Supporting Information

Efficient blue TADF-type organic afterglow material via boric acid-assisted confinement

Song Shen, Yuena Sun, Donghui Wang, Zhen Zhang, Yu-e Shi*, Zhenguang Wang*

Key Laboratory of Chemical Biology of Hebei Province, Key Laboratory of Medicinal Chemistry and Molecular Diagnosis, Ministry of Education, College of Chemistry & Environmental Science, Hebei University, Baoding 071002, China; Email: zgwang@hbu.edu.cn

EXPERIMENTAL SECTION

Materials

BA (99.9%) and norfloxacin (99%) were obtained from Aladdin.

Instrumentation

The delay and prompt PL spectra of samples were recorded on a F-7000 spectrometer (Hitachi, Japan). The phosphorescence decay curves were recorded by an Edinburgh FS5 fluorescence spectrophotometer the kinetic scan model. The absolute photoluminescence and phosphorescence QY of products were directly measured on an Edinburgh FLSP920 fluorescence spectrophotometer equipped with an integrating sphere. An environmental scanning electron microscope (ESEM, FEI/Philips XL30) was used to study the morphologies of the products. Fourier transformed infrared (FTIR) spectra were recorded on a Nicolet IS10 FTIR spectrometer (Thermo, USA). XPS spectra were recorded on an ESCALAB-MKII 250 photoelectron spectrometer (Thermo, USA). Powder XRD measurements were carried out on a Bruker D8 Advance X-ray diffractometer with Cu Kα radiation. EPR spectra were measured on an X-band (ν_{mw} = 9.84 GHz) EMXmicro BRUKER spectrometer. The electron paramagnetic resonance (EPR) spectra of elemental boron were measured on a Bruker A300 EPR Spectrometer.

Preparation of blue afterglow materials

BA (3 g) and NFX were added into 40 mL of ultrapure water in a 100 mL beaker, which was covered with a layer of foil. Then, the mixture was heated under 140 ^{o}C for 6 h, until transferring the solution into solid state. A white powder was obtained after grinding the products, which presented blue emission under 365 nm UV light. Similarly, heated BA was prepared by heat treatment the aqueous solution of 3 g BA dissolved in 40 mL of water.

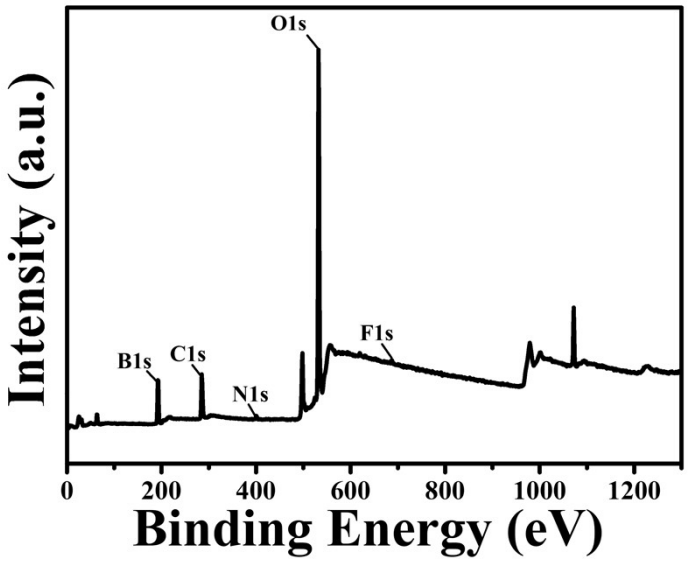

Figure S1. Full scan XPS spectrum of BNFX.

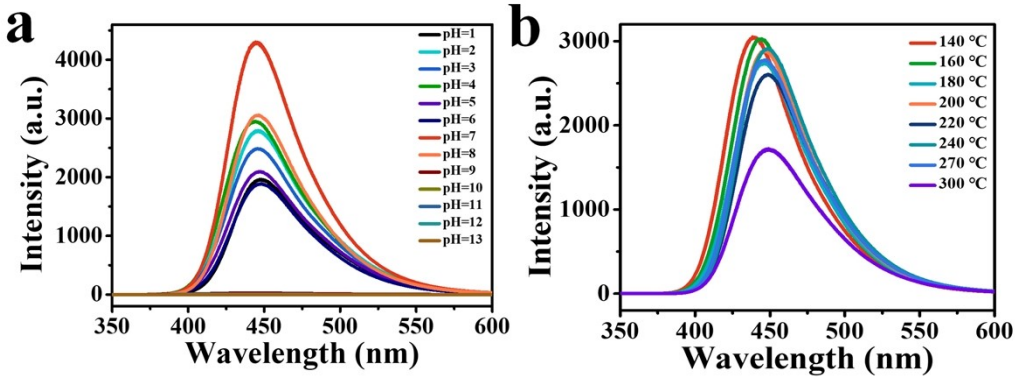

Figure S2. Delay PL spectra of BNFX produced under different pH (a) and at different heating temperatures (b). All the spectra were collected under the excitation of 310 nm.

