

Supporting Information

Endowing Hydrochromism to Fluorans via Bio-inspired Alteration of Molecular Structures and Microenvironments and Expanding Their Potential for Rewritable Paper

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1. Experimental section

Materials. 3-nitrophthalic anhydride (98%), N, N-diethyl-3-aminophenol (98%), Pd/C (10%) and o-Phthalic anhydride (98%) were purchased from Energy Chemical (Shanghai, China). Rhodamine B ($C_{28}H_{31}ClN_2O_3$) (95%), 4-methoxy-2-methyldiphenylamine (98%) were purchased from Aladdin (Shanghai, China). Unless otherwise noted, all the other materials were purchased from Sinopharm Chemical Reagent Beijing Co., without further purification. Deionized water was purified by Milli-Q system. PEG 20000 (molecular weight: 17,000-22,000) was purchased from Guangfu Fine Chemical Research Institute (Tianjin, China). PVA was purchased from Ying Jia Industrial Development Co., Ltd. (Shanghai, China). Cellulose filter paper (Whatman-Xinhua, grade 91, Hangzhou, China) is selected as the paper substrate. A4 printing commercial paper was purchased from Tianyi Company (Beijing, China).

Instrument. Absorption spectra were measured using a Shimadzu UV-2550 PC double-beam spectrophotometer. The fluorescence quantum yields (Φ_f) and lifetime were measured on FLS 920 lifetime and steady state spectrometer. Steady State fluorescence spectra were measured using a Shimadzu RF-5301 PC spectrophotometer. Reflective UV-Vis spectroscopy of water-jet rewritable paper (**WJRP**) before and after addition of water and *in situ* kinetic measurement was tested via reflective mode of integrating sphere on Analitik Jena Specord@210 plus UV/VIS spectrophotometer, using $BaSO_4$ as background, path length was 1 cm. The writing-erasing cycles experiment for **WJRP** is recorded by Maya 2000PRO fiber optical spectrometer with Ocean DH-2000-BAL UV-Vis-NIR light source. Microscopy images of **WJRPs** were measured by LEICA DM 4000/MLED. Single-crystal X-ray diffraction data for **NO₂-ODB** was recorded on a Rigaku RAXIS-PRID diffractometer using the ω -scan mode with graphite monochromator Mo-K α radiation ($\lambda = 0.71073\text{\AA}$). 1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded on a Bruker AVANCE500 at room temperature. LC-HRMS analysis was performed on an Agilent 1290-micro TOF-Q II mass spectrometer. Melting point was determined using a SGW X-4B microscopy melting point apparatus (Shanghai, China). Surface morphologies were characterized using JEOL-6700F field emission scanning electron microscopy (SEM) at an accelerating voltage of 3KV.

Theoretical Calculations. All the Density functional theory (DFT) calculations were carried out using the GAUSSIAN 09 series of programs.^{S1} DFT and B3LYP with a standard 6-31G (d, p) basis set were used for geometry optimizations. Solvent effects with the polarizable continuum model (PCM) was considered. Harmonic vibrational frequency calculations were performed for all stationary points to determine whether they are local minima or transition structure and to derive thermochemical corrections for the free energies.

Preparation of choosing dyes in MeCN/H₂O binary solvent with different volume of water. First prepare a stock solution of choosing dyes (i.e., RhB, NH₂-RhB, NO₂-RhB, ODB, NO₂-ODB and FLu) in MeCN ($C = 1 \times 10^{-4}$ M). And 1

mL stock solution has been transferred to ten 10 mL volumetric flasks, respectively. Then add 0, 1, 2, 3, 4, 5, 6, 7, 8, 9 mL deionized water to the ten flasks and finally fill the flasks to the mark with MeCN. Seal the flasks and invert them to thoroughly mix the solution. The solution was allowed to stand at room temperature for 30 minutes to achieve the balance. Then the solution of choosing dyes ($C = 1 \times 10^{-5}$ M) in MeCN/H₂O with increasing percentage of water by volume from 0 to 90% have been obtained for the spectrum test.

Preparation of WJRPs. The **WJRP** integrated with **NH₂-RhB** was prepared in a layer-by-layer manner, which referred to our previous work.^{S2} The filter paper substrate was coated with a layer of 10 wt% PEG aqueous solution and dried at 70 °C. Then EtOH/H₂O (2/3 by volume) solution of **NH₂-RhB** (0.08 mmol L⁻¹) containing 6 wt% PEG / PVA is coated over the initial PEG layer. Lastly, another protective layer of PEG was coated on the top using 10% PEG aqueous solution after the first two layers were dried completely. The methods used for **NH₂-RhB** were used for the fabrication of **WJRPs** based on **NO₂-ODB** and **FLu**. Owing to the different molar absorption coefficient of these molecules, the contents of each hydrochromic dyes varied slightly. The concentration of **NO₂-ODB** is 0.8 mmol L⁻¹, and the concentration of **FLu** is 0.4 mmol L⁻¹.

Preparation of WJRPs with hygroscopic salts. The filter paper was coated with a layer of 10 wt% PEG aqueous solution and dried at 70 °C. Then the paper was coated with a layer of 30 wt % or saturated hygroscopic salts aqueous solution and dried at 70 °C. After that the paper was coated with EtOH/H₂O (2/3 by volume) solution of **NH₂-RhB** ($C = 0.08$ mmol L⁻¹) containing 6 wt% PEG and dried completely.

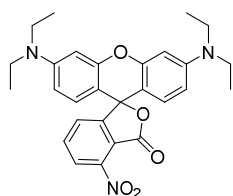
Preparation of WJRPs with polyhydroxy compounds. The polyhydroxy compound/H₂O (2/3 by volume) solution was added on the filter paper which is initially treated with 10 wt% PEG and heated at 110 °C for 15 min. Then the paper was coated with EtOH/H₂O (2/3 by volume) solution of **NH₂-RhB** ($C = 0.08$ mmol L⁻¹) containing 6 wt% PEG and dried completely.

Erasing process of WJRPs with PVA. The used rewritable paper integrated with **NH₂-RhB** was treated with steam fumigation by humidifier or put into the water-jet printer to print water on all over the paper for wetting. After the paper turned to completely magenta, heat the paper at 80 °C on a heater or put the paper in the printer using the heat of printing to evaporate the water (the details have been shown in Movie S3), the paper converted to its original blank state for the next round of usage.

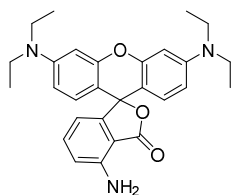
Cytotoxicity assay. HeLa cells (a human epithelial cervical cancer cell line) were cultured at 37 °C under humidified 5% CO₂ in Dulbecco's modified Eagle's medium, supplemented with 10% fetal bovine serum. HeLa cells (5,000/well) were seeded on 96-well tissue culture plates and incubated at 37 °C overnight. Then cells were treated with **NH₂-RhB**, **FLu** and **NO₂-ODB** at a concentration ranging from 0.05 to

1.00 mM for 24 h, respectively. Cytotoxicity of the dyes was evaluated by determining cell viability after incubation with various final concentrations of **NH₂-RhB**, **FLu** and **NO₂-ODB**. The number of viable cells was determined by estimating their mitochondrial reductase activity using the tetrazolium-based colorimetric method (MTT conversion test) with a Microplate Reader (GF-M3000 ELISA ANALYZER, Caihong, China) at a wavelength of 570 nm. The relative cell viability (%) was calculated as: test/control (DMSO) × 100.

