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Antioxidant Activity of Some Vanillic Mannich Bases

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The antioxidant activity of newly synthesized Mannich base 2-[1-(*N*-phenylamino)-1-(4-hydroxy-3-methoxyphenyl)]methylcyclohexanone (**MB-H**) and 2-[1-(*N*-4-chlorophenylamino)-1-(4-hydroxy-3-methoxyphenyl)]methylcyclohexanone (**MB-Cl**) was determined by DPPH assay (Figure 1, Table 1).[1] Both investigated compounds interact well with DPPH, and exhibit high activity, slightly lower than the reference compound NDGA. This interaction can be attributed to the common behaviour of phenolic compounds.

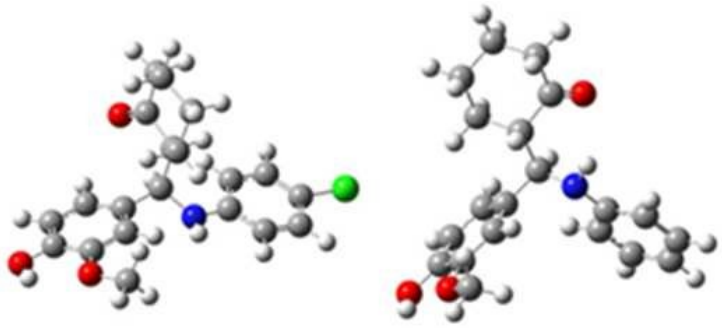

Figure 1. The optimized structures of **MB-Cl** and **MB-H**

Table 1. Interaction of the examined and reference compounds with the stable free radical DPPH

	MB-H		**MB-Cl**		**NDGA**	
concentration (μM)	inhibition (%)					
	20 min	60 min	20 min	60 min	20 min	60 min
100	89.8	91.6	90.9	92.1	96.2	96.2
50	83.6	89.6	87.9	91.7	94.8	95.9
25	72.3	84.9	78.7	86.9	94.1	95.4
IC_{50} (μM)	14.5		11.3			

In order to determine the most probable radical scavenging mechanism Density Functional Theory (m052x/6-311+g(d,p)) was applied (Table 2).[2] It was established that the most probable mechanism is Hydrogen Atom Transfer.

Table 2. Parameters for free radical scavenging activity of the Mannich bases (kJ/mol)

	HAT	SPLET		SET-PT	
	BDE	PA	ETE	IP	PDE
MB-H	339.6	144.3	195.2	367.8	-28.4
MB-Cl	338.8	144.6	194.0	315.4	23.2

(1) Kontogiorgis C., Hadjipavlou-Litina D., *J. Enzym. Inhib. Med. Chem*. **2003**, *18*, 63.
(2) Zhao Y., Schultz N. E., Truhlar D. G., *J. Chem. Theory Comput*. **2006**, *2*, 364.