

Experimental and theoretical study on antioxidant activity of structurally related 4-hydroxycinnamic and 4-hydroxybenzoic acids

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The effect of substituent on the pKa value and antioxidant activity reflected by the TEAC (Trolox equivalent antioxidant capacity) value of series of 4-hydroxybenzoic acids and 4-hydroxycinnamic acids was investigated. It was shown that the TEAC value of both 4-hydroxybenzoic and 4-hydroxycinnamic acids increases significantly with increasing pH of the surrounding environment. Comparison of the experimental data with quantum chemically computed parameters indicates that the antioxidant behavior of the monoanionic forms of 4-hydroxybenzoic acids and 4-hydroxycinnamic acids is not determined by the tendency of the molecule to donate an electron but rather by its ability to donate a hydrogen atom. Results of our experiments and computations explain qualitatively the effect of substituent on the antioxidant behavior of both 4-hydroxybenzoic and 4-hydroxycinnamic acids. Our results confirm that in the wide pH range (5-10) 4-hydroxycinnamic acids are more efficient antioxidants than structurally related 4-hydroxybenzoic acids. It is stressed that 4-hydroxycinnamic acids are potent antioxidants already in weakly acidic media (pH ~ 6).