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Author: Belygona Barare Mustafa Yıldız Gökhan Alpaslan Nefise Dilek Hüseyin Ünver Solomon Tadesse Kadir Aslan

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ACCEPTED MANUSCRIPT

2	anion sensing applications of 1-[(E)-[(6-methoxy-1,3-benzothiazol-2-yl)imino]methyl]naphthalen-2-ol
4 5 6	Belygona Barare ^a , Mustafa Yıldız ^{b,c,*} , Gökhan Alpaslan ^d , Nefise Dilek ^e , Hüseyin Ünver ^f , Solomon Tadesse ^a and Kadir Aslan ^{a,*}
7 8	^a Morgan State University, Department of Chemistry, 1700 East Cold Spring Lane, Baltimore, MD 21251, USA
9 0	^b Department of Chemistry, Faculty of Arts and Sciences, Çanakkale Onsekiz Mart University, 17100 Çanakkale, Turkey
1	^c Nanoscience and Technology Research and Application Center (NANORAC), Çanakkale Onsekiz Mart University, Çanakkale, Turkey
3	^d Department of Medical Services and Techniques, Vocational School of Health Services, Giresun University, TR-28200 Giresun, Turkey
5	^e Department of Physics, Faculty of Arts and Sciences, Aksaray University, Aksaray, Turkey
6 7	f Department of Physics, Faculty of Science, Ankara University, 06100 Besevler, Ankara, Turkey
8	*Corresponding Authors: <u>myildiz@comu.edu.tr</u> and <u>kadir.aslan@morgan.edu</u>
9	ABSTRACT
20	We report the synthesis of a Schiff base 1-(E)-[(6-methoxy-1,3-benzothiazol-2-
21	yl)imino]methyl]naphthalen-2-ol from the reaction of 2-hydroxy-1-naphtaldehyde with 2-
22	amino-6-methoxybenzothiazole. The molecular structure of the title compound was
23	experimentally determined using X-ray single-crystal data and was compared to the structure
24	predicted by theoretical calculations using density functional theory (DFT). In addition,
25	nonlinear optical (NLO) effects of the title compound was predicted using DFT. The
26	colorimetric response of the title compound in DMSO to the addition of equivalent amount of
27	anions (F, CN, H ₂ PO ₄ , OH, Br, I, SCN, ClO ₄ , HSO ₄ , N ₃ and AcO) was investigated. In
28	this regard, while the addition of F-, CN-, H ₂ PO ₄ -, OH-, and AcO- anions into the solution
9	containing the title compound resulted in a significant color change, the addition of Br-, I-,
80	SCN ⁻ , ClO ₄ ⁻ , HSO ₄ ⁻ and N ₃ ⁻ anions resulted in no color change. The most discernable color
31	change in the title compound was caused by CN-, which demonstrated that the title compound
32	can be used to selectively detect CN The order of anion-binding power of the title compound
3	was determined to be OH->CN->F-~AcO->H2PO4 The interactions between the receptor and
34	anions were investigated using ¹ H-NMR titration method. Theoretical and UV-VIS

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