

INVESTIGATION ON EFFICIENCY FACTORS OF SINGLET OXYGEN GENERATION BY PHOTOPHYSICAL STUDIES OF VARIOUS PHOTSENSITIZERS

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Photophysical studies of the anthraquinone OH derivatives, the O-,S- core-modified tetraphenylporphyrins, and the core-expanded tetrathiarubyrin and of the photoinduced singlet oxygen generation were performed by means of steady-state spectroscopies, time-resolved luminescence, time-resolved transient absorption, and time-resolved thermal lens method. From the studies, the direction of structural modification for better functionalities of photosensitizer in PDT application was suggested. The singlet oxygen quantum yield is affected by various photophysical factors of the photosensitizers. For the anthraquinone OH derivatives, the singlet oxygen generation efficiency is lowered due to the excited state intramolecular proton transfer. When the oxygen and sulfur atoms are core-substituted in tetraphenylporphyrin, the triplet state quantum yield increases due to the enhanced spin-orbit coupling cross section and, therefore, the singlet oxygen quantum yield also increases up to 0.57. However, the structural distortion which is caused by the heavy atom substitution reduces the energy transfer efficiency to the triplet oxygen due to the enhanced $T_1 \rightarrow S_0$ relaxation. In the case of tetrathiarubyrin, the triplet state quantum yield increases and the singlet oxygen quantum yield is 0.52. Therefore, it is considered, as expected, that the singlet oxygen quantum yield increases with the increment of the triplet state quantum yield. However, in the case of the heavy structural distortion of photosensitizer or the existence of other energy dissipation pathways such as proton transfer and charge transfer complex, the singlet oxygen generation yield is influenced to be decreased. It is concluded that the enhancement of the triplet quantum yield and the prevention of other various energy dissipation pathways caused by nonradiative relaxation photophysics due to proton transfer and charge transfer and inter/intra-molecular vibrationally coupled structural distortions should be considered in designing new synthesized PDT photosensitizers

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