

**Synthesis, optical properties, and acid-base indicating performance of novel ketene
hydroxybenzylidene nopinone derivatives**

Jinlai Yang,^{abc} Xu Xu,^{ad} Yiqin Yang,^e Jian Rui,^a Yan Zhang,^a Hongbo Kuang,^a Shifa
Wang,^{*ad} Liangru Wu^{*bc}

Supplementary data

*Corresponding author: Dr. and Prof. Shifa Wang

College of Chemical Engineering, Nanjing Forestry University, Nanjing, Jiangsu
210037, China

Jiangsu Key Lab of Biomass-based green Fuels and Chemicals, Nanjing, Jiangsu
210037, China

Phone: +86-25-85427812; Fax: +86-25-85427812

Email: wangshifa65@163.com

Table S1. Crystal data, diffraction data, and refinement data of compound **1**.

empirical formula	C ₁₆ H ₁₈ O ₂
formula weight	242.30
crystal system	monoclinic
space group	P 212121
a [Å]	8.938(4)
b [Å]	11.742(5)
c [Å]	12.745(6)
α [deg]	90
β [deg]	90
γ [deg]	90
volume [Å ³]	1337.7(10)
Z	27
D _c [g/cm ⁻³]	1.203
F (000)	520
T [K]	299
wavelength [Å]	0.71073
absorption coefficient [mm ⁻¹]	0.078
completeness to theta	29.40 (100.0%)
reflections collected/unique	12714/3703 [R(int) = 0.0255]
data/restraints/parameters	3703/0/163
R ₁ , wR ₂ [I>2σ(I)]	0.0464, 0.1210
R ₁ , wR ₂ (all data)	0.0561, 0.1280
goodness of fit on F ²	1.030
largest diff. peak and hole [e.Å ⁻³]	0.254 and -0.209

