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The origin of anthocyanidins' high antioxidant activity

Anthocyanidins are flavonoid natural products responsible for the red to purple colours of many vegetables, fruits and flowers. Because of their poly-phenolic nature, they possess good antioxidant activity where some of them are more potent antioxidants than vitamins E and C which enables them to provide protection against many chronic diseases. Most experimental works have observed improved antioxidant activity as a result of the presence of 3-hydroxyl group and/or catecholic moiety that can donate two-hydrogen atoms and forms stable quinones. DFT calculation was performed to identify the favored path of the two-hydrogen atom donation process and determine the roles of the 3-hydroxyl group and other OH and OMe groups in stabilizing the resulted radicals and thus controlling the antioxidant efficiency in a series of 3-oxy-(and de-oxy) anthocyanidins with catecholic and non-catecholic moieties. Results showed that all 3-oxyanthocyanidins were non-planer while their 3-radicals were planer that allows better unpaired electron delocalization and explains the lowest BDE of 3-OH group in all the examined anthocyanidins. In non-catecholic compounds, the presence of two stabilizing OMe groups ortho to 4'-OH causes the two-hydrogen atom donation to take place through 3, 4'-OH; otherwise, the donation occurs through 3, 5-OH. In all catecholic anthocyanidins, it was found that two-hydrogen atom donation through 3, 4'-OH path was more favored than that of the catecholic hydroxyl groups (4', 3'-path) by 10-23 Kcal/mol while the role of the catecholic 3'-OH is stabilizing 4'-radicals by H-bonding. HOMO and spin density distribution supported the stabilization of 3, 4'-diradicals.

Biography

Hussein Mohamed Galal El-Din Ali has completed his Master's (1982) in Biochemistry from Agricultural Biochemistry Department, Ain Shams University, Egypt and PhD in Organic Chemistry from Michigan State University, USA, 1990. He is working as a Professor of Chemistry in Agricultural Biochemistry Department, Ain Shams University, Egypt from 2000 till date, and served as Head of the Department (2007-2010). He is member of the Permanent Scientific Committee of Promoting Professors and Associate Professors Egypt (2008-2010). He served as Visiting Professor at Umm Al-Qura (1994-2000) and Dammam Universities (2010-2015) SA. He is regular referee of some reputed journals (IF 2.0-4.0). His research experience is in: Agricultural & Food Chemistry, Enzyme Kinetics & Inhibition, Computational Chemistry, QSAR and Spectroscopy. He has published > 40 papers, most of them in international journals with IF 1.0-4.5.

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