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ORIGINAL PAPER

DFT study of free radical scavenging activity of erodiol

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Antioxidant activity of erodiol was examined at the M05-2X/6-311+G(d,p) level of theory in the gas and aqueous phases. The structure and energy of radicals and anions of the most stable erodiol rotamer were analyzed. To estimate antioxidant potential of erodiol, different molecular properties were examined: bond dissociation enthalpy, proton affinity together with electron transfer energy, and ionization potential followed by proton dissociation enthalpy. It was found that hydrogen atom transfer is the prevailing mechanism of erodiol behavior in gas; whereas single electron transfer followed by proton transfer and sequential proton loss electron transfer mechanisms represent the thermodynamically preferred reaction paths in water.

Keywords: depside, erodiol, free radical scavenging mechanisms, BDE, IP, PA

Introduction

Depsides are polyphenolic compounds composed of two or more aromatic rings bound by a phenolic oxygen-ester linkage. They are most often found in lichens, but have also been isolated from higher plants (Ono et al., 2002; Hillenbrand et al., 2004; Reynertson et al., 2006). It has been suggested that some depsides act as antipyretic, analgesic, antibacterial, antiviral, anti HIV-1 integrase, anticancer, and antiproliferative agents (Proksa et al., 1994; Yamamoto et al., 1995; Neamati et al., 1997; Kumar & Müller, 1999; Nielsen et al., 1999). In addition, depsides inhibit biosynthesis of prostaglandin and leukotriene B4, and they act as powerful nonsteroidal antiinflammatories (Kumar & Müller, 2000; Reynertson et al., 2006; Lv et al., 2009). A new depside, erodiol (Fig. 1), has been isolated from the aqueous extract of the dried aerial parts of *Erodium cicutarum* (Fecka & Cisowski, 2005).

Depsides are electron-rich and highly conjugated chemical systems. Due to these features they easily

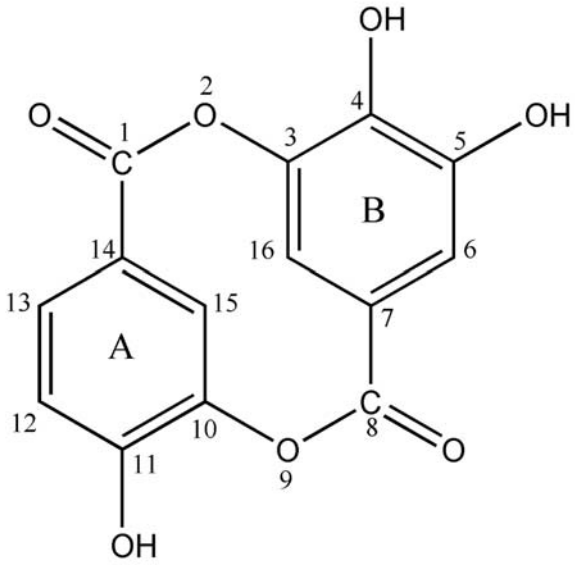

Fig. 1. Structural formula of erodiol. Labels on the atoms are used throughout the paper.

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