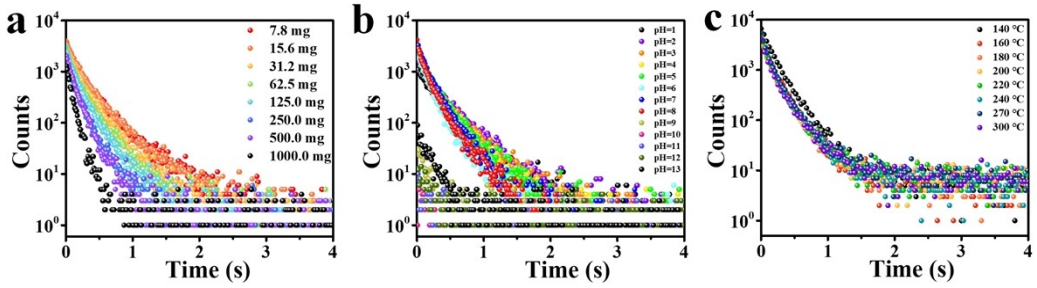

Figure S3. Delay PL decay curves BNFX produced by loading different amounts of NFX (a), under different pH (b) and at different heating temperatures (c). All the curves were collected under the excitation of 310 nm and recorded at 450 nm.

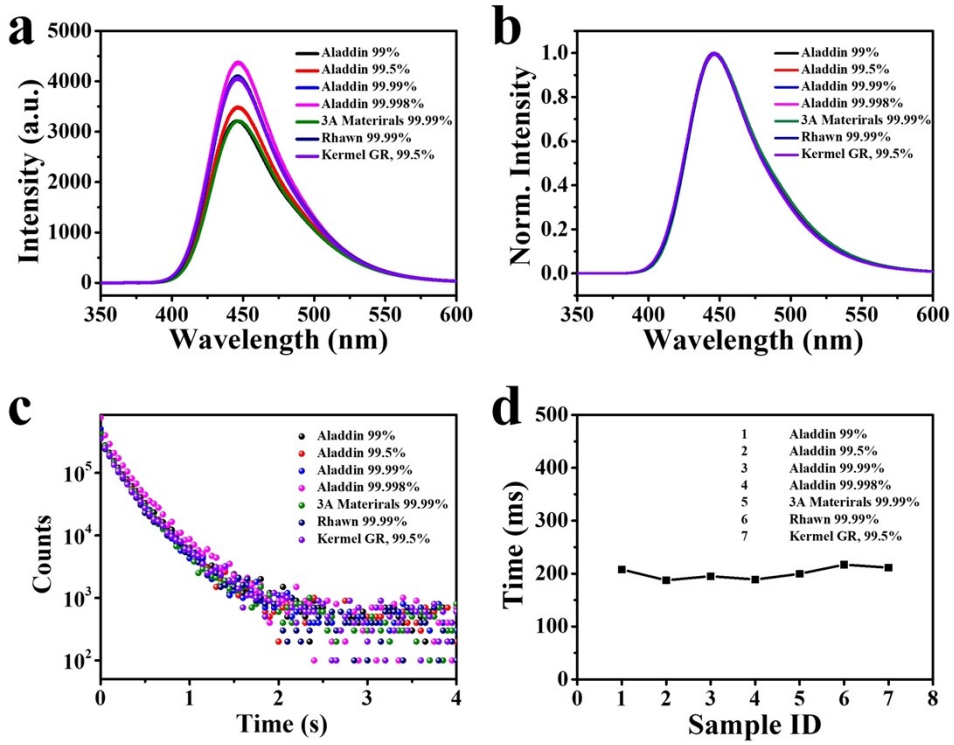

Figure S4. Delay PL spectra (a), normalized delay PL spectra (b), decay curves (c), and average emission lifetime (d) of BNFX produced by using BA from different manufacturers with different purity, as indicated on the frame.

