BENZOTHIAZOLE ANALOGUES OF BODIPY DYES WITH A QUADRUPOLAR (D-π-A-π-D) ARCHITECTURE FOR BIOIMAGING

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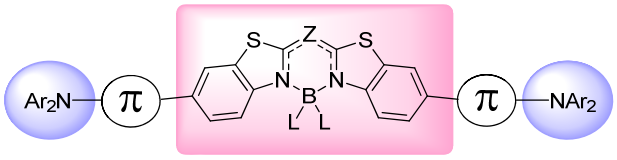
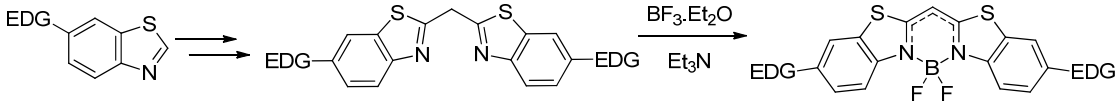
BODIPY dyes are frequently employed as fluorescent markers but they find use also in various optoelectronic applications.[1,2] We prepared a hitherto unexplored series of donor-substituted bis(benzothiazole)methanes and corresponding BODIPY-like dyes with a quadrupolar (D-π-A-π-D) setup, which are predicted to display large two-photon absorption (TPA) cross-sections (> 1000 GM) in the near-IR region (800-1000 nm) on the basis of our quantum-chemical calculations. In connection with high fluorescence quantum yields, these dyes may serve as efficient TPA sensitizers in a high-resolution laser fluorescence microscopy.



π-bridge = -, -C_6H_4-, -CH=CH-C_6H_4-, -CC-C_6H_4- ...
L = F, CN, Et, Ph; Z = CH, C(CN), N ...

The target dyes were prepared from donor-substitued benzothiazoles, which were transformed to corresponding aminothiophenols by hydrazine or NaOH, followed by the cyclocondensation with malononitrile and complexation with boron trifluoride.



Besides the effect of π-conjugation length and composition of the π-bridge, the influence of substituents directly bound to the boron atom and modification of the central methine group on absorption and fluorescence characteristics as well as TPA activity was also explored.

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[1] Kowada, T.; Maeda, H.; Kikuchi, K. *Chem. Soc. Rev.* **2015**, *44*, 4953–4972.

[2] Loudet, A.; Burgess, K. *Chem. Rev.* **2007**, *107*, 4891–4932.