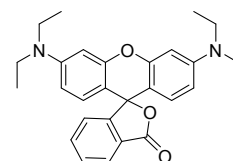
2. Preparation / synthesis of NO₂-RhB, NH₂-RhB, RhB (lactone form), ODB, and NO₂-ODB



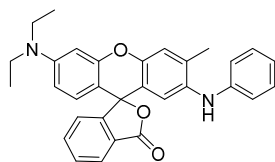
NO₂-RhB was synthesized according to reported literature.^{S3} ¹H NMR (500 MHz, DMSO-d₆): δ (TMS, ppm): 8.11 (d, *J* = 7.8 Hz, 1 H), 7.86 (t, *J* = 7.8 Hz, 1 H), 7.57 (d, *J* = 7.7 Hz, 1 H), 6.74 (d, *J* = 9.0 Hz, 2 H), 6.68-6.56 (m, 4 H), 3.44 (q, *J* = 7.0 Hz, 8 H), 1.13 (t, *J* = 7.0 Hz, 12 H). LC-HRMS: *m/z* calculated for [*M* + *H*]⁺ 488.2180, found 488.2186.



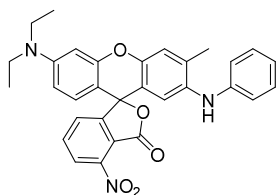
NH₂-RhB was synthesized according to reported literature.^{S3} ¹H NMR (500 MHz, CDCl₃): δ (TMS, ppm): 7.33 (m, *J* = 7.5, 8.0 Hz, 1H), 6.70 (d, *J* = 9.0 Hz, 2H), 6.66 (d, *J* = 8.0 Hz, 1H), 6.44-6.39 (m, 3H), 6.35 (dd, *J* = 9.0, 2.5 Hz, 2H), 5.35 (s, 2 H), 3.36 (q, *J* = 7.0 Hz, 8H), 1.17 (t, *J* = 7.0 Hz, 12H). LC-HRMS: *m/z* calculated for [*M* + *H*]⁺ 458.2438, found 458.2431.



Synthesis of **RhB** (lactone form). 2 M. aqueous NaOH (20 mL) was added to a solution of RhB hydrochloride (0.48 g, 1 mmol) in hexane (35 mL) and stirred overnight, and the resulting colorless hexane solution was evaporated under vacuum to get light pink solid. (0.37 g, 85% yield). ¹H NMR (500 MHz, CDCl₃): δ (TMS, ppm): 7.99 (d, *J* = 7.5 Hz, 1 H), 7.63 (m, *J* = 7.0, 7.5 Hz, 1H), 7.57 (m, *J* = 7.0, 7.5 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1 H), 6.56 (d, *J* = 9.0 Hz, 2 H), 6.44 (s, 2 H), 6.33 (d, *J* = 9.0 Hz, 2 H), 3.35 (q, *J* = 7.0 Hz, 8 H), 1.17 (t, *J* = 7.0 Hz, 12 H). LC-HRMS: *m/z* calculated for [*M* + *H*]⁺ 443.2329, found 443.2325.



ODB was synthesized according to reported literature.^{S4} ¹H NMR (500 MHz, CDCl₃): δ (TMS, ppm): 7.95 (d, *J* = 7.5 Hz, 1 H), 7.64 (t, *J* = 7.5 Hz, 1 H), 7.56 (t, *J* = 7.5 Hz, 1 H), 7.21 (d, *J* = 7.5 Hz, 1 H), 7.15 (s, 1 H), 7.08 (t, *J* = 7.5 Hz, 2 H), 6.75 (t, *J* = 7.0 Hz, 1 H), 6.63-6.54 (m, 4 H), 6.47 (s, 1 H), 6.37 (d, *J* = 7.0 Hz, 1 H), 5.23 (s, 1 H), 3.37 (q, *J* = 7.0 Hz, 4 H), 2.25 (s, 3 H), 1.19 (t, *J* = 7.0 Hz, 6 H). LC-HRMS: *m/z* calculated for [*M* + *H*]⁺ 477.2173, found 477.2177.



Synthesis of **NO₂-ODB**. A mixture of 3-nitrophthalic anhydride (1.93 g, 10 mmol) and N, N-diethyl-3-aminophenol (1.85 g, 11 mmol) was stirred in toluene at 110°C for 5h. After removal of the solvent, dissolved in 20 mL CHCl₃, and washed with hydrochloric acid (1M, 20 mL), water twice, and 20 mL Na₂CO₃ solution (10%) three times, combined the aqueous phase, used hydrochloric acid 2 M to get pH < 3, separated the orange solid **A1** (1.38 g, 78% yield). Following this, a mixture of 4-methoxy-2-methyldiphenylamine (0.64 g, 5 mmol), **A1** (1.07 g, 3 mmol) and H₂SO₄ (98%, 6 mL) were reacted at room temperature for 24 h. The mixture was poured into ice water and filtered. The product was washed to neutral. The filter cake thus obtained was then refluxed with 20 % aq. sodium hydroxide (15 ml) and 20 ml toluene for 2 h. Extract the product from toluene. Then it was recrystallized from toluene and methonal (1:1) to give yellow solid **NO₂-ODB** (0.63 g, 40% yield). Melt point: 249.2-250.8 °C. ¹H NMR (500 MHz, CDCl₃): δ (TMS, ppm): 7.94 (d, *J* = 8.0 Hz, 1 H), 7.76 (t, *J* = 8.0 Hz, 1 H), 7.43 (d, *J* = 8.0 Hz, 1 H), 7.17 (s, 1 H), 7.12 (t, *J* = 8.0 Hz, 2 H), 6.78 (m, *J* = 7.0, 7.5 Hz, 1 H), 6.60-6.59 (m, 4 H), 6.47 (s, 1 H), 6.41 (s, 1 H), 5.26 (s, 1 H), 3.38 (q, *J* = 7.0 Hz, 4 H), 2.26 (s, 3 H), 1.20 (t, *J* = 7.0 Hz, 6 H). ¹³C NMR (126 MHz, CDCl₃): δ (TMS, ppm): 163.40, 156.10, 153.00, 149.87, 147.81, 146.29, 144.66, 136.38, 135.62, 135.54, 129.30, 129.06, 128.69, 128.29, 128.25, 125.32, 124.38, 120.64, 119.84, 119.18, 118.94, 116.15, 115.31, 108.50, 103.22, 97.53, 83.40, 44.40, 18.09, 12.52, 1.09. LC-HRMS: *m/z* calculated for [*M* + H]⁺ 522.1984, found 522.1990.

3. Single crystal of NO₂-ODB

Single crystals of **NO₂-ODB** were grown by vapor diffusion of acetone/hexane into a CH₂Cl₂ solution of **NO₂-ODB**.

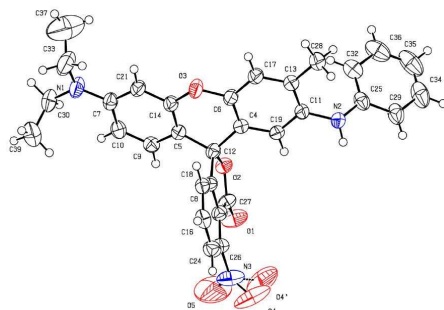


Figure S1. Single-crystal X-ray structure of **NO₂-ODB** (50% probability ellipsoids).

Table S1. Summary of crystal data and intensity collection parameters for **NO₂-ODB**.