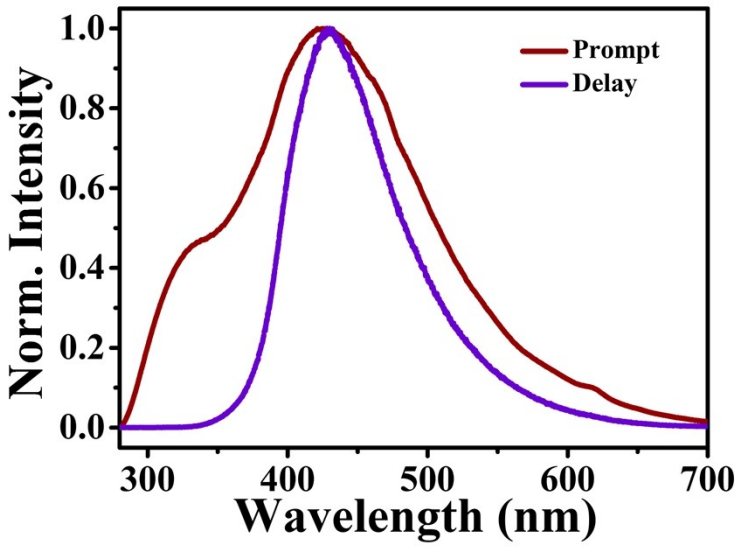

Figure S5. Normalized prompt and delay PL spectra of heated BA, under the excitation of 250 nm.

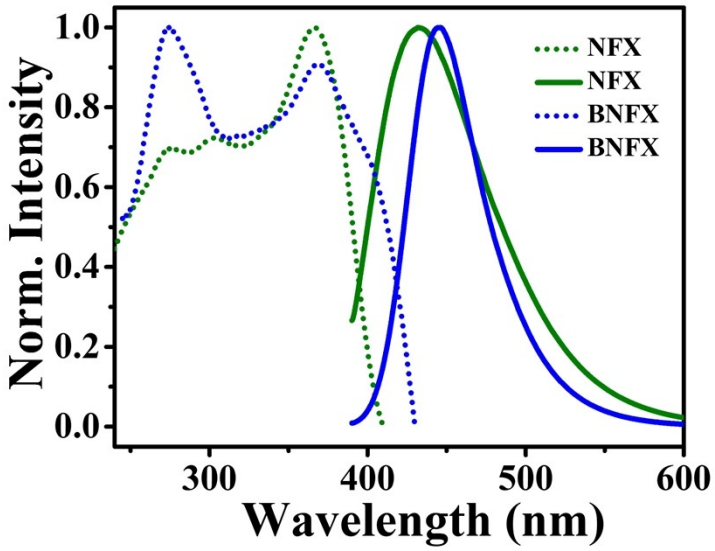

Figure S6. Normalized prompt PL emission (solid line) and excitation (dotted line) of BNFX (blue line) and NFX (green line).

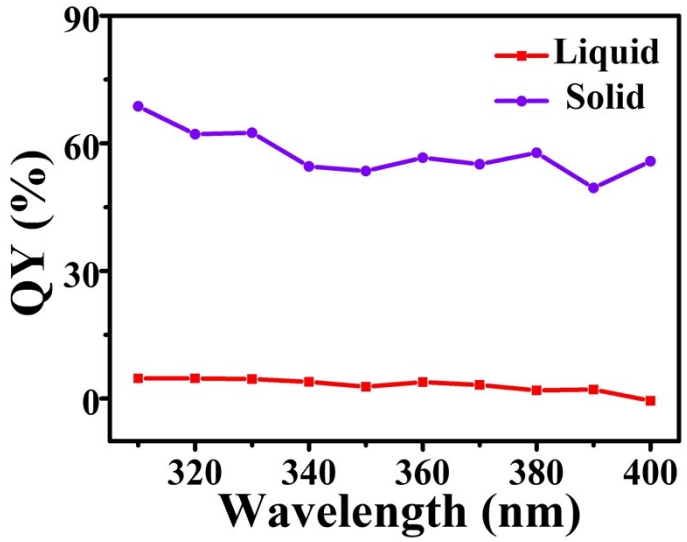

Figure S7. Evolution of PL QY of norfloxacin in solution (red line) and BNFX (purple line), as a function of excitation wavelengths.

