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Aggregation induced emissive pyrimido fused tetraphenylethene benzothiazole probe for sensitive and selective detection of Fe^{3+} ions

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The synthesis and photophysical properties of a novel pyrimido fused benzothiazole-tetraphenylethene (TPE-1) chromophore, incorporating both electron-donating ($-SCH_3$) and electron-withdrawing (–CN) groups, are reported. TPE-1 exhibits aggregation-induced emission (AIE), mechanochromic, and electrochemical characteristics. The recognition behavior of TPE-1 towards various metal cations is investigated by fluorescence spectroscopy. TPE-1 shows a selective and sensitive response towards ferric (Fe^{3+}) ion over other tested cations in DMSO: water (90:10, *v/v* ratio) with a limit of detection of 102 nM. Time-correlated single photon counting (TCSPC) plot displays dynamic and static quenching of TPE-1 with the addition of Fe^{3+} ions. Computational studies have been performed to demonstrate the binding mode of TPE-1 towards Fe^{3+} ions. Most importantly, the application of TPE-1 in the detection of Fe^{3+} ions in various water sources showcases its promising utility in environmental monitoring and pollution control, underscoring its potential for substantial contributions to environmental chemistry and sensor technology.

Keywords: Benzothiazole, Tetraphenylethylene, Pyrimido, Fe^{3+} ions, Sensor