Compound	NO ₂ -ODB
Formula	C ₃₁ H ₂₇ N ₃ O ₅
Formula mass	521.56
Space group	triclinic, P -1
<i>a</i> / Å	10.558(2)
<i>b</i> / Å	11.152(2)
<i>c</i> / Å	11.868(2)
<i>α</i> / °	89.94(3)
<i>β</i> / °	86.75(3)
<i>γ</i> / °	72.15(3)
<i>V</i> / Å ³	1327.8(5)
<i>Z</i>	2
<i>ρ</i> / g.cm ⁻³	1.304
<i>μ</i> / mm ⁻¹	0.090
<i>F</i> ₀₀₀	548.0
Temp, (K)	293 K
No. of collected reflns.	10429
No. of unique reflns. (<i>R</i> _{int})	4654(0.0316)
Data/restraints/parameters	4654/0/369
<i>R</i> ₁ , <i>wR</i> ₂ [obs <i>I</i> > 2σ (<i>I</i>)]	0.0568, 0.1542
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0799, 0.1674
Residual peak/ hole e.Å ⁻³	0.49/ -0.355
Goodness-of-fit on <i>F</i> ₂	1.088
CCDC numbers	1486791

4. UV-Vis spectra of fluoran dyes in different solvents

(1) UV-Vis spectra of **RhB**, **NH₂-RhB** and **NO₂-RhB** in different solvents

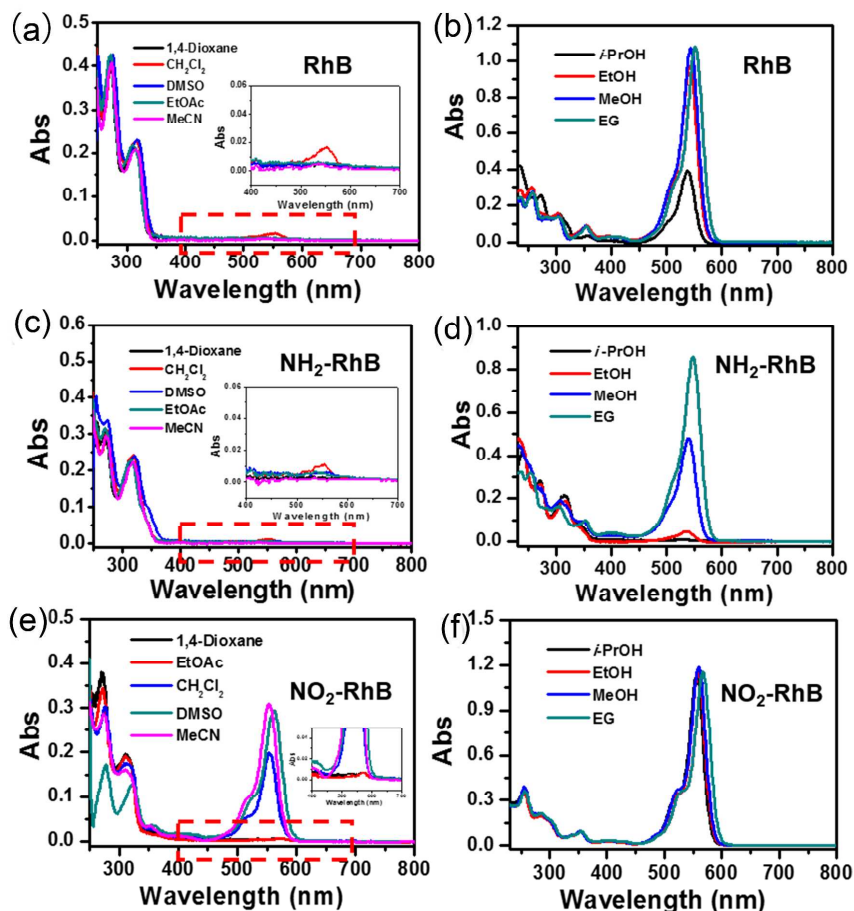


Figure S2. UV-Vis spectra of **RhB**, **NH₂-RhB** and **NO₂-RhB** (1×10^{-5} mol L⁻¹) in different (a), (c), (e) aprotic solvents and (b), (d), (f) protic solvents at 20 °C, respectively.

As shown in Figure S2 a and b, **RhB** and **NH₂-RhB** nearly have no absorption peak in visible spectra, which indicates they are not favorable to exist as zwitterionic forms in aprotic solvents no matter how strong the dipolarity of the solvent is; while their lactone forms and zwitterionic forms coexist in protic solvents. These results indicate hydrogen bonds (H-bond) play important roles. Compared to **RhB**, **NH₂-RhB** is more stable in lactone form as *i*-PrOH cannot switch **NH₂-RhB** open. From Figure S2 e and f, we can see for **NO₂-RhB**, its lactone and zwitterionic forms can coexist in strong dipolarity solvents, and it can nearly completely exist as zwitterionic forms in protic solvents. It indicates introduction of nitro promotes the equilibrium of **NO₂-RhB** shifting to zwitterionic isomers. These results show that molecular substituents and microenvironment

have great effect on equilibrium positions of **RhB** derivatives. It is worth noting that the dynamic equilibria between their lactone forms and zwitterionic forms have always been existing even in unfavorable aprotic solvents, which is easy to be ignored. In addition, **RhB**, **NH₂-RhB** show obvious ring-open in CH₂Cl₂ compared to other aprotic solvents (see amplified insets of a and b), which might be due to the moderate hydrogen bonding donating ability of CH₂Cl₂ from its multiple directions dipole.

(2) UV-Vis spectra of **ODB** and **NO₂-ODB** in different solvents

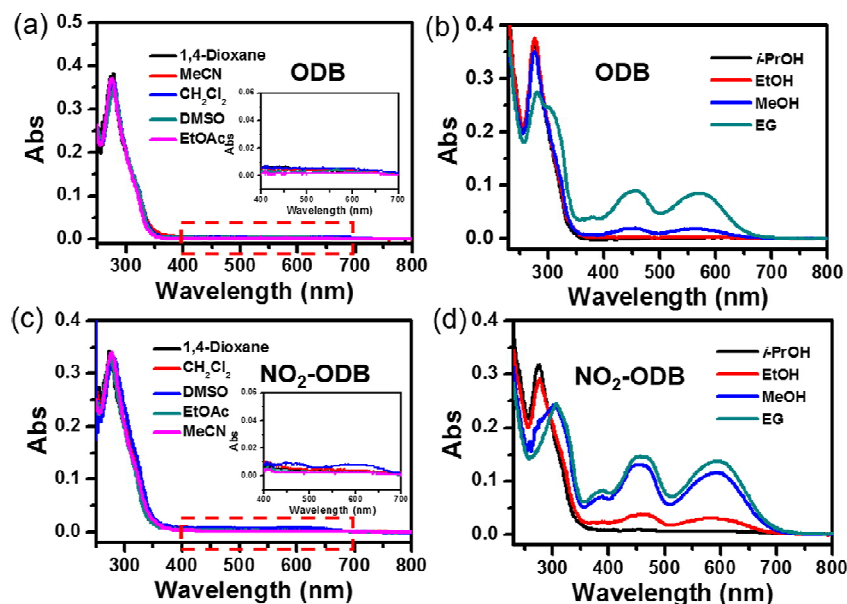


Figure S3. UV-Vis spectra of **ODB** and **NO₂-ODB** (1×10^{-5} mol L⁻¹) in different (a), (c) aprotic and (b), (d) protic solvents at 20 °C, respectively.

