Synthesis of new fluorophores based on 2-methyltetrahydroquinazoline *N*-oxide

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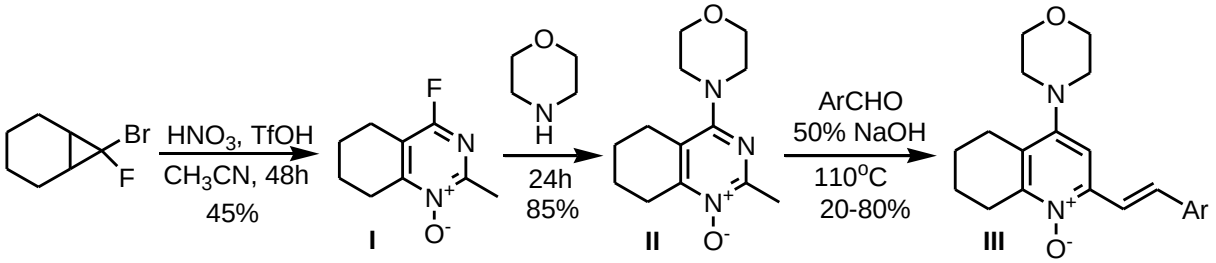
Pyrimidine represents a highly π-deficient aromatic heterocycle, which can therefore be used as electron withdrawing part in push-pull structures for intramolecular charge transfer (ICT). An effective ICT along the scaffold of the molecule can also induce luminescence properties. Such materials find widespread application in photonics, electronics and bioresearch. Pyrimidine *N*-oxide is even more π-deficient heterocycle that makes its derivatives promising exploration target. Nevertheless, the information about synthesis, application and photo-physical properties of pyrimidine *N*-oxide derivatives is quite limited due to low synthetic accessibility of these compounds.

Recently, an effective approach leading to easily functionalizable 4-fluoropyrimidine *N*-oxides **I** was found in our laboratory [1]. In present work, we describe synthesis and photo-physical study of new fluorophores **III** based on tetrahydroquinazoline *N*-oxide core.



Ar = Ph (**a**); 2,5-dimethylphenyl (**b**); 4-methoxyphenyl (**c**); 4-ethoxyphenyl (**d**); 3,4,5-trimethoxyphenyl (**e**); 4-formylphenyl (**f**); 4-(diethoxymethyl)phenyl (**g**); 4-(2-phenylvinyl)phenyl (**h**); -CH=CH-Ph (**i**)

A series of previously unknown heterocyclic compounds **III** was synthesized from tetrahydroquinazoline *N*-oxide **I** via aromatic nucleophilic substitution of fluorine and subsequent condensation of 4-aminosubstituted heterocycles **II** with aromatic aldehydes in basic conditions.

It was found that absorption wavelengths maxima for the compounds obtained were located in visible region (384–416 nm); the emission wavelengths maxima were located in range 527–560 nm (except for compound **IIIf**). The best result was obtained for tetrahydroquinazoline **IIIf**, containing an aldehyde function in *p*-position of phenyl fragment, that redshifts the longest-wavelength emission maximum to λ_{em} = 600 nm, nearer to therapeutic window (700–950 nm) and could be used for further design of new fluorescent probes for medical imaging.

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References

[1]. Sedenkova K.N., Averina E.B., Grishin Yu.K., Bacunov A.B., Troyanov S.L., Morozov I.V., Deeva E.B., Merkulova A.V., Kuznetsova T.S., Zefirov N.S. *Tetrahedron Lett.* **2015**, *56*, 4927