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Structural analysis, theoretical studies, and chemosensing properties of novel 2-hydroxy naphthalene based hydrazide as highly selective and sensitive turn-on fluorescent probe for detection of Al^{3+}

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ABSTRACT

In solvent methanol, ethylcarbazate and 2-hydroxy-naphthaldehyde were stirred in the presence of catalytic amounts of glacial acetic acid to synthesise the target chemical ethyl (Z)-2-((2-hydroxynaphthalen-1-yl)methylene)hydrazine-1-carboxylate (HL). The structure of the target compound $C_{14}H_{14}N_2O_3$, has been determined by X-ray crystallographic analysis and crystallizes in monoclinic crystal system with P21/c space group possessing one molecules per asymmetrical unit, with unit cell dimensions a=14.675(4) Å, b=5.8089(11) Å, c=16.497(4), β= 112.758(9)°. Characteristic feature of crystal packing is the existence of hydrogen bonding followed by CH…Pi, lp…Pi and Pi…Pi stacking interactions. Hirshfeld surface analysis, which includes the assessment of several energy frameworks reveals that the molecular sheets are mainly composed of hydrogen bonds, and their stability is predominantly influenced by the electrostatic energy contribution. Investigation of binding test indicated that probe HL could sensitively and selectively detect Al^{3+} ion with striking fluorescent signalling responses in methanol solvent. Results from Job's plot, UV–Vis titration, fluorescent titration, and IR experiments indicated a 1:1 binding ratio between probe HL and Al^{3+}, with a binding constant of 1.57 $\times 10^5$ M^{-1}. The optimized structure and electronic transitions were confirmed by DFT and TD-DFT studies utilizing wB97XD/def2tzvp level of theory with the solvation model of SMD in methanol. Probe HL undergoes ESIPT upon complexation and excitation and the shoulder band located around 426 nm is due to the radiative decay of enol (S1) while the longer-wavelength emission (445 nm) is from keto form (S1). Probe HL exhibits excellent selectivity and reversibility feature towards sequential detection of Al^{3+} ions. The limit of detection for Al^{3+} is 8.08 $\times 10^{-8}$ M, which is significantly lower than the US EPA and FDA standard of 7.41 μM Al^{3+} for bottled drinking water and low for the detection of Al^{3+} ions when compared to literature studies.

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