From Figure S3 we can see that none of the aprotic solvents switched **ODB**, no matter how strong their dipolarity was. **ODB** and **NO₂-ODB** could partially exist in zwitterions in protic solvents, such as MeOH and EG. The results indicate hydrogen bonds (H-bond) play important roles. In contrast with **ODB**, **NO₂-ODB** is much easier to be switched open as its lactone and zwitterion coexist even in EtOH. From inset of Figure S3c, the aprotic solvent with large dipolarity (i.e., DMSO) can also switch **NO₂-ODB** open, which might be due to the strong electron-withdrawing property of the nitro group enhance dipole of ortho lactones (-CO-O-). Besides, owing to the two peak contributes one color, the molar absorption coefficients of **ODB** and **NO₂-ODB** is low.

(3) UV-Vis spectra of **FLu** in different solvents

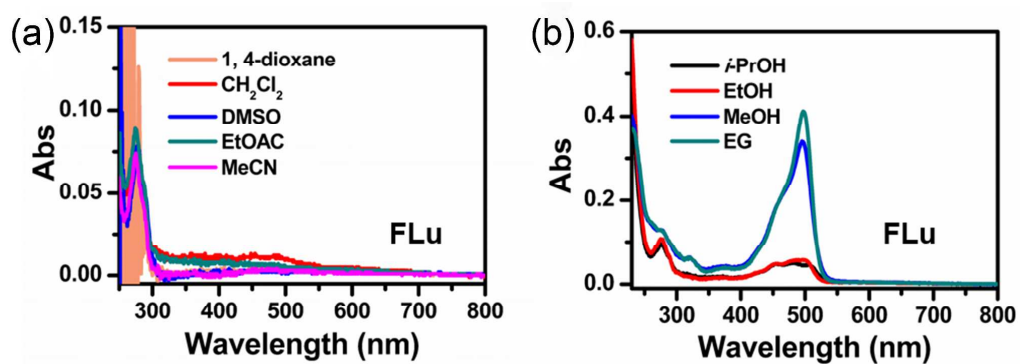


Figure S4. UV-Vis spectra of **FLu** (1 × 10⁻⁵ mol L⁻¹) in different (a) aprotic and (b) protic solvents at 20 °C.

5. Theoretical calculations for optimized structures and energy of lactone, zwitterion and transition state of $\text{NH}_2\text{-RhB}$, RhB and $\text{NO}_2\text{-RhB}$

Table S2. The energy of each optimized structure from lactone form to zwitterionic form was calculated using B3LYP/6-31G (d, p).

	E (lactone) / a.u.	E (transition state) / a.u.	E (zwitterion) / a.u.
RhB	-1420.3053	-1420.2959	-1420.2962
$\text{NH}_2\text{-RhB}$	-1475.6743	---- ^a	---- ^a
$\text{NO}_2\text{-RhB}$	-1624.7953	-1624.7865	-1624.7894

a) The zwitterionic structure of **$\text{NH}_2\text{-RhB}$** is not obtained by B3LYP/6-31G (d, p) calculations because it is not stable in acetonitrile.

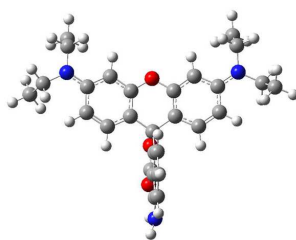


Figure S5. The optimized structure of **$\text{NH}_2\text{-RhB}$** lactone in acetonitrile with B3LYP/6-31G (d, p) calculations.

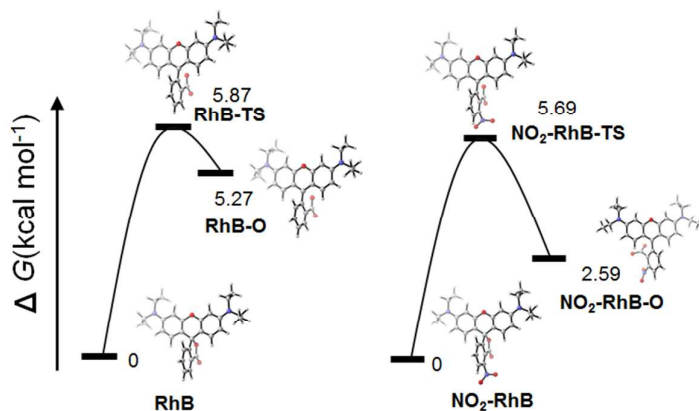


Figure S6. The optimized structures and Gibbs free energy of lactone, transition state (TS) and zwitterionic isomers (O) of **RhB** and **$\text{NO}_2\text{-RhB}$** in acetonitrile with B3LYP/6-31G (d, p) calculations. Zero-point corrected Gibbs free energies of the main stationary points on the ground-state potential Gibbs free energy surface of lactone forms of **RhB** and **$\text{NO}_2\text{-RhB}$** , respectively.

6. Molar extinction coefficient of fluoran dyes

Table S3. Molar extinction coefficient of **RhB**, **NH₂-RhB**, **NO₂-RhB**, **ODB**, **NO₂-ODB** and **FLu**, respectively.

	RhB	NH₂-RhB	NO₂-RhB	ODB	NO₂-ODB	FLu
λ_{max} / nm	557	552	568	444/581	447/604	490
ϵ / L • mol ⁻¹ • cm ⁻¹ × 10 ⁴	12.1	11.2	12.2	1.83/2.11	1.96/1.93	7.75

The molar absorption coefficients of the fluoran dyes colored form at the peak maximum were in the range (3.8-12.2) × 10⁴ L • mol⁻¹ • cm⁻¹ in MeCN/H₂O=1/1 (v/v) after addition of CF₃COOH or t-BuONa (for **FLu**). Besides, owing to the two peaks contribute one color, the molar absorption coefficients of **ODB** and **NO₂-ODB** are low.

7. Stability of $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$ in aqueous solution.

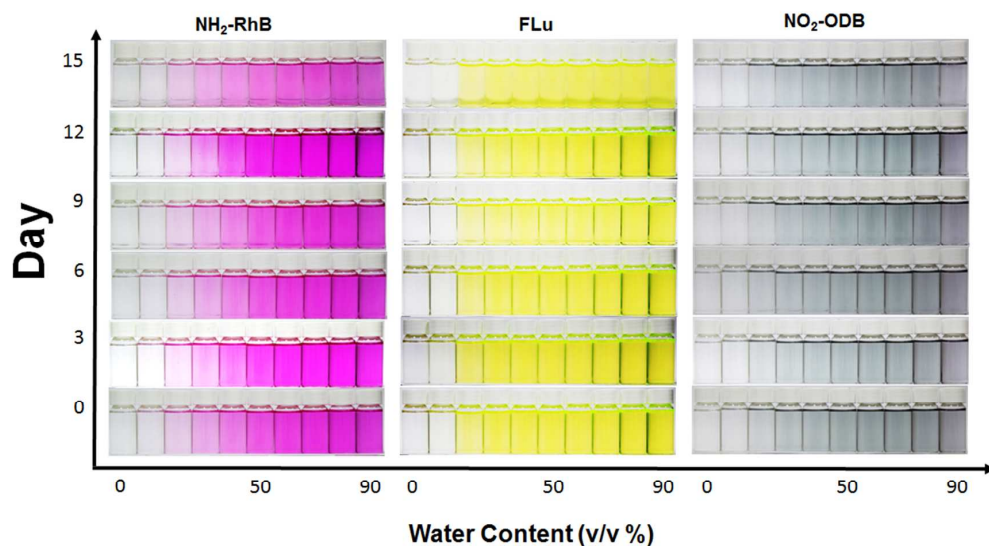


Figure S7. Photographs of the solution of $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$ in their zwitterionic forms ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) in $\text{MeCN}/\text{H}_2\text{O}$ with different amount of water (from 0% to 90%) over time.

