THEORETICAL CALCULATIONS, BIOLOGICAL ACTIVITIES, ANION SENSING APPLICATIONS AND CRYSTALLOGRAPHIC STUDIES OF (E)-2-((3,5-BIS (TRIFLUOROMETHYL) PHENYLIMINO) METHYL)-4,6-DIMETHOXYPHENOL

[1]BAHADIR BOYACIOGLU, [2]HUSEYİN UNVER, [3]MUSTAFA YILDIZ, [4]NESLİHAN DEMIR, [5]NURAY YILDIRIM, [6]CELAL TUGRUL ZEYREK, [7]AYHAN ELMALI

[1]Vocational School of Health Services, Ankara University, TR-06290 Keçioren-Ankara, Turkey
[2]Department of Physics, Faculty of Science, Ankara University, 06100 Beşevler-Ankara, Turkey
[3]Department of Chemistry, Faculty of Arts and Sciences, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey
[4]Department of Biology, Faculty of Arts and Sciences, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey
[5]Vocational School of Health Services, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey
[6]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, TR-06100 Ankara, Turkey
[7]Department of Physics Engineering, Faculty of Engineering, Ankara University, 06100 Beşevler-Ankara, Turkey
E-mail: [1]bboyacioglu@ankara.edu.tr, [2]huseyin.unver@ankara.edu.tr, [3]myildiz@comu.edu.tr, [4]neslihandemir@comu.edu.tr, [5]ny.nuray@gmail.com, [6]ctzeyrek@gmail.com, [7]elmali@eng.ankara.edu.tr

Abstract- We report the synthesis of (E)-2-((3,5-bistrifluoromethyl)phenylimino)methyl)-4,6-dimethoxyphenol from the reaction of 3,5-bismethoxysalicylaldehyde with 3,5-bistrifluoromethylaniline.The molecular structure of the title compound was experimentally determined using X-ray single-crystal data and was compared to the structure predicted by theoretical calculations using density functional theory (DFT). In addition, nonlinear optical (NLO) effects of the title compound was predicted using DFT. Theoretical and UV-VIS spectroscopy studies of the interactions between the title compound and calf thymus DNA (CT-DNA)showed that the title compound interacts with CT-DNA. The colorimetric response of the title compound in DMSO to the addition of equivalent amount of anions (F^-, CN^-, $H_2PO_4^-$, OH^-, Br^-, I^-, SCN^-, ClO_4^-, HSO_4^- N_3^- and AcO^-) was investigated.
This study is supported by a grant (Project Number: TÜBİTAK 115F253) from the Scientific and Technical Research Council of Turkey.

Keywords- Density Functional Theory, 3,5-Bismethoxysalicylaldehyde, X-ray Crystallography, Calf Thymus-DNA.