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THEORETICAL AND EXPERIMENTAL ANALYSIS OF THE ANTIOXIDANT FEATURES OF PHENOL AND ANILINE MODEL COMPOUNDS

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Reactive oxygen and nitrogen species (ROS/RNS) have been implicated in the aging process and numerous diseases including cancer, cardiovascular diseases, neurodegenerative diseases and diabetes. Several natural products such as polyphenols including resveratrol have been investigated as potential antioxidants preventing and/or treating diseases related to oxidative stress. We intend to gain better insight into the mechanism of action of these bioactive molecules and ultimately develop new derivatives with improved antioxidant capacity. Our computational and experimental studies on resveratrol-inspired hydrazone derivatives have shown that an -NH group may act as a better radical scavenger than the phenolic-OH that is commonly found in natural polyphenols. To assess this idea, several simple phenol and aniline derivatives were selected as model compounds and basic structural, energetic and electronic features of these compounds were calculated by density functional theory (DFT) to determine the structural characteristics that has major effect on the radical scavenging activity. The structures were analyzed at the B3LYP/6-31G(d,p) level of theory using Gaussian09 to identify the ionization potential, N-H dissociation enthalpy, proton affinity, HOMO/LUMO energies, and the band gaps. This data was correlated with the experimental antioxidant activity determined in three assays: 2,2-diphenyl-1-picrylhydrazyl (DPPH), 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulphonic acid) (ABTS), and oxygen radical absorbance capacity (ORAC). The % radical scavenging has been analyzed as a function of the above determined structural parameters in order to identify the role of the structural, energetic and electronic features in determining the antioxidant activity.

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