



Synthesis, Crystal Structure and Hirshfeld Surface Analysis of 1-[5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl]-3-p-tolyl-prop-2-en-1-one

M. K. Usha^{1*}, M. Manjula², Nitin Chandra³, Balakrishna Kalluraya⁴
and D. Revannasiddaiah⁵

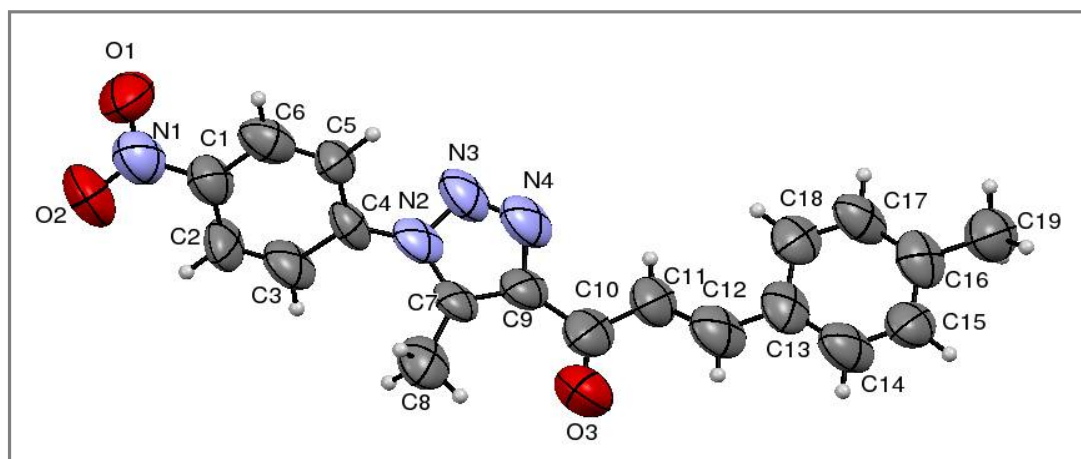
1. P. G. Department of Physics, K. L. E. Society's S. Nijalingappa College, Bengaluru, **INDIA**
2. Department of Physics, Jain University School of Sciences, Bengaluru-560027, Karnataka, **INDIA**
3. Narcotics and Chemistry Division, Karnataka State Forensic Science Laboratory
Bengaluru-560068, Karnataka, **INDIA**
4. Department of Studies in Chemistry, Mangalore University, Mangalore, **INDIA**
5. P. G. Department of Physics, St. Philomena's College (Autonomous), Mysuru, **INDIA**
Email: usha.rao.mk@gmail.com

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ABSTRACT

The title compound 1-[5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl]-3-p-tolylprop-2-en-1-one is synthesized and the structure was confirmed by HNMR, IR, and single crystal X-ray diffraction. The title compound is a chalcone derivative which is known for potential pharmacological activities. The compound crystallizes in the monoclinic space group $P21/c$ with cell parameters $a=8.2925(8)$ Å, $b=13.4045(12)$ Å, $c=15.5791(14)$ Å, $\alpha=90^\circ$, $\beta=94.584(5)^\circ$, $\gamma=15.5791(14)^\circ$, $Z=4$ at 293 K. Hirshfeld surface analysis shows that the major intermolecular interaction is due to H...H contacts.

Graphical Abstract



ORTEP diagram of the title compound

Keywords: Crystal structure, X-ray crystallography, Hirshfeld surface analysis, Chalcones, Triazoles, fingerprint plots.