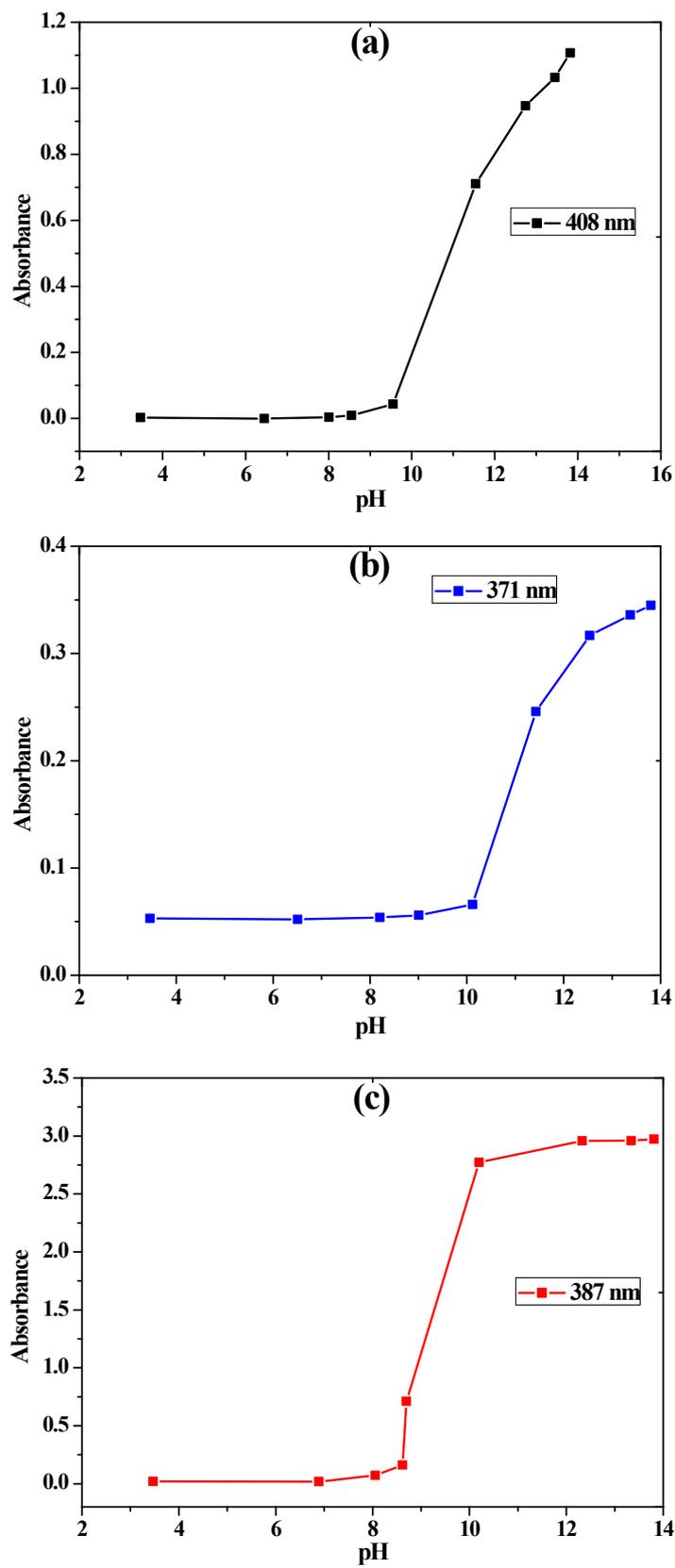


Fig. S1 The relationship between absorbance and pH of compounds **1** (a), **2** (b) and **3** (c).

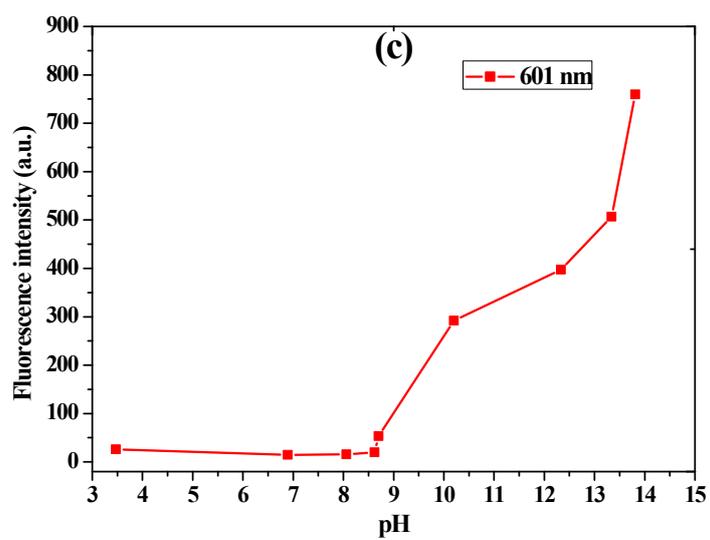
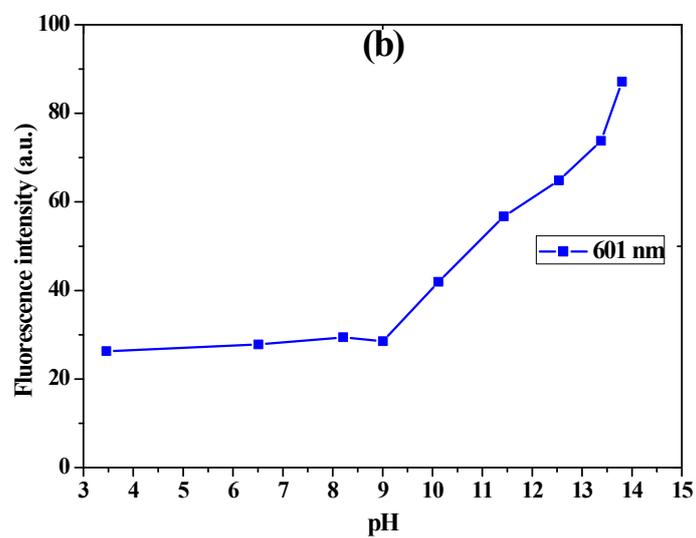
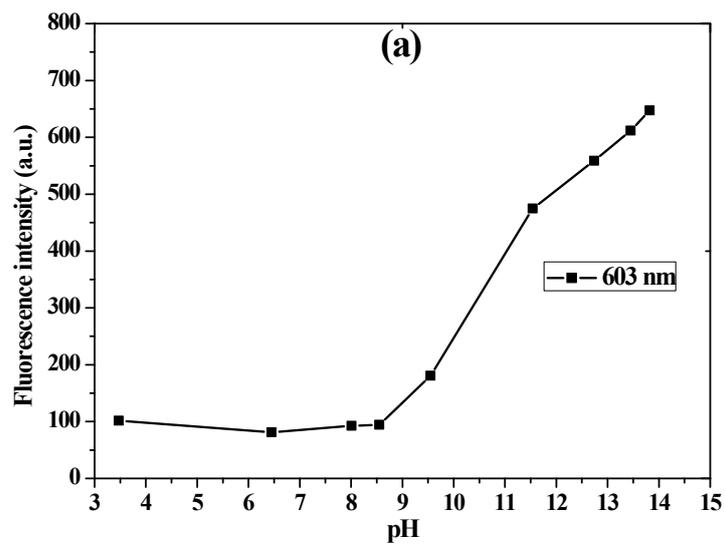


Fig. S2 The relationship between fluorescence intensity and pH of compounds 1 (a), 2 (b) and 3 (c).