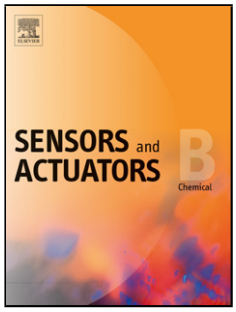

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Synthesis, characterization, theoretical calculations, DNA binding and colorimetric anion sensing applications of 1-[(*E*)-[(6-methoxy-1,3-benzothiazol-2-yl)imino]methyl]naphthalen-2-ol

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ABSTRACT

We report the synthesis of a Schiff base 1-(*E*)-[(6-methoxy-1,3-benzothiazol-2-yl)imino]methyl]naphthalen-2-ol from the reaction of 2-hydroxy-1-naphtaldehyde with 2-amino-6-methoxybenzothiazole. 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. 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. In this regard, while the addition of F^-, CN^-, $H_2PO_4^-$, OH^-, and AcO^- anions into the solution containing the title compound resulted in a significant color change, the addition of Br^-, I^-, SCN^-, ClO_4^-, HSO_4^- and N_3^- anions resulted in no color change. The most discernable color change in the title compound was caused by CN^-, which demonstrated that the title compound can be used to selectively detect CN^-. The order of anion-binding power of the title compound was determined to be $OH^->CN^->F^-\sim AcO^->H_2PO_4^-$. The interactions between the receptor and anions were investigated using ^{1}H-NMR titration method. Theoretical and UV-VIS