Goncagul Serdaroglu, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

The DFT Calculations on relationship between Solvation Energies and aromaticity of THβC, DHβC, βC

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The βC, which are naturally extracted from plants and obtained as secondary metabolism products from human tissues and marine organisms, have a very important place in many research fields because of their pharmacological properties such as inhibition activity against to the human cancer cell lines, antimalarial, fungicidal, convulsant, and so on. Here, this study used computational chemistry tools to predict the possible chemical behavior of these non-aromatic, half-aromatic and full aromatic compounds in the living body. Geometry optimization and frequency calculations have been performed in the three basis set levels, both in the gas and in the aqueous phases. The stabilization free energies increase in the following order as 0 (9.32 kcal) < 1 (9.50 kcal) < 2 (10.18 kcal) with B3LYP/6311++G** basis set in water phases. The electron density on molecular surface have changed in the following order: 2 (0.128) < 1 (0.123) < 0 (0.114) with the B3LYP/6-311++G** level of theory in water phase. It seems to be the structure 2 is the most reactive structure because it has the lowest negative and the highest positive charge centers and it seems to be the most reactive and most aromatic and less stable structure.

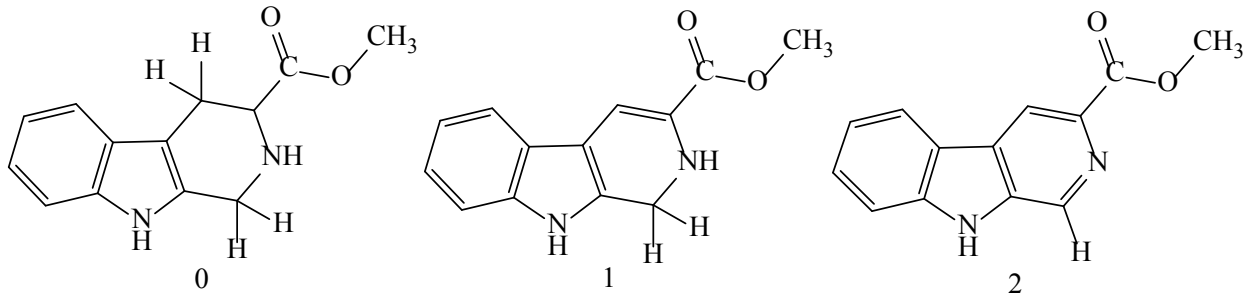

Figure 1. The β-Carbolines given as 0 (THβC-3-carboxylic acid methyl ester), 1 (DHβC-3-carboxylic acid methyl ester), 2 (βC-3-carboxylic acid methyl ester)

Biography

Goncagul Serdaroğlu has completed his PhD from Cumhuriyet University (2008) and postdoctoral studies from Auburn University (2013). She works on the structural properties and chemical behavior of biologically and pharmacologically important molecules by using computational tools.

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