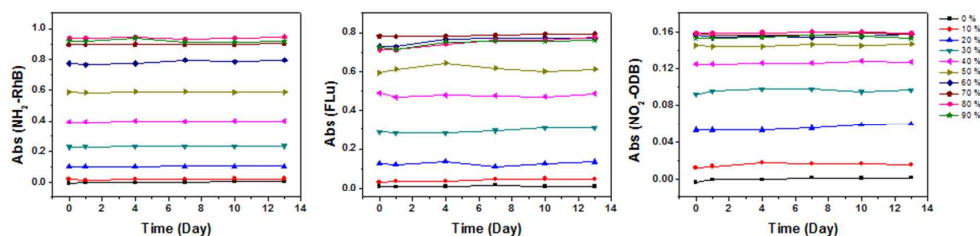


Figure S8. Plots of maximum absorbance intensity for $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$ in visible region in their zwitterionic forms ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) in $\text{MeCN}/\text{H}_2\text{O}$ against increasing percentage of water by volume from 0% to 90% over time.

8. Hydrochromism of $\text{NH}_2\text{-RhB}$ compared with its acidochromism in UV-Vis spectra

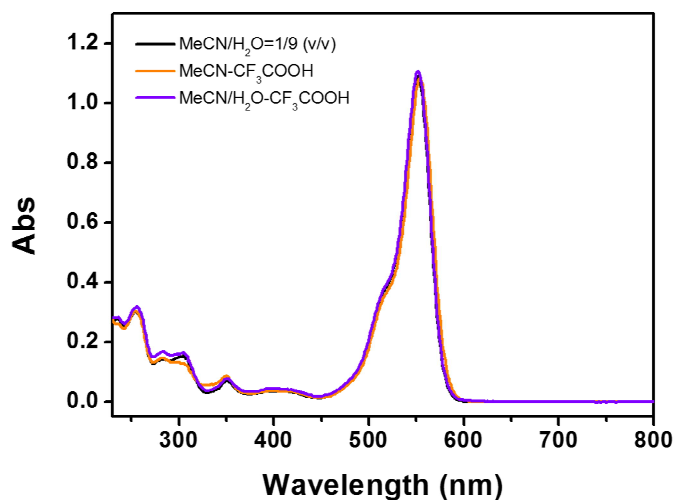


Figure S9. UV-Vis spectra of $\text{NH}_2\text{-RhB}$ in MeCN/ H_2O ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) with water content of 90% (v/v) without and with CF_3COOH and in MeCN ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) with CF_3COOH .

9. Ring-closing of $\text{NH}_2\text{-RhB}$ in MeCN/ H_2O as MeCN content increases

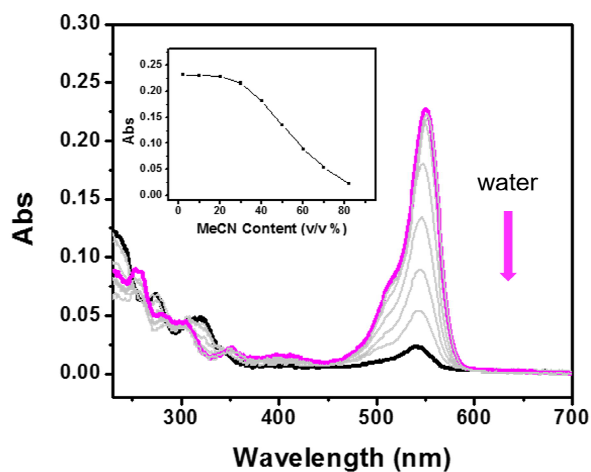


Figure S10. UV-Vis absorption spectra of $\text{NH}_2\text{-RhB}$ in variable mixtures of MeCN and water with increasing percentage of MeCN by volume from 2% to 82% ($C = 2 \times 10^{-6} \text{ mol L}^{-1}$). Inset: Plot of absorbance at λ_{max} as MeCN content increases.

10. Fluorescent properties of $\text{NH}_2\text{-RhB}$ in solution

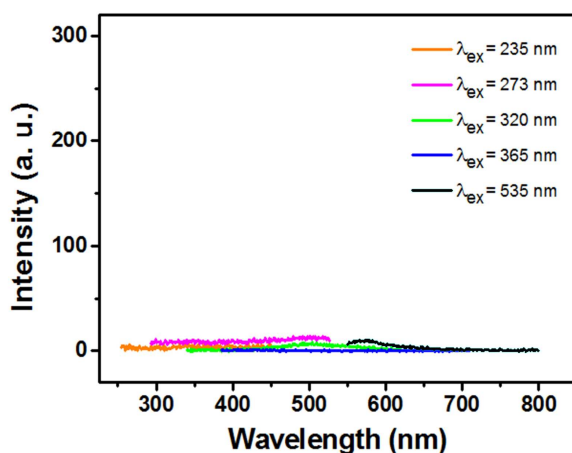


Figure S11. Fluorescence spectra of $\text{NH}_2\text{-RhB}$ in MeCN ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) with five excitation wavelength of 235, 273, 320, 365 and 535 nm, respectively.

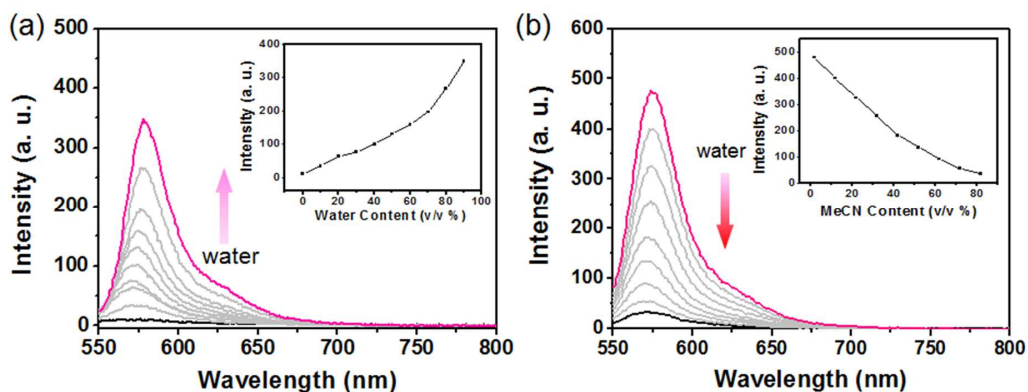


Figure S12. (a) Fluorescence spectra of $\text{NH}_2\text{-RhB}$ in variable mixtures of MeCN and water with increasing percentage of water by volume from 0 to 90% ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) with an excitation wavelength of 535 nm. Inset: Plot of fluorescent intensity at λ_{max} as water content increases. (b) Fluorescence spectra of $\text{NH}_2\text{-RhB}$ in variable mixtures of MeCN and water with increasing percentage of MeCN by volume from 2% to 82% ($C = 2 \times 10^{-6} \text{ mol L}^{-1}$) with an excitation wavelength of 535 nm. Inset: Plot of fluorescent intensity at λ_{max} as MeCN content increases.

