عنوان مقاله:

Photosensitization of coronene–purine hybrids for photodynamic therapy

محل انتشار:

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خلاصه مقاله:

Photosensitization properties of coronene-purine (Cor-P) hybrids for photodynamic therapy (PDT) have been investigated in this work. Eight hybrid Cor-P models have been designed by the additional of adenine (A) and guanine (G) nucleobase to Cor species. The evaluated absorption and emission energies indicated that the singular models are not good at all for PDT process whereas their hybrid models are very much useful for the purpose. Although the Cor-A models are very much better for visible region, but the Cor-G models could be also used in the near-infrared region. The main point of these materials is to generate singlet molecular oxygen, in which all investigated Cor-P hybrids could supply the required energy for triplet to singlet conversion of molecular oxygen. This work has been done based on the advantage of quantum computation for solving the problems in living systems.

کلمات کلیدی:

photodynamic therapy, photosensitizer, coronene, adenine, guanine