**Single crystal, density functional theory, biological and sensor studies of (*E*)-2-[(3,5-bis(trifluoromethyl)phenylimino)methyl]-4,6-dichlorophenol**

**C.T. Zeyrek1, B. Boyacıoğlu2, N. Demir3, Y. Tümer4, A. Kiraz5, M. Yıldız6, H. Ünver7**

*1Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, TR-06100 Besevler-Ankara, Turkey*

*2Vocational School of Health Services, Ankara University, TR-06290 Kecioren-Ankara, Turkey*

*3Department of Biology, Faculty of Arts and Sciences, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey.*

*4Department of Chemistry, Faculty of Science, Karabük University, TR-78050 Karabük, Turkey.*

*5Near East University, Ataturk Faculty of Education, Nicosia, Mersin TR-10 Turkey.*

*6Department of Chemistry, Faculty of Arts and Sciences, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey.*

*7Department of Physics, Faculty of Science, Ankara University, TR-06100 Beşevler-Ankara, Turkey*

*E*-mail:  [Huseyin.Unver@ankara.edu.tr](mailto:myildiz@comu.edu.tr)

We report here the synthesis and characterization, biological activity, antioxidant activity, colorimetric anion sensors properties, and computational density functional theory (DFT) study of a novel Schiff base (*E*)-2-[(3,5-bis(trifluoromethyl)phenylimino)methyl]-4,6-dichlorophenol. The molecular structure of the title compound was experimentally determined by using X-ray single-crystal data and was compared to the structure predicted by theoretical calculations using DFT. The antimicrobial activities of the title compound have been studied for their minimum inhibitory concentrations (MIC) against some bacteria and fungi. Besides, we have examined the interaction of the title compound with DNA by UV-Vis and agarose gel electrophoresis methods. The antioxidant activity of the compound was measured by the DPPH method, and its activity was found to be lower than butylated hydroxytoluene (BHT). Also, the colorimetric response of the Schiff base receptors in DMSO has been investigated before and after the addition of the equivalent amount of each anion to evaluate the anion recognition properties

1. Alorabi, A. Q., Abdelbaset, M., and Zabin, S. A., Chemosensors,  2020, vols. 8, p. 1. [doi.org/10.3390/chemosensors8010001](https://doi.org/10.3390/chemosensors8010001)
2. Barare, B., Yıldız, M., Alpaslan, G., Dilek, N., Ünver, H., Tadesse, S., and Aslan, K., *Sens. Actuators B Chem.,* 2015, vols. 215, p. 52. [doi.org/10.1016/j.snb.2015.03.025](https://dx.doi.org/10.1016/j.snb.2015.03.025)
3. Ünver, H., Boyacıoğlu, B., Zeyrek, C. T., Yıldız, M., Demir, N., Yıldırım, N., Karaosmanoğlu, O., Sivas, H., and Elmalı, A., *J. Mol. Struct.,* 2016, vols. 1125, p. 162. [doi.org/10.1016/j.molstruc.2016.06.058](https://dx.doi.org/10.1016/j.molstruc.2016.06.058)