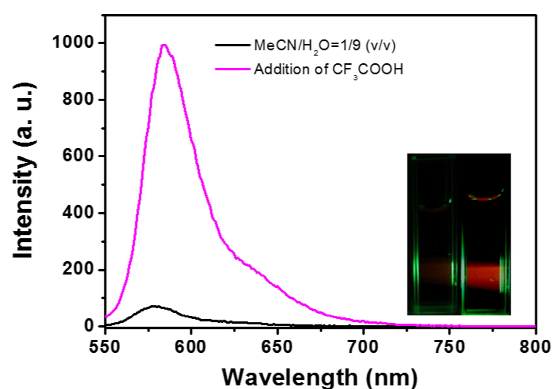


Figure S13. Fluorescence spectra ($\lambda_{\text{ex}} = 535 \text{ nm}$) of **NH₂-RhB** ($C = 1 \times 10^{-5} \text{ mol L}^{-1}$) in MeCN/H₂O with water content of 90% before ($\Phi_f = 0.95$) and after ($\Phi_f = 8.42$) addition of CF₃COOH, respectively. Inset: Photographs of **NH₂-RhB** in MeCN/H₂O (v/v 1/9) before (left) and after (right) addition of CF₃COOH excited with wavelength of 535 nm.

11. Hydrochromism of NH₂-RhB compared with its acidochromism in ¹H NMR spectroscopy

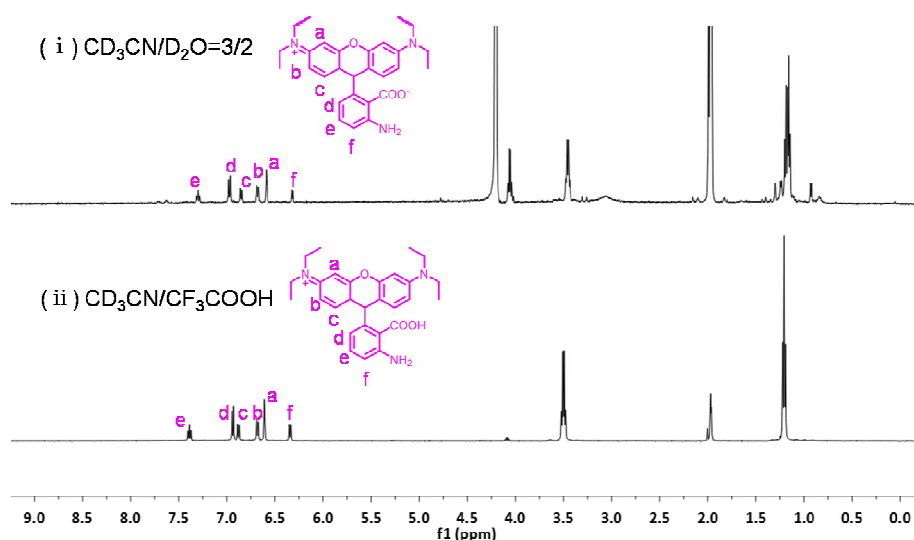


Figure S14. ¹H NMR spectra of **NH₂-RhB** (5 mg) in 0.5 mL (i) CD₃CN/D₂O = 3/2 (v/v), (ii) CD₃CN with the addition of 1 equiv. (0.74 μL) CF₃COOH.

12. Acido-, baso- and hydro-chromism of FLu

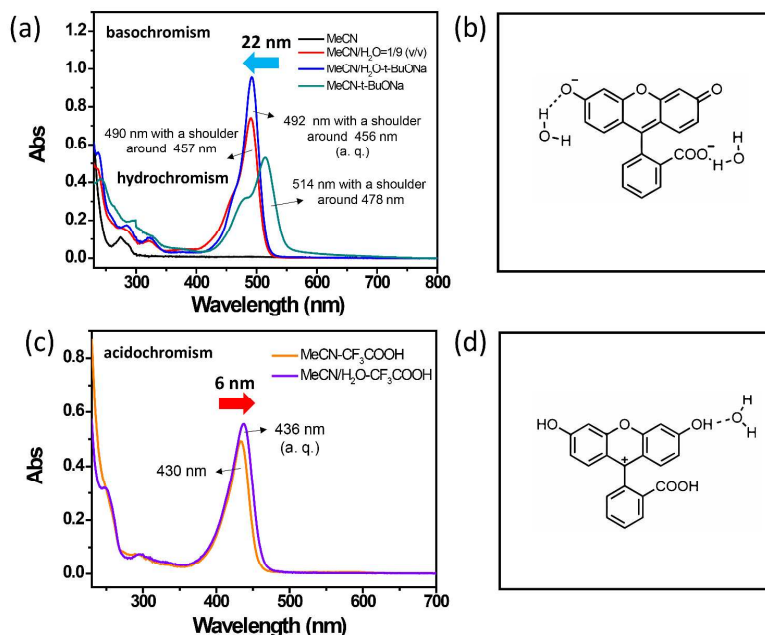


Figure S15. (a) UV-Vis absorption spectra of **FLu** (1×10^{-5} mol L⁻¹) in MeCN or in MeCN/H₂O (v/v 1/9) with or without t-BuONa. (b) The main isomer of **FLu** in MeCN/H₂O (v/v 1/9). (c) UV-Vis absorption spectra of **FLu** (1×10^{-5} mol L⁻¹) in MeCN or in MeCN/H₂O (v/v 1/9) with CF₃COOH. (d) The main isomer of **FLu** in MeCN/H₂O (v/v 1/9) with acid.

Table S4. Different states of **FLu** in aqueous solution with various pH and their corresponding λ_{max} .^{S5,S6}

pH	states	isomers	λ_{max} (nm)
< 2	cation		436
around 3.3	neutral species		434 and 475 (shoulder)
around 5.5	anion		472 and 453
>8	dianion		490 and 475 (shoulder)

13. Effect of PEG on WJRPs

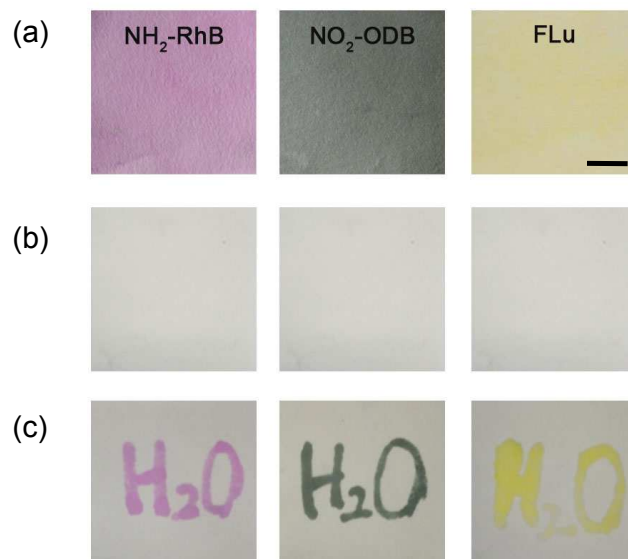


Figure S16. Photographs of WJRPs based on $\text{NH}_2\text{-RhB}$, $\text{NO}_2\text{-ODB}$ and FLu (a) without and with PEG (b) before and (c) after writing with water, respectively (scale bar = 1 cm).

