

## Abstract

In this research, the kinetics and mechanism of the reaction between the DPPH• radical and two antioxidant compounds (gallic acid and methyl gallate) were investigated in different solvents. For this purpose, kinetic parameters such as pseudo-first-order rate constant, second-order rate constant, hydrogen bond donor ability of antioxidant, and some other parameters related to DPPH• test such as steric accessibility to the DPPH• radical site, IC<sub>50</sub>, the stoichiometry of the reaction were calculated. Studies were performed by monitoring the decrease of DPPH• absorbance in the range of 517-520 nm, at constant DPPH• concentration (~60 μM) and variable concentrations of antioxidants. The values showed a significantly higher second-order rate constant in alcoholic solvents, indicating that the kinetic solvent effects may lead to changes in the reaction mechanism from the main hydrogen atom transfer (HAT) to electron transfer (SPLET), which may be related to the solvent properties such as supporting the antioxidant ionization or regeneration of antioxidant structure by a nucleophilic attack. Exploiting the initial reaction rate and the  $\Delta\text{DPPH}_f/\Delta\text{DPPH}_i$  ratio in each antioxidant, gallic acid and methyl gallate reactions with DPPH• could be divided into three groups: rapid, medium, and slow. The results also showed that the steric accessibility as well as the effect of antioxidant structure and solvent type on the antioxidant closeness to the radical reaction site affect the reaction kinetics dramatically. Finally, methyl gallate showed weaker results than gallic acid regarding the IC<sub>50</sub> and reaction stoichiometry, which this can be related to the steric freedom and better access of gallic acid to the radical reaction site.

**Keywords:** Antioxidant activity, DPPH radical, gallic acid, kinetic, methyl gallate, solvent, steric accessibility.