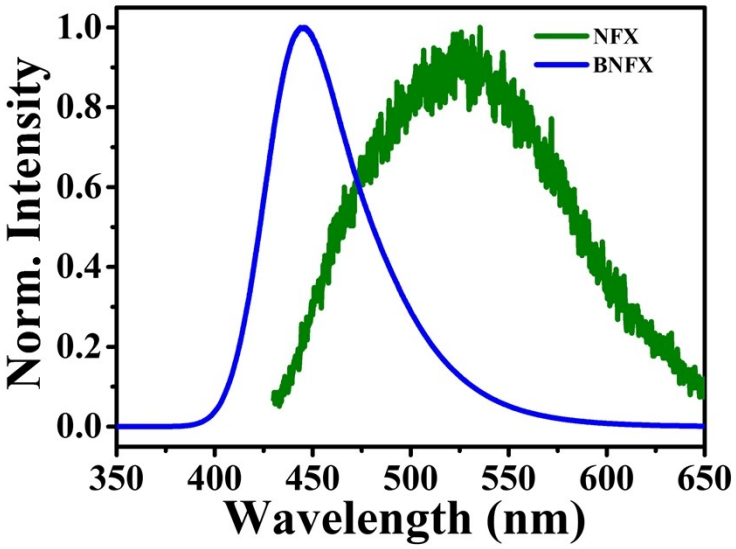

Figure S8. Normalized delay PL emission spectra of BNFX (blue line) and NFX (green line). All the curves of recorded under the excitation of 310 nm.

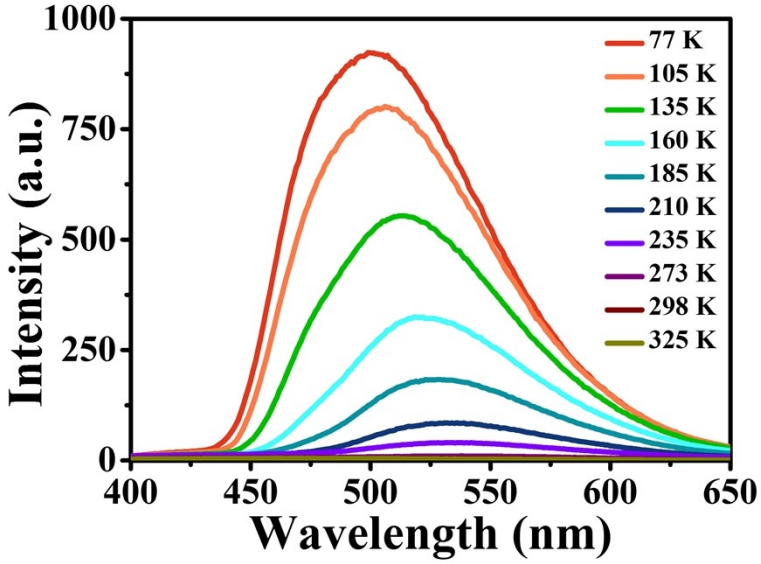

Figure S9. Delay PL emission spectra of pure norfloxacin, under the excitation of 310 nm, at different detection temperatures.

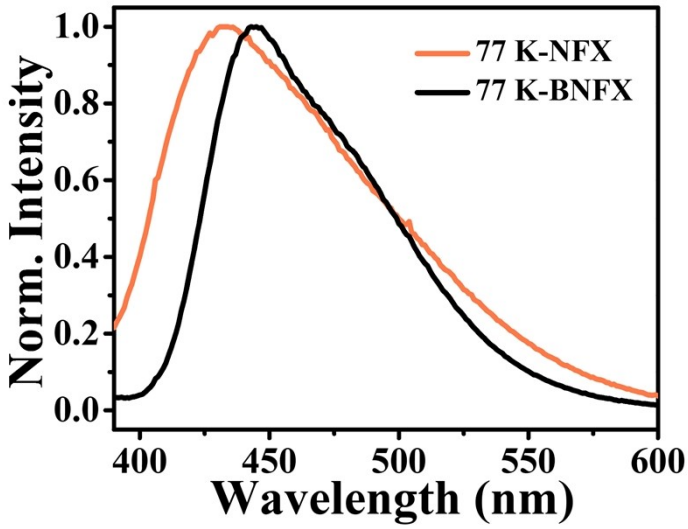

Figure S10. Prompt PL emission spectra of pure norfloxacin (yellow line) and BNFX (black line), under the excitation of 310 nm.

