Substituted BODIPYs for PDT and bioimaging

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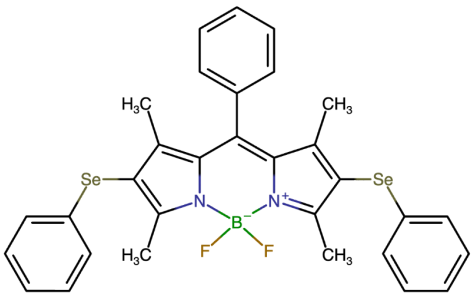
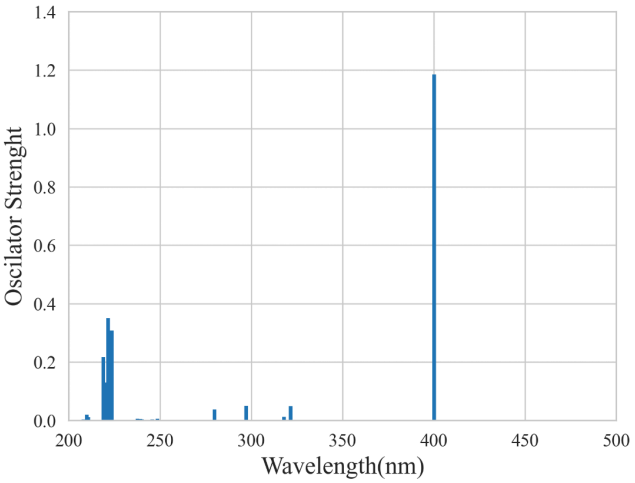
Photodynamic therapy (PDT) is a selective and minimally invasive treatment that destroys target cells by irradiating a photosensitizer with light, generating highly reactive oxygen species (ROS). Key properties of photosensitizers for cancer treatment include the efficiency to generate reactive oxygen species and good biocompatibility. Some photosensitizers are also used as bioimaging probes due to their bright fluorescence and emission in the near-infrared(NIR) [1]. Recent research focuses on developing high-performance photosensitizers able to be used simultaneously for PDT and bioimaging, allowing real-time monitoring of tumor response. Bioimaging excites the photosensitizer at 400 nm, while it requires excitation between 600-800 nm to generate ROS. We seek a photosensitizer that can absorb in both regions. In this sense, BODIPY is a class of compounds that present high fluorescence, great photostability and are highly versatile regarding its derivatives. In this work, we used TD-DFT and DLPNO-CCSD(T) to compare the emission and Stokes shift of a known 2,6-BODIPYs containing Selenium and other substitutes [2]. The selenium BODIPY shows a strong absorption in 400nm.





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