

## Imidazole derivatives with $\pi$ -extended chromophore - synthesis and optical properties

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The main purpose of my work was to synthesize and investigate the photophysical properties of previously unknown  $\pi$ -conjugated polycyclic compounds possessing imidazole core. To achieve this goal, it was necessary to examine the scope of reactivity and to deepen the understanding of the electronic requirements of intramolecular coupling of aromatic compounds containing imidazole as a central unit. I started my research from the synthesis of a series of imidazole derivatives exhibiting excited state intramolecular proton transfer (ESIPT), in particular I focused on the synthesis of unexplored  $\pi$ -expanded imidazoles possessing multiple conjugated aromatic rings. As a result, I obtained a series of imidazole derivatives which exhibit large fluorescence quantum yields (up to 50%) and significant Stokes shift (up to 15000  $\text{cm}^{-1}$ ). In order to further improve the photophysical properties, I subsequently focused on methods that enabled formation of  $\text{C}_{\text{Ar}}\text{-C}_{\text{Ar}}$  bonds between aromatic rings at different positions of imidazole core. My meticulous studies of intramolecular oxidative aromatic coupling have proven that this reaction is much more problematic in the case of imidazole derivatives compared with typical polycyclic aromatic compounds. Still, I was able to show that it is possible to selectively form  $\text{C}_{\text{Ar}}\text{-C}_{\text{Ar}}$  bonds if the aryl substituents are activated with alkoxy groups. In the next phase of the project I decided to use other methods of intramolecular aromatic coupling reactions including direct arylation catalyzed by palladium. In the course of this study, I discovered that imidazole derivatives possessing 2-halogenoaryl substituents at position 2, undergo intramolecular direct arylation promoted by ultraviolet radiation. The discovered photochemical method is very efficient, regardless of the electronic or steric effects, and it can be carried out in solid state. It is noteworthy that this reaction occurs also for derivatives possessing free phenolic OH group. Based on this observation, I designed and synthesized a number of substituted imidazo[1,2-*f*]phenanthridines displaying ESIPT. As I suspected, they exhibit larger fluorescence quantum yields compared to less conjugated imidazole analogs, up to 80% in both non-polar and polar solvents, which is a very important requirement for the potential use as probes in fluorescence imaging. The methods that I developed have proven to be an excellent tool in the synthesis of structurally unique imidazo[1,2-*f*]phenanthridines and other  $\pi$ -conjugated imidazole derivatives having favorable optical properties. The developed syntheses of these novel compounds are efficient and inexpensive, and the optical properties of products makes them suitable candidates in optoelectronic applications.