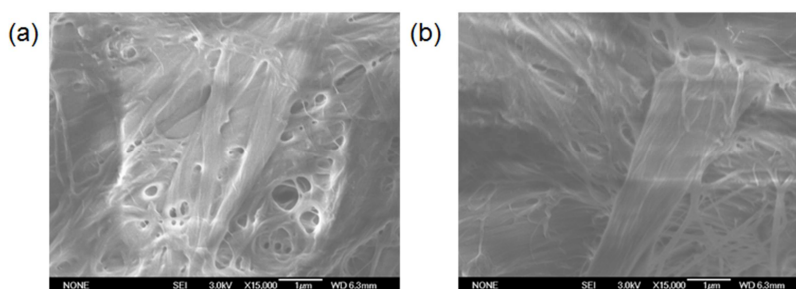


Figure S17. SEM images of the surface of (a) filter paper and (b) filter paper treated with PEG.

14. Effect of different hygroscopic compounds on retaining time of water-writings on $\text{NH}_2\text{-RhB}$ based WJRP

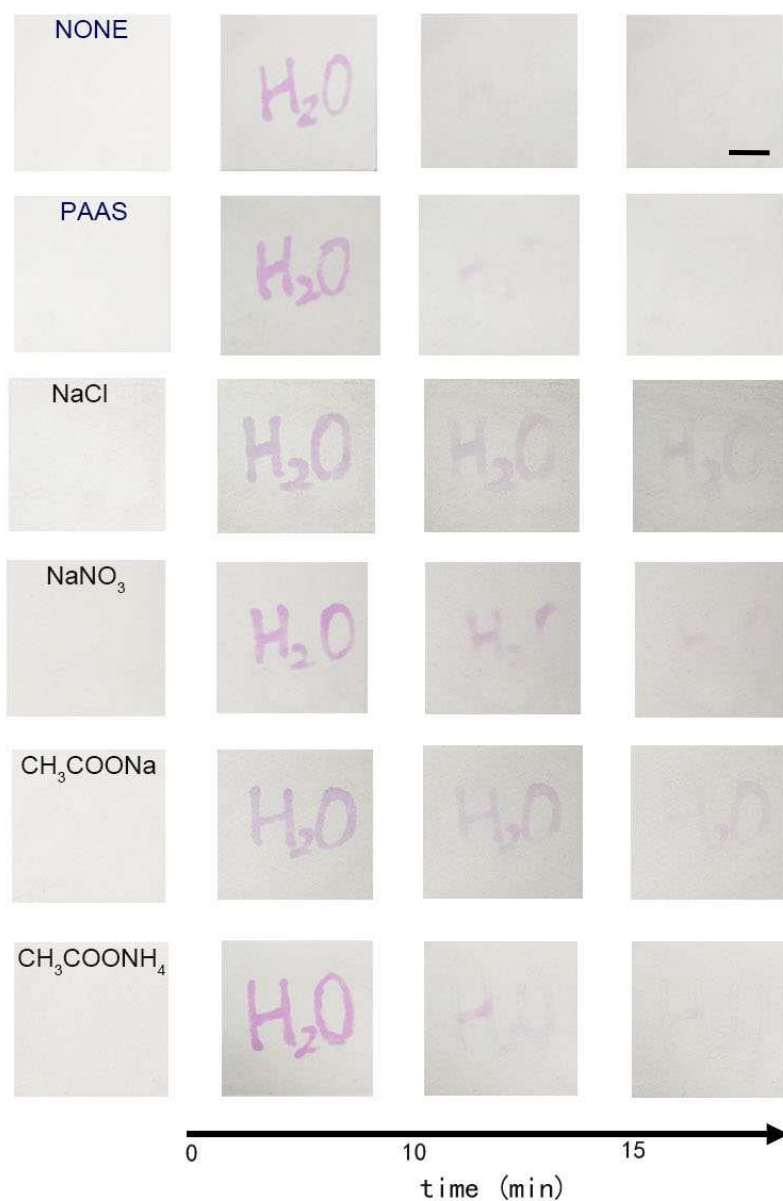


Figure S18. Photographs of WJRP based on $\text{NH}_2\text{-RhB}$ with different hygroscopic salts, such as sodium polyacrylate (PAAS), NaCl, NaNO₃, CH₃COONa and CH₃COONH₄ to replace glycerin written by water as time passed by (scale bar = 1 cm).

15. Effect of glycerin on retaining time of water-writings on $\text{NH}_2\text{-RhB}$ based WJRP

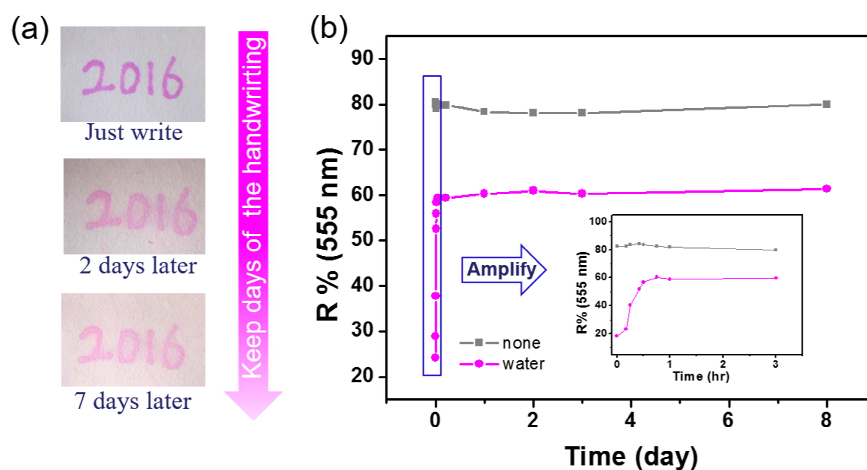


Figure S19. (a) Contrast photos of "2016" via handwriting on the $\text{NH}_2\text{-RhB}$ based WJRP with different keep days. (b) Time-dependent reflective visible spectra of the WJRP at 555 nm before (gray dots) and after (magenta dots) addition of water. Inset: Amplified plot of time-dependent reflection at 555 nm of rewritable paper in 3 hours written by water.

16. Effect of different polyhydroxy compounds on retaining time of water-writings on $\text{NH}_2\text{-RhB}$ based WJRP

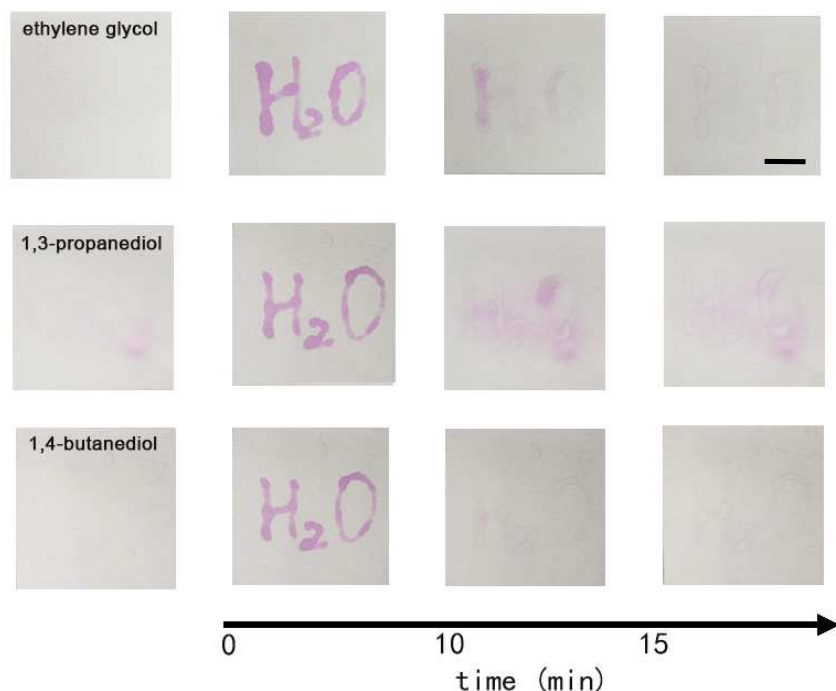


Figure S20. Photographs of WJRPs based on $\text{NH}_2\text{-RhB}$ with some polyhydroxy compounds, such as ethylene glycol, 1, 3-propanediol and 1, 4-butanediol written by water as time passed by (scale bar = 1 cm).

