

**P-44****A DFT Study Of Structure-Antioxidant Activity Relationship of a New Series of 2-Methoxybezohydrazide Schiff Bases**

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Natural and synthetic Schiff bases are known for their diverse biological activities and potent antioxidant and free radical scavenging activity. A series of 31 Schiff bases (*e.g.* **2**) were synthesized through the condensation of 2-methoxybenzohydrazide (**1**) and different aldehydes in methanol. The antioxidant activities of these Schiff bases were evaluated by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) test. To rationalize their structure-antioxidant activity relationship, density functional theory (DFT) calculations have been performed at B3P86/6-31+G(d,p) level in gas phase and in solvent using a polarizable continuum model (PCM). Both experimental and DFT results emphasize the importance of the (i) catechol moiety, (ii) number of OH groups, (iii) delocalization of spin density (such as in **3**), and (iv) bond dissociation enthalpies (BDE for a first hydrogen atom transfer and BDE<sub>d</sub> for a second hydrogen atom transfer) in the antioxidant activity of that series of Schiff bases. Thermodynamic and kinetic studies of the reactivity of Schiff bases with free radicals (*e.g.* DPPH and •OOCH<sub>3</sub>) have shown that the coupled proton electron transfer (CP-ET) is the major mechanism to scavenge free radicals due to low free activation barriers as compared to the electron transfer proton transfer (ET-PT) mechanism.

**Keywords:** DFT, antioxidant activity, Schiff bases.

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