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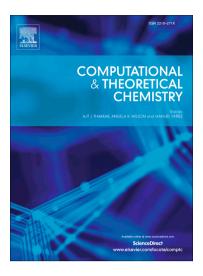
PII: S2210-271X(18)30156-7

DOI: https://doi.org/10.1016/j.comptc.2018.05.002

Reference: COMPTC 2788

To appear in: Computational & Theoretical Chemistry

Received Date: 29 March 2018 Revised Date: 2 May 2018 Accepted Date: 2 May 2018



Please cite this article as: L. Lespade, Ab initio molecular dynamics of electron transfer from gallic acid to small radicals: a comparative study between hydroxyl and nitrogen dioxide radicals., *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.05.002

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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.

Laure Lespade

Institut des Sciences Moléculaires, UMR 5255, Univ. Bordeaux, 351 crs de la Libération, 33400 Talence, France laure.lespade@u-bordeaux.fr

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:

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