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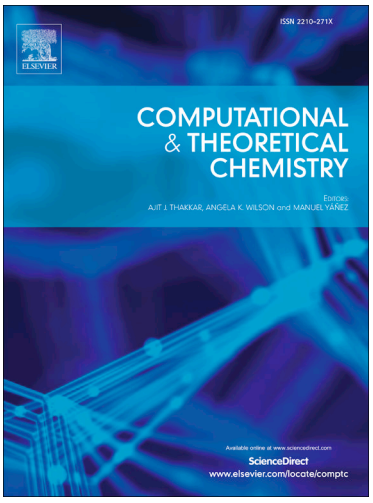

Ab initio molecular dynamics of electron transfer from gallic acid to small radicals: a comparative study between hydroxyl and nitrogen dioxide radicals.

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Ab initio molecular dynamics of electron transfer from gallic acid to small radicals: a comparative study between hydroxyl and nitrogen dioxide radicals.

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Abstract : Gallic acid moiety is found in a large variety of natural molecules and has shown strong radical scavenging properties in vitro. In vivo, it exhibits both prooxidant and antioxidant behavior. This study focuses on the radical scavenging activity of gallic acid towards two radicals: hydroxyl and nitrogen dioxide in aqueous cluster. The reactivity was analyzed by ab initio molecular dynamics using CPMD code. For both radicals, the reaction consists in an electron transfer from gallate anion to the radical. The transfer occurs through water molecules chains forming a loop with the reactants. This study shows that the electron transfer occurs before the formation of adduct. It is the main channel excluding other types of reactivity.

Keywords: