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Influence of Nonpolar Medium on Antioxidant Capacity of Bergaptol and Xanthotoxol—Kinetic DFT Study †

Žiko Milanović [1,2,*], Marko Antonijević [2], Jelena Đorović Jovanović [2], Edina Avdović [2], Dejan Milenković [2] and Zoran Marković [2]

[1] Department of Chemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia
[2] Department of Science, Institute for Information Technologies, University of Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Serbia; mantonijevic@uni.kg.ac.rs (M.A.); j.djorovic@uni.kg.ac.rs (J.Đ.J.); edina.avdovic@pmf.kg.ac.rs (E.A.); deki82@kg.ac.rs (D.M.); zmarkovic@uni.kg.ac.rs (Z.M.)
* Correspondence: ziko.milanovic@pmf.kg.ac.rs; Tel.: +381-34-335-039
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Abstract: Within this study, the antioxidant capacity of bergaptol (BER) and xanthotoxol (XAN) in a nonpolar environment (benzene) was investigated against the reference standard trolox (Tx). The ability to inactivate HO• radicals from the kinetic aspect was examined through hydrogen atom transfer (HAT), single-electron transfer–proton transfer (SET-PT), sequential proton loss electron transfer (SPLET) and radical adduct formation (RAF) mechanisms. The rate constants of the chemical reaction were calculated using the conventional transition state theory (TST) and Eckart method (ZCT_0). The research is based on a QM-ORSA (Quantum Mechanics–based test for Overall free-Radical Scavenging Activity) protocol. For this purpose, the *Gaussian 09* software package with the M06-2X/6-311++G(d,p) theoretical model was used. It has been shown that both compounds in benzene can inactivate the HO• radical via HAT and RAF mechanisms. The calculated kinetic parameters indicate that the TST method, in some positions, is not suitable for calculating reaction rate constants at room temperature. Based on relative antioxidant capacity (r^T), both compounds showed better antioxidant capacity than Tx, and it should be emphasized that BER showed better activity than XAN. Based on the relative amount of products (Γ_i) of both compounds, it was concluded that the formation of a radical adduct in positions C-3, C-5, C-8, and C-2' is the most represented.

Keywords: bergaptol; xanthotoxol; QM-ORSA; DFT; kinetic approach

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