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Fine Tuning the emission wavelengths of the 7-hydroxy-1-indanone based nano-structure dyes: Near-infrared (NIR) dual emission generation with large Stokes Shifts

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Abstract

Near-infrared (NIR) fluorescent dyes have recently gained special attention due to their applications to use as molecular probes for imaging of biological targets and sensitive determination. In this study, photophysical properties of the 7-hydroxy-1-indanone based fluorophors **A1, A2, A3, B1, B2** and **3R-B2 (**R = CF_3, NH_2, NO_2 and OMe) in the gas and three solution phases were probed using TD-DFT method at PBE0/6-311++G(d,p) and M06-2X/6-311++G(d,p) levels of theory. In addition to structural and photophysical properties as well as ESIPT mechanism of all mentioned molecules, the FC and relaxed potential energy surfaces of **B2** and **3R-B2** (R = CF_3 and NH_2) molecules were explored in gas phase and acetonitrile, cyclohexane and water solvents. It is predicted that the **A1**, **A3** and **3R-B2** chromophores afford normal (615-670 nm) and NIR fluorescence emissions (770-940 nm; biological window) with the large Stokes shifts of >160 and >300 nm, respectively. A good aggrement was found between theoretical and experimental results. In sum, these new types of dyes may render the new approaches for the development of the most efficient NIR fluorescent probes for enhanced image contrast and optimal apparent brightness in biological applications.

Keywords: Near-infrared (NIR) fluorescent; 7-hydroxy-1-indanone; ESIPT; PBE0; M06-2X; Stokes shift.

1. Introduction

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