**A feasible sulphur-atom engineering in peryleneimides: a conformational tweak to boost luminogen characteristics, efficient photosensitizer for the effective photodynamic anticancer therapy**

Mst Nasima Khatun, Parameswar Krishnan Iyer\*

\*Department of Chemistry, Indian Institute of Technology Guwahati, Assam, India.

\*Centre for Nanotechnology, Indian Institute of Technology Guwahati, Assam, India.

Email of Author: *nasim176122016@iitg.ac.in*

**Abstract:**

A novel yet simple design strategy of sulphur (S)-atom engineering, a conformational tweak regulate the potential condensed state emission (with large stoke shift >140 nm) and prominent photosensitization characteristics. In this contribution, S-atom has been intentionally incorporated into the functional group in planar rigid peryleneimide (**PNI**) to block the notorious π-π stacking interaction and potentially alter the aggregation caused quenching (ACQ) fluorophores to aggregation induced enhanced emission (AIEE) luminogens. Hertein, **API** AIEEgen perform efficient biomimaging characteristics due to its spontaneously formed micrrose assemebly. Besides, the regulation of the ACQ-to-AIEE characteristics, the S-atom engineering at the carbonyl positions in **PNI** such as **PPI, THPI** and **API** form thiobased **PNI** (**PNIS)** such as **PPIS, THPIS** and **APIS** that leads to totally quench its emission (photoluminescence quantum yield ,ΦPL ≈ 0) in their condensed state, revealed higher reactive excited triplet formation. Interestingly, **THPIS** shows efficient photodynamic therapy (PDT) effect due to its enhanced donor-acceptor strength via Type 1 and Type 2 mechanisms in cancer cell with minimal side effects towards normal cell upon white light irradiation that opens up a new approach for both hypoxia and normoxia tumor treatment. Thus, this precise conformational tweaking of S-atom into the functional unit and at the carbonyl position could be the key hypothesis for the ACQ-to-AIEE transformation for potential practical application including bioimaging**,** as well as to achieve efficient PDT in future, respectively.

**Keywords:** AIEE, PDT, Type 1 and Type 2 PS