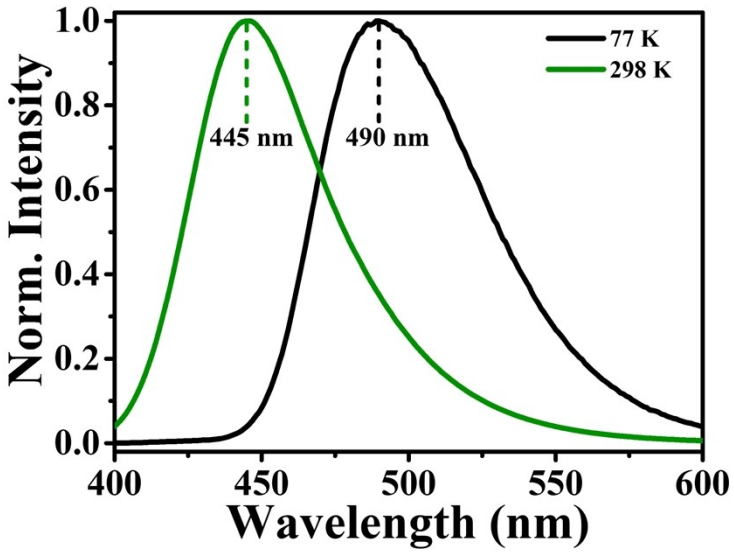

Figure S11. Prompt PL spectra of BNFX under 298 K, excited at 310 nm (green line); Delay PL spectra of BNFX under 77 K, excited at 280 nm (black line).

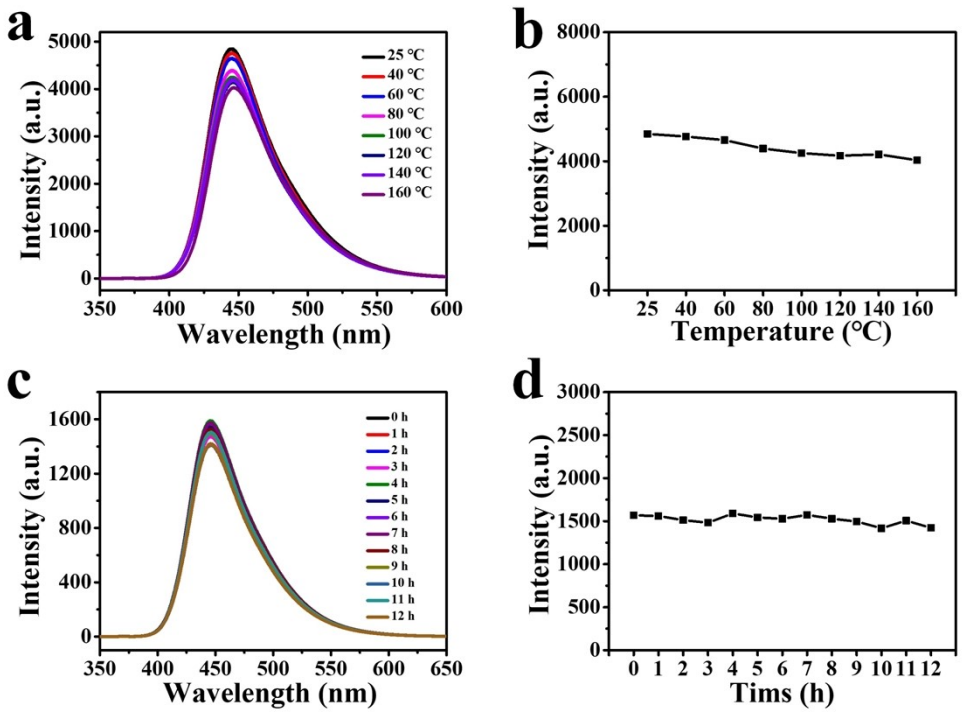

Figure 12. Evolution of delay PL spectra (a), PL intensity (b) of BNFX, as a function of heating temperature; Evolution of delay PL spectra (c), PL intensity (d) of BNFX, as a function of heating time. All the spectra were collected under the excitation of 310 nm, and all the PL intensities were recorded on corresponding spectra at 450 nm.

