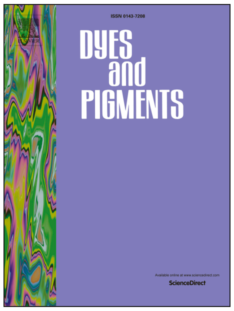

Does the length matter? - Synthesis, photophysical, and theoretical study of novel quinolines based on carbazoles with different length of alkyl chain

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Does the length matter? - Synthesis, photophysical, and theoretical study of novel quinolines based on carbazoles with different length of alkyl chain

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Abstract

Donor-acceptor (D-A) system based on 2,4-dicarbazolyl-substituted quinolines (**Q2-Q5**) with different length of alkyl chain at carbazole, viz -CH_3 (**Q3**), -C_8H_{17} (**Q4**), -$C_{10}H_{21}$ (**Q5**), and different attachment of carbazole to quinoline core, and in addition a 4-bromo-(9*H*-carbaz-2-yl)-quinoline (**Q1**) was designed and synthesized via Suzuki-Miyaura cross-coupling reaction to examine the influence of alkyl chain length on their photophysical behavior. The study shows a strong dependence of optical and electrochemical properties on the number of carbazole units in the molecule as well as the position of substitution of carbazole and mainly length of alkyl chain on carbazole units of studied quinoline derivatives. Emission (PL) spectra exhibit that the extension of alkyl chain length to -C_8H_{17} enhances the fluorescence quantum yield and lifetime of compounds but the introduction of -$C_{10}H_{21}$ into molecule results in a significant reduction of luminescence ability. Additional PL spectra at 77 K of **Q4** (-C_8H_{17}) and **Q5** (-$C_{10}H_{21}$) reveal that intersystem crossing takes place with higher efficiency in **Q5** and plays a superior role than possible intramolecular photoinduced electron transfer (PET) mechanism than in the case of **Q4**. The study of the geometry of the first singlet (S_1) and triplet (T_1) excited states of **Q4** and **Q5** demonstrate that the energy of the excited state in **Q5** may be mostly spread as a result of the oscillations within the aliphatic hydrocarbons and in **Q4** the intersystem crossing processes amplify the deactivation in the radiative path. The electrochemical investigation indicates that the oxidation potential is lower for molecules with carbazole substituted at 2- than 3-position, and among **Q3-Q5** decreases significantly from