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Colorimetric anion sensors based on positional effect of nitro group for recognition of biologically relevant anions in organic and aqueous medium, insight real -life application and DFT studies

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Abstract

A new six colorimetric receptors A1-A6 were designed and synthesized, characterized by typical common spectroscopic techniques like FT-IR, UV-Visible, ^{1}H NMR, ^{13}C NMR and ESI-MS. The receptor A1 and A2 exhibit a significant naked-eye response towards F^- and AcO^- ions in DMSO. Due to presences of the NO_2 group at para and ortho position with extended π-conjugation of naphthyl group carrying -OH as a binding site. Compared to receptor A2, A1 is extremely capable of detecting F^- and AcO^- ions present in the form of sodium salts in an aqueous medium. This is owed to the occurrence of $–NO_2$ group at para position induced in increasing the acidity of -OH proton. Consequently, it easily gets deprotonated in aqueous media. The detection limit of receptor A1 was turned out to be 0.40 and 0.35 ppm for F^- and AcO^- ions which is beneath WHO permission level (1.0 ppm). Receptor A1 shows a solitary property of solvatochromism in different aprotic solvents in presence of AcO^-ion. Receptor A1 depicts high selectivity towards AcO^-ion in DMSO: HEPES buffer (9:1, v/v). Receptor A1 proved itself for real life application by detecting anion in solution and solid state. The binding mechanism of receptor A1 with $AcO^-$and F^- ions was monitored from ^{1}HNMR titration and DFT study.

Keywords: Fluoride; Acetate; Sensor; Coloimetric; DFT calculation