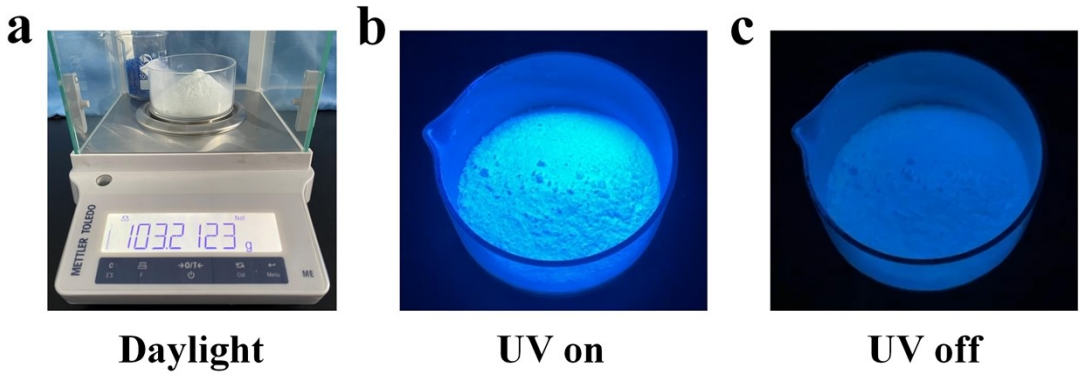

Figure S13. Photographs of BNFX produced by the large-scale methods under daylight (a), 365 nm UV light (b) and switching off of UV light (c).

Table S1. Emission lifetimes ($\tau_{1\text{-}2}$, ms) and fractions of the emission intensity ($f_{1\text{-}2}$,%) obtained from the fitting of experimental emission decay data by two-exponential functions of BNFX, produced under different pH, from which the average emission lifetimes (τ_{avg}, ms) were calculated. All the curves were detected at 450 nm, under the excitation of 370 nm.

pH	τ_1 (f_1)	τ_2 (f_2)	τ_{avg}
pH=1	129.6 (37.9)	349.1 (62.1)	265.9
pH=2	114.2 (33.9)	340.1 (66.2)	263.6
pH=3	112.6 (39.5)	333.3 (60.5)	246.2
pH=4	121.2 (48.6)	392.1 (51.4)	228.1
pH=5	113.74 (41.8)	297.3 (59.2)	225.5
pH=6	101.9 (60.7)	257.1 (39.3)	162.9
pH=7	87.2 (36.9)	229.7 (63.1)	177.1
pH=8	96.4 (58.4)	262.4 (41.6)	165.4
pH=9	50.0 (25.2)	433.1 (74.8)	336.6
pH=10	119.7 (40.3)	344.1 (59.7)	253.7
pH=11	50.9 (70.3)	1355.76 (29.7)	438.8
pH=12	141.1 (13.0)	524.3 (87.0)	489.9
pH=13	149.1 (94.2)	666.5 (5.8)	179.2

Table S2. Emission lifetimes ($\tau_{1\text{-}2}$, ms) and fractions of the emission intensity ($f_{1\text{-}2}$,%) obtained from the fitting of experimental emission decay data by two-exponential functions of BNFX, produced by loading different amount of NFX, from which the average emission lifetimes (τ_{avg}, ms) were calculated. All the curves were detected at 450 nm, under the excitation of 370 nm.

Amount of Norfloxacin	τ_1 (f_1)	τ_2 (f_2)	τ_{avg}
7.8 mg	136.7 (45.9)	344.4 (54.1)	248.9
15.6 mg	126.1 (43.2)	321.7 (56.8)	237.2
31.3 mg	105.9 (45.2)	292.5 (54.8)	208.1
62.5 mg	108.2 (46.3)	297.8 (53.7)	200.3
125 mg	83.9 (45.0)	230.9 (55.0)	164.8
250 mg	82.4 (48.9)	209.1 (51.1)	147.1
500 mg	66.5 (37.6)	159.3 (62.4)	124.4
1000 mg	60.1 (57.2)	105.2 (42.8)	79.4

Table S3. Emission lifetimes ($\tau_{1\text{-}2}$, ms) and fractions of the emission intensity ($f_{1\text{-}2}$,%) obtained from the fitting of experimental emission decay data by two-exponential functions of BNFX, produced at different heating temperature, from which the average emission lifetimes (τ_{avg}, ms) were calculated. All the curves were detected at 450 nm, under the excitation of 370 nm.

Temperature	τ_1 (f_1)	τ_2 (f_2)	τ_{avg}
140 °C	74.9 (26.8)	202.1 (73.2)	168.0
160 °C	85.2 (35.2)	205.5 (71.8)	186.3
180 °C	189.5 (72.9)	68.3 (27.1)	156.7

200 °C	128.1 (58.6)	323.2 (41.4)	208.8
220 °C	61.6 (30.6)	188.1 (69.4)	149.3
240 °C	69.2 (34.7)	198.8 (65.3)	153.8
270 °C	63.3 (27.6)	197.3 (72.4)	160.3
300 °C	55.3 (24.3)	197.9 (75.7)	163.3