Due to over exploitation of minerals, depletion of non-renewable energy sources and energy crisis, alternative and sustainable pathways are getting attention such as renewable sources of energy. Photovoltaic technology, including solar cells of many types like OSCs, perovskite solar cells, polymer solar cells and dye-sensitized cells is potential candidate for eco-friendly conversion of solar energy from sun into electrical energy. With development of NFAs, PCE of organic solar cells has reached 20%. Key objective of this study is designing and synthesis of non-fused NFAs based on benzothiadiazole as core material to analyze their applications and performance in photovoltaic activity. The molecular properties and electronic behavior of BTD-based NFAs are predicted with the use of computational modelling, which can shed light on the potential of these NFAs to optimize charge transport and light absorption. Computational analysis of compound E1 and E2 based on optimization of geometry, DFT calculation, molecular electrostatic potential, TD-DFT calculation based transition density matrix, physio-chemical parameters and global chemical reactivity discriptors, demonstrates the optoelectronic properties of both compounds and better photovoltaic performance of E1 due to small energy gap and better charge transfer. In synthetic approach, BTD based core is used to synthesize novel non-fused ring non-fullerene acceptors via multi-step synthesis. Due to adjustability in molecular design and electron-withdrawing nature, benzothiadiazole core based acceptors have excellent performance in photovoltaic and better PCE. UV-visible spectra confirm the formation of targeted compounds with extended conjugation. In FT-IR spectrum analysis, the presence of distinct peaks confirms the presence of discrete functionalities in newly synthesized compounds. These materials have better performance, more efficient and stable and so, are good candidates for high-performance organic photovoltaic.