Dual State Fluorescence Emissive Fluorinated Pyrimido[5,4-*h*]quinazolines: Synthesis, Structure, and Photophysical and Halochromic Properties

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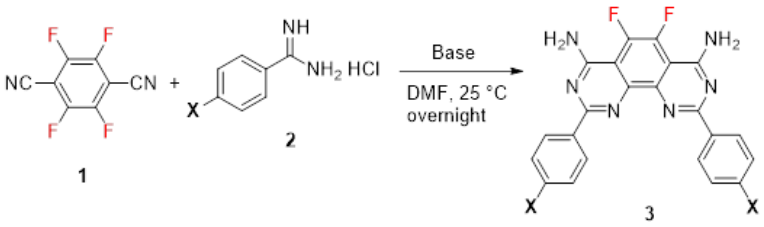
A series of the novel tricyclic fluorophore with the core moiety pyrimido[5,4-*h*]quinazoline (**3**), has been designed and synthesized via the condensation reaction of tetrafluoroterephthalonitrile and derivatives of benzimidamine hydrochloride in presence of base. To address the need for a fluorophore with enhanced stability, selectivity, and versatility across various applications, this new compound incorporates additional nitrogen atoms, offering superior performance to traditional fluorophores like 1,10-phenanthroline. Mechanistic insights emphasized the importance of selecting a suitable base to guarantee its efficiency and success.

NMR and single-crystal X-ray studies confirmed the structure of **3**, while spectroscopic measurements showed that these fluorophores are dual-state (solution and solid-state) emissive under UV-visible light. Photophysical studies highlighted the red-shifted fluorescence spectra in the solid state rather than the solution state. Further investigation revealed the formation of aggregates in the solid state. DFT calculations showed that the electron-withdrawing capability of **3** stabilized the energy levels. Electrochemical properties were also investigated, which were in good agreement with the results of DFT calculations. High decomposition temperature in the TG-DTA experiment proved the thermal stability of **3** at elevated temperatures. Due to the presence of protonable protons in **3**, it gave the positive Halochromism.[1] These fluorophores are anticipated to have enhanced chelation, leading to more stable metal complexes, which will increase their potential applications for further studies in future.



1) S Kothavale, N. Sekar, *Dyes and Pigments*. **2017**, *136*, 31-45.