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The Thesis Submitted for the Degree of Master of Science
(In the field of Analytical Chemistry)

Computational study on the anti-breast cancer activity of flavonoid derivatives as protein kinase inhibitors

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Abstract

Flavonoids are polyphenolic compounds with antioxidant and radical scavenging activities, which are found in almost all natural products. The main reasons for the antioxidant activity of flavonoids are the position and the number of hydroxyl groups attached to the carbon skeleton and the possibility of formation of intramolecular hydrogen bonds. It seems that changing electronic properties of rings (A and B) leads to change of overall electronic properties, which affects on inhibitory strength of structure. It is expected that this method can optimize some of properties of structure and control side effects of it. In this research, initial structures of some natural flavonoid derivatives are optimized using quantum mechanical computations and then effect of different substituents on structural parameters, electron charge densities at the hydrogen bonds (HB_1 and HB_2) critical points and at the ring ones, donor-acceptor energies and electrostatic potentials of structures are evaluated. The electron-donating substituents on the A ring lead to increase in strength of both HBs. In the case of B ring, the electron-donating substituents strengthen HB_1, while the electron-withdrawing substituents strengthen HB_2.

Keywords: Flavonoid, quantum mechanics, intramolecular hydrogen bond, Inhibitor