PHOTOPHYSICAL AND PHOTOTHERMAL PROPERTIES OF AGGREGATED BODIPY DYES FOR ANTIMICROBIAL APPLICATIONS

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The recent spreading of nanomedicine has boosted the search for suitable molecular platforms for applications in photodynamic therapy and photopharmacology. Molecular aggregates, obtained by self-assembly of different dyes often have peculiar spectroscopic properties, which make them suitable candidates for antimicrobic applications. [1]

Six BODIPYs functionalized with a crown ether and charged species are proposed, divided into two families based on the presence or absence of two bromine atoms. Their spectroscopic properties were firstly investigated in acetonitrile. The non-brominated compounds exhibit good fluorescence yields while the brominated counterparts show significantly reduced emission yields due to triplet formation (Φ_Δ 17-59%). Transient absorption spectroscopy confirmed this finding, revealing triplet formation in less than 1 ns for the brominated compounds and possible charge transfer between the BODIPY core and the appended crown ether for all the investigated compounds.

These water-insoluble BODIPYs were then studied in mixed acetonitrile-water solutions with varying acetonitrile-water ratios (from 1:10 to 1:100). Water addition lead to aggregates formation, as confirmed by the broadening of absorption bands and a significant red shift. Transient absorption spectroscopy revealed accelerated decay kinetics as compared to what observed in acetonitrile. Triplet formation was no longer observed for the aggregates indicating the quenching of the heavy atom effect upon aggregation. The aggregate morphology was characterized with SEM microscopy, revealing the formation of spherical particles, with dimensions of around 100 nm

The photothermal efficiency of the compounds was then evaluated allowing the calculation of the photothermal conversion efficiency. The obtained values, ranging from 70 to 98% confirm that the presence of the heavy atom is not a key factor for their photothermal conversion ability, paving the way for the development of bio-compatible antimicrobial compounds. Finally, the biological activity of one of these BODIPYs was successfully evaluated through preliminary tests on bacterial cultures; further measurements will be carried out.

REFERENCES

[1] Y. Dai, J. Sun, X. Zhang, J. Zhao, W. Yang, J. Zhou, Z. Gao, Q. Wang, F. Yu, and B. Wang, "Supramolecular assembly boosting the phototherapy performances of BODIPYs," Coordination Chemistry Reviews, vol. 517, p. 216054, 2024.