

Molecular Interactions Driven Pyridoindole Based Materials for Switchable Fluorescence and Chemo/ Bio-Sensing

Bahadur Sk^a, Pilendra K Thakre^b, Raghuvir Singh Tomar^b and Abhijit Patra^{a*}

^aDepartment of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal

^bDepartment of Biological Sciences, Indian Institute of Science Education and Research (IISER) Bhopal

Development of new functional molecules and materials with pre-defined properties employing simple chemical methods is significant both from fundamental and application perspectives.¹ Our earlier study established biologically important heterocycle, pyrido[1,2-a]indoles (PI), as a new class of fluorophore with promising potential in cell imaging.² However, this molecule shows complete quenching of fluorescence in water as well as in aggregated phase. To augment the fluorescence properties of PI in the solid state, we coupled it with a classic aggregation induced emission (AIE) active core of tetraphenylethylene (TE). A simple Schiff base condensation involving PI and TE unit results strong π - π stacked non-fluorescent PITE1 (Fig. 1a). Circumventing the problem of planarity and π - π stacking in PITE1, we synthesized a C-C coupled molecule, PITE2 (Fig. 1b), exhibiting strong emission in the solution, nanoparticle, and solid state. The crystal structure analysis of PITE2 indicates multiple C-H... π and C-H...H-C intra/intermolecular interactions rigidifying the molecule in aggregated state leading to strong fluorescence.³ The lone pair of electrons on nitrogen in PITE2 involve in conjugation and responsible for pH-sensitive fluorescence. The presence of four propyl groups and multiple phenyl rings make PITE2 substantially hydrophobic and established it as lipid droplets (LDs) targeting bioprobe in multiple cell lines. Thus, PITE2 is a promising molecular optical material for pH-based sensing and lipid droplets tracking.

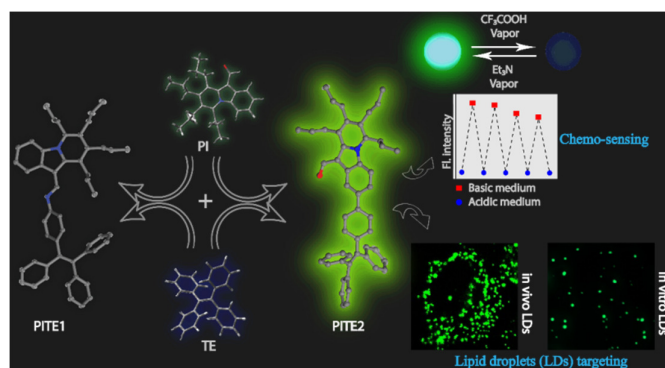


Fig 1: Schematic illustration of pyridoindole based molecules and their applications.

References:

1. Mei, J.; Leung, N. L. C.; Kwok, R. T. K.; Lam, J. W. Y.; Tang, B. Z. *Chem. Rev.* **2015**, *115*, 11718-11940.
2. Samala, S.; Pallavi, P.; Kumar, R.; Arigela, R. K.; Singh, G.; Ampapathi, R. S.; Priya, A.; Datta, S.; Patra, A.; Kundu, B. *Chem. Eur. J.* **2014**, *20*, 14344 – 14350.
3. Sk, B.; Patra, A. *Cryst Eng Comm.* **2016**, *18*, 4290-4294.