

Molecular Structure of the Analogue of Chalcone C₂₀H₂₂N₁O₃

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The Malaria is a tropical disease that affects about 200 million people per year mainly in Africa, Asia and Brazilian Amazon. It is caused by agents of the genus *Plasmodium* presenting species of the *Plasmodium falciparum* as responsible for the disease in its most severe form and resistant to existing drugs. In order to develop new drugs some compounds of the class of chalcones have shown great potential for the treatment of this disease^{1,2}. In the search for new drugs the analogue of chalcone (1E,4E)-1-(4-nitrophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)-penta-1,4-dien-3-one (Figure 1) was obtained from the coupling of the β -ionona with *p*-nitrobenzaldehyde under the presence lithium hydroxide as catalyst.

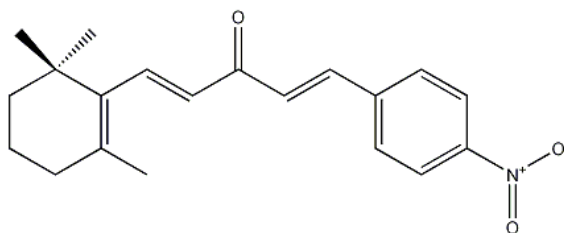


Figure 1: Structural representation of C₂₀H₂₂N₁O₃.

Diffraction data were collected in a CCD diffractometer using MoK α radiation. The structure was solved by Direct Methods and refined on F² by the Least Squares method. Non H atoms were refined anisotropically. All H atoms were placed geometrically. All calculations were performed using the WINGX package^{3,4}. **Crystallographic Data:** a = 11.593(2) Å, b = 11.715(2) Å, c = 14.202(2) Å, $\alpha = \gamma = 90^\circ$ and $\beta = 110^\circ$, Monoclinic, space group P2₁/c, Z = 4, V = 1810.8(4) Å³, d_c = 0.30 Mg.m⁻³. Empiric Formula: C₂₀H₂₂N₁O₃. 1908 measured reflections with 3211 unique and 2166 observed [I > 4 σ (I)]. Final indices R₁ = 0.042 for 226 refined parameters.

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