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Substituent effect on reactivity of βCCM: A computational study

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βC compounds used in the treatment of many disease as a effective drug are obtained from both plants and marine organism as a secondary metabolism product. Here, all DFT calculations conducted with 3 basis set such as 631G(d,p), 631+G(d,p) and 6311++G(d,p) in both the gas phase and the water phase have been performed to predict the most reactive structure among the studied C1-substituted- N9-methyl-βCCM derivatives, which the substituent groups are that A (anthracen-9-yl), B (naphthalene-1-yl), C (naphthalene-2-yl), D (6-methoxynaphthalene-2-yl), E (phenanthrene-9-yl). The structure A is predicted as the most reactive structure in according to the quantum chemical descriptors such as the Energy Gap and global hardness values, that is, the Energy Gap of structure A has the lowest value than the other structures. Also it is determined as the soft molecule among the studied structures. As seem from Table 1, the calculated parameters are mostly compatible with each other to detemine the most reactive structure ot the less reactive structure. This work is to aim to contribute to the future development of the new drug molecules using the computational tools based on the quantum chemical descriptors.

Biography

Goncagul Serdaroglu has completed his PhD from Cumhuriyet University (2008) and postdoctoral studies from Auburn University (2013). Her major research interests are on structural properties and chemical behavior of biologically and pharmacologically important molecules by using computational tools.

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