**DFT CALCULATIONS, HIRSHFELD SURFACE ANALYSIS AND MOLECULAR DOCKING STUDIES OF (1E,4E)-1,5-BIS (4-ETHOXYPHENYL) PENTA-1,4-DIEN-3-ONE**

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| **ABSTRACT**  Monocarbonyl analogues of curcumin are among the pharmaceutical scaffolds exhibiting a range of pharmacological actions, such as antibacterial, anticancer, antioxidant, and antityrosinase properties [1]. In this study, quantum chemical electronic structure, Hirshfeld surface and molecular docking studies of (1E,4E)-1,5-Bis(4-toxyphenyl)penta-1,4-dien-3-one that is a curcumin analogue were performed. The intermolecular interactions were analyzed using the Hirshfeld surface method. In order to understand molecular stability, quantum chemical descriptors calculated at the time-dependent density functional theory (TD-DFT) were investigated by visualization of frontier molecular orbitals. All calculations of the compound were conducted with the Gaussian16W package program [2] at the three-parameter hybrid functional of Becke based on the correlation functional of Lee, Yang, and Parr (B3LYP). Quantum chemical calculations show good agreement between calculated and experimental parameters obtained from the literature. The antibacterial activity of the title compound docked into the active sites of the target protein was studied from docking parameters.  **References:**  [1] Chantrapromma S.,Ruanwasa P., Boonnak N. (2016). Synthesis, Antityrosinase Activity of Curcumin Analogues, and Crystal Structure of (1E,4E)-1,5-Bis(4-ethoxyphenyl)penta-1,4-dien-3-one, *Crystallography Reports*, 61, 1081–1085.  [2] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016. |

# Keywords: DFT, Hirshfeld Surface Analysis, Molecular Docking, HOMO-LUMO.