule and it was found that between β-carbolines and the two substrates, besides the structural similarity, there are similarities in the electronic structures. For example, for serotonin, harmana, and harmaline, the lowest fluorescente state S1 are ($\pi\ \pi^*$) and it was originated from eletronic transition between indole N to benzene C. The HOMO and LUMO energies in eV are: (5.08 and 0.96), (5.62 and 0.98) and (5.03 and 0.94) respectively. The possible explanations for the inhibition of MAO, mode of action of β-carbolines and the interacion of these molecules with the biological material are discussed.

Key-words:density functional theory, β-carbolines, serotonin

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