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THEORETICAL INVESTIGATION INTO THE ANTENNAL RECEPTOR SITE OF THE AMERICAN CORN ROOTWORN DIABROTICA VIRGIFERA VIRGIFERA LECONTI (COLEOPTERA: CHRYSOMELIDAE) FROM THE BEST ATTRACTANT MOLECULE, 4-METHOXYCINNAMALDEHYDE



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## ABSTRACT

highest attractivity to adults of the American western corn rootworm (WCR) Diabrotica virgifera virgifera Leconte. The comparisons of geometry of 4-methoxycinnamaldehyde among other attractive phenylpropanoids can be used to investigate the distance between the antennal receptor sites of WCR adults. Density functional theory (DFT) at pBP level with DN\*\* basis set produced very good accuracy in obtaining the molecular geometry of 4-methoxycinnamaldehyde. The electrostatic charges of the oxygen atom of para-CH<sub>3</sub>O group, the carbon atoms on benzene ring and the carbonyl carbon supported the previous proposed interactions with three receptor sites of WCR adults that the first active site strongly interacted with the oxygen atom of para-CH<sub>3</sub>O group by hydrogen bonding, the second active site interacted with the benzene ring and the third active site interact with the carbonyl carbon by dipole-dipole interaction. The internuclear distances between specific pairs of atoms in the optimized structure of 4methoxycinnamaldehyde were used to estimate the distance between the first and the second active site and the distance between the second and the third active site which were 2.346 Å and 4.910 Å, respectively.