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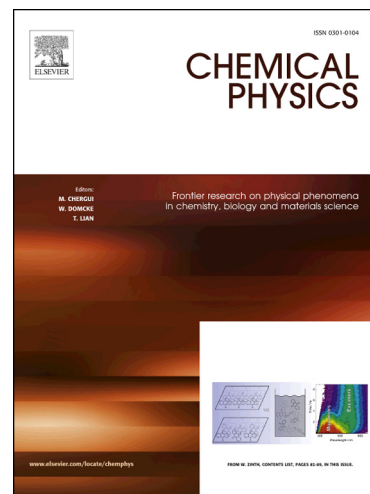
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An experimental and DFT study on free radical scavenging activity of hesperetin Schiff bases

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Abstract

Three hesperetin Schiff bases N-[2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chromen-4-ylidene]thiosemicarbazide (**HTSC**), N-[2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chromen-4-ylidene]isonicotinohydrazide (**HIN**) and N-[2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)chromen-4-ylidene]benzhydrazide (**HHSB**) were synthesized and evaluated for their electronic and physicochemical properties using experimental and theoretical methods. In order to determine antioxidant activity of the above mentioned compounds a detailed kinetic study of hesperetin analogues has been performed and comprehensive results have been reported with DPPH[•] assay using UV-Vis and ¹H NMR spectroscopy. Using DPPH assay, the order of the antioxidant activity increase was established as HTSC > HIN > HHSB > hesperetin. Based on the theoretical DFT(B3LYP) calculations it was concluded that in polar solvents (methanol

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