Title:	Design and Development of Fluorescent Sensors with Mixed Aromatic Bicyclic Fused Rings and Pyridyl Groups: Solid Mediated Selective Detection of 2,4,6-Trinitrophenol in Water
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Keywords:	Picric Acid Metal-Organic Frameworks Aromatic Nitro Compound Hydrocarbons, Aromatic compounds,
Issue Date:	2018
Publisher:	American Chemical Society
Citation:	ACS Omega, 3(3), pp. 3248–3256
Abstract:	For a strategic incorporation of both π-electron-rich moieties and Lewis basic moieties acting as hydrogen bonding recognition sites in the same molecule, two new fluorescent sensors, N,N′-bis(anthracen-9-ylmethyl)-N,N′-bis(pyridin-2-ylmethyl)butane-1,4-diamine (banthbpbn, 1) and N,N′-bis(naphthalen-1-ylmethyl)-N,N′-bis(pyridin-2-ylmethyl)butane-1,4-diamine (bnaphbpbn, 2), have been developed for the selective detection of highly explosive 2,4,6-trinitrophenol (TNP) in water. Each of the two identical ends of these sensors that are linked with a flexible tetra-methylene spacer contains a mixed aromatic bicyclic fused ring (anthracene or naphthalene) and a pyridyl group. These are synthesized via the simple reduced Schiff base chemistry, followed by the nucleophilic substitution reaction under basic conditions in high yields. Both 1 and 2 were characterized by Fourier transform infrared, UV–vis, and NMR (1H and 13C) spectroscopy, and high-resolution mass spectrometry. The bulk phase purity of 1 and 2 and their stability in water were confirmed by powder X-ray diffraction (PXRD). Utilizing the effect of solvents on their emission spectra as determined by fluorescence spectroscopy, spectral responses for 1 and 2 toward various nitro explosives were recorded to determine a detection limit of 0.6 and 1.6 ppm, respectively, for TNP in water via the “turn-off” quenching response. Also, the detailed mechanistic investigation for their mode of action through spectral overlap, lifetime measurements, Stern–Volmer plots, and density functional theory calculations reveals that resonance energy transfer and photoinduced electron transfer processes, and electrostatic interactions are the key aspects for the turn-off response toward TNP by 1 and 2. In addition, the selectivity for TNP has been found to be more in 1 compared to 2. Both exhibit good recyclability and stability after sensing experiments, which is confirmed by PXRD and field-emission scanning electron microscopy.
URI:	https://pubs.acs.org/doi/abs/10.1021/acsomega.8b00080 (https://pubs.acs.org/doi/abs/10.1021/acsomega.8b00080) http://hdl.handle.net/123456789/2210 (http://hdl.handle.net/123456789/2210)
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