Topology Delimited Radical-Scavenging Propensity of Monohydroxycinnamic Acids

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May 5, 2020

Abstract

Hydroxyl derivatives of cinnamic acid, both natural and synthetic, are well-known antioxidants. However, not all of them feature the same radical-scavenging propensity. Establishing the relation between structure and reactivity towards radical of those species plays a crucial role in the design of novel antioxidant pharmaceuticals founded on the same parent structure. The study aims at clarifying the relationship between topology, geometry, electron and spin density distribution and the radical-scavenging activity. Different mechanisms are discussed based on the enthalpies of the possible structures generated in the process of dissociation of the OH-bonds. All structures are modelled utilizing first principles methods and accounting for the polar medium at neutral pH (B3LYP/6-311++G**/PCM). A hybrid mechanism is suggested applicable not only to hydroxylated cinnamic acids but to phenolic acids in polar environment in general.

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