Current Topics in Biophysics (Zagadnienia Biofizyki Współczesnej) vol. 24 (2), 2000, 101-108

Effect of substitution pattern on TEAC antioxidant activity of mono- and dihydroxyflavones

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The effect of position of the hydroxyl substituent on the antioxidant activity reflected by the so-called TEAC value of a series of mono- and dihydroxyflavones was investigated in pH ranging from 5 to 9.5. The TEAC value of flavones substituted by hydroxyl group at C3, C5 or C6 position significantly increases with increasing pH of the environment. Flavones with hydroxyl groups at C4' and C7 positions are essentially not active over the whole pH range studied. Surprisingly some combinations of double OH substitutions in the flavone system like 7,3'-diOH or 7,4'-diOH were found to be also not active. Comparison of the experimental data to calculated ionization potentials indicates that the hydroxyl moiety at the C3 or C5 position in the flavone system (in the vicinity of the C4=O group) is an important structural element causing an increase in the antioxidant activity (TEAC value) of the mono- and dihydroxyflavones. The presence of catechol moiety at 3'4' position as well as at 6,7 position and 7,8 position at the A ring was found to be necessary for any antioxidant action of dihydroxyflavones if hydroxyl group at the C3 or C5 position is absent.