SYNTHESIS OF A NEW BENZOXANTHENE FLUOROPHORE WITH EMISSION IN THE NEAR-IR REGION

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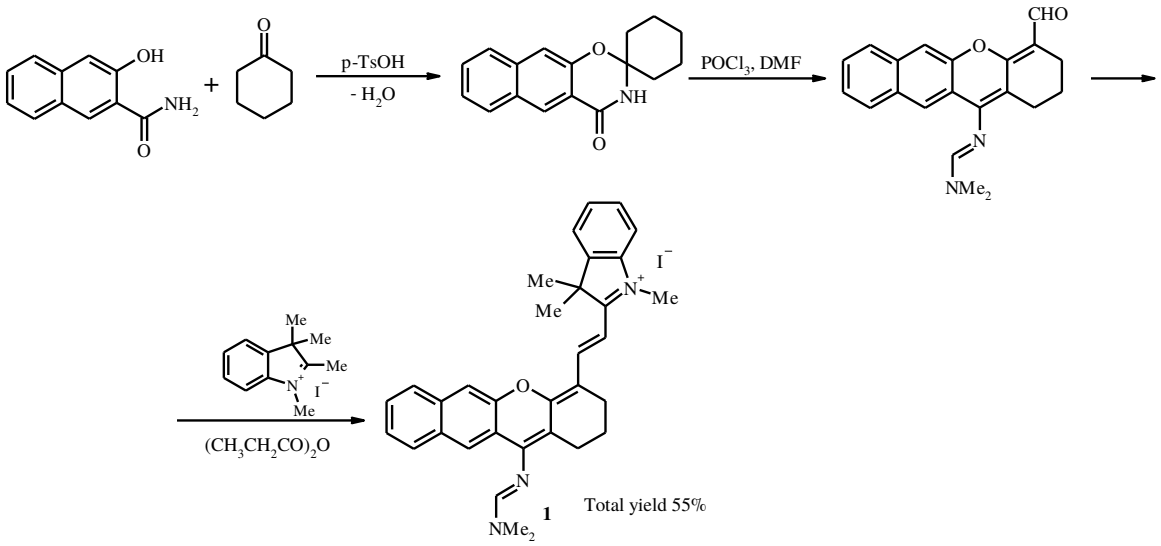
Xanthenes, including benzoxanthene derivatives, are of great interest for chemical biology. This is an important class of heterocyclic compounds for both photophysical and medicinal chemistry. Benzoxanthenes are used as fluorescent materials for the recognition of biologically important molecules. Their ability to transform light allows them to be used from optical fibers to light filters. Some xanthene dyes with radiation in the near infrared (NIR) region of the electromagnetic spectrum are used as markers for the diagnosis of various diseases.

We developed a scheme for the synthesis of a new benzoxanthene fluorophore in three stages starting from 3-hydroxy-2-naphthamide (Scheme 1).



Scheme 1. Synthesis of benzoxanthene fluorophore

Absorption and emission spectra for the synthesized dye 1 were recorded in four solvents (Table 1). The longest absorption maximum for compound 1 is observed in dichloromethane and THF (667 nm and 665 nm, respectively), and the longest emission maximum is observed in methanol (701 nm). The highest relative fluorescence quantum yield (2.18%) and extinction coefficient for this compound is also observed in methanol. From the data given in Table 1, it can be seen that dye 1 has small Stokes shifts in all investigated solvents and emits in the near-IR region, which allows us to recommend this dye for further research as a fluorescent probe.

Table 1. Spectral characteristics of benzoxanthene dye 1 in various solvents

Solvent	Solvent polarity, E_T^N	$\lambda_{abs\text{-}max}$ (nm)	$\lambda_{Em\text{-}max}$ (nm)	$\varepsilon_{max}x10^4$ (M^{-1} cm^{-1})	Φ_F[a], %	Stokes shift, nm/cm^{-1}
THF	0.207	665	694	6.59	1.71	29/630
CH_2Cl_2	0.309	667	698	6.56	1.67	31/670
MeCN	0.460	659	690	6.68	2.12	31/680
MeOH	0.762	661	701	6.70	2.18	40/870

[a]Quantum yields (Φ_F) determined at 20 °C using rhodamine B (Φ_F = 0.68 in EtOH) as a standard.