Quinoline-fused BODIPYs

Li et al. describe the synthesis and properties of a type of compound known as quinoline-fused BODIPYs.

Synthesis: The quinoline-fused BODIPYs were synthesized through a series of chemical reactions. The process involved two main steps:

Reduction of nitrophenyl-substituted BODIPYs: Initially, nitrophenyl-substituted BODIPY molecules were reduced. This step likely involved the conversion of nitro groups (NO2) to amino groups (NH2).

Pictet-Spengler cyclization: After the reduction step, the molecules underwent a Pictet-Spengler cyclization reaction. This type of reaction typically involves the formation of a ring structure, often involving nitrogen atoms, in the molecule.

Structure: The resulting compounds had a unique structure consisting of a BODIPY core (a specific type of organic dye) fused with quinoline rings. This fusion of the BODIPY core with quinoline rings led to a distinctive molecular conformation. The key characteristic of this conformation was that it was significantly twisted, with an approximately 20.0° deviation from coplanarity. This information was determined through X-ray crystal structure analysis.

Properties: These quinoline-fused BODIPYs displayed several noteworthy properties:

Reduced LUMO (Lowest Unoccupied Molecular Orbital): The lowest unoccupied molecular orbital is an energy level important in the context of electronic properties. The quinoline-fused BODIPYs had a reduced LUMO, indicating specific electronic properties that could be advantageous for certain applications. Redshifted Absorption/Emission Bands: The absorption and emission spectra of these compounds were shifted toward longer wavelengths (redshifted), which can be significant in applications like light absorption or emission. High Molar Extinction Coefficients: This indicates that these compounds efficiently absorb light, which can be crucial in applications such as photodynamic therapy or light-harvesting materials.

Reactive Oxygen Species (ROS) Generation Efficiency: The compounds showed a satisfactory ability to generate reactive oxygen species, with an efficiency level of up to 0.56. ROS are chemically active molecules and are often important in biological and photodynamic applications.

Potential Use as Photosensitizers: The unique combination of properties in these quinoline-fused BODIPYs makes them promising candidates for use as photosensitizers. Photosensitizers are compounds that can absorb light energy and convert it into reactive species, often used in medical and environmental applications, particularly in the context of photodynamic therapy and pollution control.

In summary, the study describes the synthesis of quinoline-fused BODIPY compounds with distinct twisted conformations and various desirable properties, making them potentially useful as photosensitizers in applications where heavy-atom-free compounds are preferred [1].

1)
Li W, Gong Q, Wu Q, Guo L, Guo X, Guo D, Jiao L, Hao E. Pictet-Spengler synthesis of twisted quinoline-fused BODIPYs as heavy-atom-free photosensitizers. Chem Commun (Camb). 2023 Sep 27. doi: 10.1039/d3cc04460b. Epub ahead of print. PMID: 37753618.