# ABSTRACT

Energy resources and their availability is closely linked to stability and a sustainable economy of any country. Recent advancements in π-conjugated semiconducting materials have demonstrated their promise as essential components for developing efficient light-based devices, whether for light harvesting in solar cells or light emitting in OLEDs. The introduction of materials like Y6 has catalyzed numerous innovative designs, and this trend continues to evolve. Each year brings new discoveries, and the exploration of various molecular architectures—from fullerenes to non-fullerene, fused to non-fused and symmetrical to asymmetrical designs. In response to current research trends, this study presents a novel quinoxaline (Qx) molecular system, designated as (Z)-2-(2-((11,12-bis(2-ethylhexyl)-11,12-dihydrothieno[2',3':4,5]pyrrolo[3,2-f]thieno [2',3':4,5] pyrrolo[2,3-h] quinoxalin-2-yl) methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile. This unique structure has the potential to serve as a versatile starting material for a variety of new molecules. The progress in synthesizing this compound is clearly characterized through rigorous physical characterization techniques, ensuring the purity of each step via column chromatography. Additionally, computational analysis has been conducted in comparison with its benzothiadiazole (BT) analogue to explore its potential advantages over the commonly utilized BT core. This comprehensive approach highlights the exciting possibilities that lie ahead in the field of organic semiconductors.



**Key words:**

Quinoxaline, Benzothiadiazole, Organic solar cells, photovoltaic, asymmetry