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www.elsevier.com/locate/talanta

PII: S0039-9140(18)30357-6
DOI: https://doi.org/10.1016/j.talanta.2018.04.017
Reference: TAL18556

To appear in: *Talanta*

Received date: 14 December 2017
Revised date: 23 March 2018
Accepted date: 7 April 2018

Cite this article as: Liu Chen, Yu-Jia Fu, Wen-Le Fang, Xiao-Feng Guo and Hong Wang, Screening of a highly effective fluorescent derivatization reagent for carbonyl compounds and its application in HPLC with fluorescence detection, *Talanta,* https://doi.org/10.1016/j.talanta.2018.04.017

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ABSTRACT:

Carbonyl compounds are widely distributed in organisms, and the commonly used methods for determination of them like UV/fluorescence/mass spectrometry always require derivatization reagents. However, the reported derivatization reagents have significant difference in reactivity, which is very unfavorable for developing highly reactive reagent. In this study, we theoretically investigated the factors affecting the reactivity of hydrazine-based derivatization reagents, and proposed a strategy for filtering highly reactive reagents by quantum chemical calculation. With this strategy,