New derivatives of diketopyrrolopyrroles – synthesis and photophysical properties

Anna Kamila Purc

Supervisor: Prof. Daniel T. Gryko

The primary goal of the dissertation was the synthesis of diketopyrrolopyrrole derivatives possessing useful optical properties. This task was achieved through the synthesis of diketopyrrolopyrroles comprising two benzofuran units attached to the core in position 2. Despite the need to develop new variants of cyanobenzofuranes' synthesis, I was able to synthesize 12 *N*,*N'*-dialkyl-bis(benzofuranyl)diketopyrrolopyrroles. The best optical properties were observed for dyes bearing dialkylamino substituents at the position 6 of benzofuranes. The dyes were characterized by a green color and a high molar absorption coefficient. Fluorescence and two-photon absorption were also very strong.

I synthesized a library of *N*,*N'*-dialkyl-bis(pyridyl)diketopyrrolopyrroles, so that I was able to examine the relationship between their structure and optical properties. The obtained compounds were characterized by interesting optical properties. Only in one case, when the morpholine substituent was located in the *meta* position relative to the chromophore core and *ortho* to the nitrogen atom, the resulting dye posessed extremely low fluorescence. Upon further research, I discovered that the absorption and fluorescence of this compound strongly depends on the pH. The addition of acid or base caused an increase in fluorescence quantum yield, which enabled biological research using fluorescence microscopy.

Investigation of reactivity of diketopyrrolo-pyrroles in reaction of 1,3-dipolar cycloaddition with *in situ* generated iminium ylides showed that the structure of diketopyrrolopyrroles posseses bonds polarized enough to be able to undergo such a reaction, but the products were characterized by very poor stability.

Moreover, I prepared a diketopyrrolopyrrole derivative possessing electron-donating aryl substituent on one of amide nitrogen atoms. The study of the dynamics of electron transfer allowed to conclude that after the excitation and charge separation the molecule stays in such a state for a relatively long time, which is especially important for potential applications in electronics and photonics.