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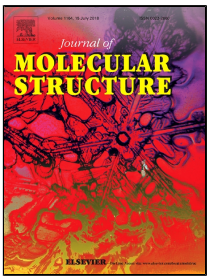

Effects of chemical structures of omega-6 fatty acids on the molecular parameters and quantum chemical descriptors

Tuğba Gocen, Sevgi Haman Bayarı, Mehmet Haluk Guven

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Effects of chemical structures of omega-6 fatty acids on the molecular parameters and quantum chemical descriptors

Tuğba Gocen [1] Sevgi Haman Bayarı [2*] Mehmet Haluk Guven[1]

[1]*Bülent Ecevit University, Department of Physics,67100 Zonguldak, Turkey*

[2] *Hacettepe University, Department of Physics Eng., 06800 Beytepe-Ankara, Turkey*

Omega-6 fatty acids are essential polyunsaturated fatty acids (PUFAs) and found in refined vegetable oils, nuts and seed that play a very important role in heart and brain function, along with normal growth and development. These acids have at least two double bonds and 18 carbon atoms (18:2) that the number of double bonds present refers to the degree of unsaturation of a fatty acid. A first phase of calculations was performed using PM3 semi-empirical method to characterize to potential energy surface of omega-6 fatty acids: Linoleic (18:2), γ-linolenic (18:3), Eicosadienoic (20:2), Dihomo-γ-linolenic (20:3), Arachidonic (20:4), Docosadienoic (22:2), Adrenic (22:4), Docosapentaenoic (22:5), Tetracosatetraenoic (24:4) and Tetracosapentaenoic (24:5). Afterwards, the lowest energy conformer of each acid was selected for the geometric optimization step and PM3 geometries were fully optimized using the DFT method at the B3LYP/ 6-311++G(d,p). The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima.

The effect of a fatty acid structure on its molecular properties were analysed.

Keywords: *Omega-6 fatty acids; PUFA, conformational analysis; molecular properties*