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EXAMINATION OF ANTIOXIDANT ACTIVITY OF THREE DIHYDROXYBENZOIC ACIDS

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ABSTRACT

In the present study the M05-2X/6-311++G(d,p)model is used to evaluate scavenging potency of 2,3-, 2,6-,and 3,4-dihydroxybenzoic acids (DHBAs).Reaction enthalpies related to the scavenging mechanisms of the studied species were calculated in water and benzene. Hydrogen atom transfer is a preferred reaction pathway in benzene, while sequential proton loss electron transfer is a predominant reaction pathway in polar solvent, water, for all the studied compounds.

INTRODUCTION

Phenolic acids represents important class of phenolic compounds which are widely distributed in the plant world, being an integral part of the human diet. Naturally occurring phenolic acids, with common basic skeleton, are divided intotwo large groups: hydroxycinnamic and hydroxybenzoicacids [1]. Phenolic acids exist in almost all vegetables, fruits, and grains. They are rarely found as free molecules in nature, more often they are found in plants in the form of esters, ethers, and acetals, or as structural components of cellulose, hemicellulose, proteins and lignin[2]. Free-radical scavenging ability of 3,4-DHBA inhibits chemical carcinogenesis and protects against hydroperoxide-induced toxicity [3]. 2,3-DHBAis also a human metabolite found in plasma and a biological marker for the detection and quantification of OH radicals.