Accepted Manuscript

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PII: S0143-7208(17)32454-3

DOI: 10.1016/j.dyepig.2018.01.016

Reference: DYPI 6490

To appear in: Dyes and Pigments

Received Date: 30 November 2017

Revised Date: 8 January 2018

Accepted Date: 10 January 2018

Please cite this article as: Li J, Zhang C, Wu S, Wen X, Xi Z, Yi L, Facile synthesis of green-light and large Stokes-shift emitting coumarins for bioconjugation, *Dyes and Pigments* (2018), doi: 10.1016/i.dyepig.2018.01.016.

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ACCEPTED MANUSCRIPT

Facile synthesis of green-light and large Stokes-shift emitting coumarins for bioconjugation

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ABSTRACT

Bright and hydrosoluble fluorescent dyes with large Stokes shifts are widely used as molecular probes and light-emitting markers in chemistry and biology. In this report, one-step synthesis of a bright green-emitting coumarin ($\Phi = 0.52$, $\lambda_{\rm em} = 505$ nm) was achieved from available reagents under neat conditions. The novel dye **1** showed very large Stokes shift ($\Delta\lambda = 138$ nm) due to strong intramolecular charge transfer (ICT) effect, which was confirmed by density functional theory (DFT) calculations. Dye **1** was hydrosoluble and displayed strong emission at a wide range of pH from 3 to 8. Importantly, the secondary amine in **1** made it extremely convenient for futher bioconjugation. Representative derivatives were showcased for various successful applications of fluorogenic enzyme assay, biolabelling and mitochondrial staining.

Keywords: Coumarin, Green-emitting, Large Stokes shift; Bioconjugation

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