Photophysical behavior of a potential drug candidate, *trans*-[2-(4-methoxystyryl)]quinoline-1-oxide tuned by environment effects.

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Streszczenie

Styryl and/or quinoline structural fragments, present in a large number of bioactive substances, inspired the design of various new drug candidates. In this paper, we describe the photophysical behavior of trans-[2-(4-methoxystyryl)]quinoline-1-oxide (trans-MSQNO) on the basis of X-ray analysis data, theoretical calculations as well as steady state and time-resolved spectroscopy experiments in various media. The molecule crystallizes in orthorhombic unit cell containing eight molecules of N-oxide, space group Pbca. The NO bond is substantially shorter in comparison with the NO bond in the ZnTPP unit [1.3052(11) Å vs. 1.335(2) Å]. Variation of emission colors from the violet (~450nm) through blue (480nm), green (525nm) and yellow (575nm) is observed in different environments. Comparable values of lifetimes estimated both at ambient temperature and at 77K suggest that excited state dynamics in this case is viscosity independent. DFT and TD DFT B3LYP/6-31G(d, p) calculations performed for four different trans-MSQNO rotamers in the gas phase, as well as nonpolar and polar media (PCM model) suggest that an equilibrium between them can be significantly altered even by a relatively weak interactions with the environment. It is suggested that varying intensity ratios of experimental absorption bands in different media may be due to the dominant share of one or more rotamers of the excited trans-MSQNO molecule. Gas phase calculations show also that the vertical ππ*, $S_0 \rightarrow S_1$, transition resulting from the HOMO→LUMO electronic configuration exhibits only a partial CT nature. On the other hand, in polar media, a substantial increment of excited state dipole moment of all rotamers compared to the ground state, its increase with increasing solvent polarity and a significant red shift in the absorption and emission spectra, point to the enhanced CT nature of the S_1 excited state. Hence, the trans-MSQNO molecule may be considered a subsequent styrylquinoline drug candidate where the CT drug-receptor interactions are of a high importance.

Słowa kluczowe

Styryl derivatives, pK(a)*, TD DFT calculations, excited states, lifetimes

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