17. Photographic images of luminescence of water-jet prints



Figure S21. Photographs of luminescence of prints on $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$ based WJRPs, respectively, after printed with water irradiated by handheld UV lamp at 365 nm (scale bar = 5 mm).

18. Microscope images of the water-jet prints

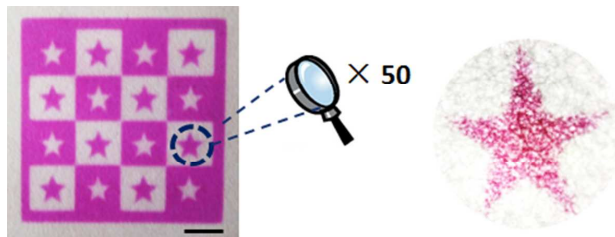


Figure S22. Water-jet prints of the intricate structure and the pattern of the water-jet prints in black circle to be magnified 50 times by microscope, scale bar = 1 cm.

19. Compared the substrate of filter paper with commercial printing paper

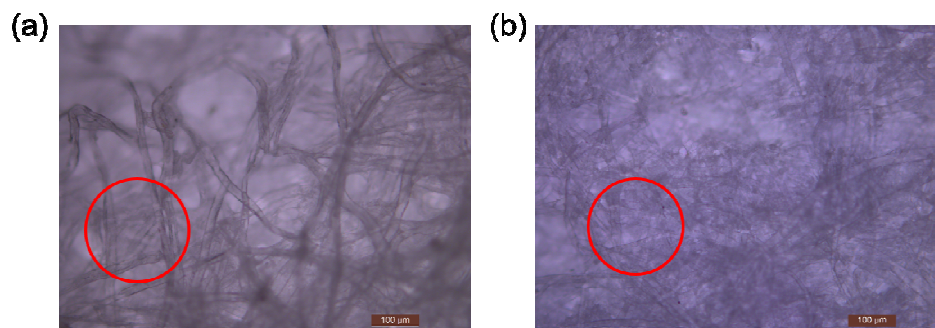


Figure S23. Microscopy images of **WJRP**s (without PVA) of **NH₂-RhB** based on substrate of (a) filter paper and (b) commercial printing paper, respectively. The voids among the fibers in filter paper are larger than that in commercial printing paper, as marked in red circles, which make the filter paper more favorable to absorb dyes showing deeper color after addition of water.

20. Cost comparisons between water-jet printing and ink-jet printing

Table S5. Cost comparisons between water-jet printing and HP ink-jet printing.

	HP ink-jet printing	Water-jet printing	Additional information
Printing paper	A4 paper	A4 paper	Paper size 21 × 29.7 cm ²
RMB¥*/sheet	0.04	0.04	---
Ink	ink	water	Take HP 704 as an example
RMB¥*/sheet	0.1	---	---
Other materials (Dosage/sheet)	---	Dyes (0.02 mg-0.2 mg) PEG (0.3 g), PVA (0.2 g) EtOH (2 mL)	---
RMB¥*/sheet	---	0.00024 +0.036+0.016+0.012 (Dyes 0.2 mg)	The bulk price of the dyes is estimated as 1200 (RMB ¥) /1 kg
Total cost for one paper	0.14	0.10	---
Total costs for 30 sheets printing	4.20	0.10	One sheet of rewritable paper can at least be used for thirty times

Notes:

* RMB ¥ is the abbreviation for Renminbi Yuan.

Market price for the other materials:

Polyethylene glycol (PEG, average Mn = 20000): 60 RMB ¥ / 500 g;

Polyvinyl alcohol (PVA, average Mn = 300-400): 30 RMB ¥ / 500 g;

Ethanol (EtOH): 4 RMB ¥/500 g;

A4 paper: 20 RMB ¥ / Pack (500 sheets, 29.7 cm × 21 cm).

Ink cartridge for HP ink-jet printer: 50 RMB ¥ (HP 704, 22 mL) (One cartridge can be limited to print 480 sheets for black mark and 200 sheet for color mark, calculated by 5% cover printing for each sheet)

21. Result of cell cytotoxicity test of $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$

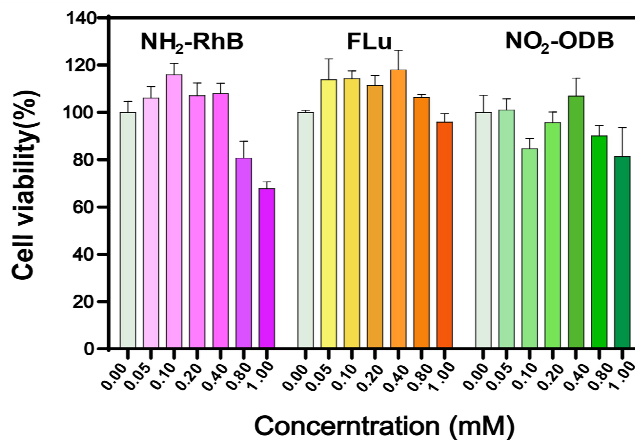


Figure S24. MTT assay of the cytotoxicity of $\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$ by the cell viability of HeLa cells incubated with various concentrations, respectively. The viability of HeLa cells after being cultured in solutions of dyes ($\text{NH}_2\text{-RhB}$, FLu and $\text{NO}_2\text{-ODB}$) at a concentration from 0.05 mM to 1.00 mM for 24 h. All three dyes showed nontoxic or very low cytotoxicity (over 90% viability) under working concentration ($\text{NH}_2\text{-RhB}$ 0.08 mM, FLu 0.4 mM and $\text{NO}_2\text{-ODB}$ 0.8 mM) within 24 h of incubation time.

22. The coordination of structures

RhB

C	0.11173800	2.87830000	-1.78610100
H	0.15501300	2.07248000	-2.51194700
C	0.13688600	4.21379700	-2.19724700
H	0.20011600	4.44367500	-3.25651300
C	0.08172300	5.26564800	-1.26818400
H	0.10292500	6.29209600	-1.62002500
C	0.00043500	4.99837600	0.09734700
H	-0.04301300	5.79572100	0.83226600
C	-0.02396500	3.66136800	0.49515200
C	0.03009700	2.61694200	-0.42058400
C	-0.01574200	1.28287400	0.30705400
C	-0.10565800	3.09148100	1.85633900
C	-1.24480300	0.46605300	0.01361200
C	-2.52416700	1.03943000	-0.07379800
H	-2.62402400	2.11664000	0.02134700
C	-3.66847200	0.28706700	-0.26867900
H	-4.61919000	0.80054400	-0.31461100
C	-3.59941700	-1.12940600	-0.39958900
C	-2.31835000	-1.71347200	-0.30122400
H	-2.16577300	-2.78121400	-0.37810000
C	-1.18550900	-0.92634700	-0.10279300
C	-6.05156100	-1.27366300	-0.72816800
H	-6.68365400	-1.95488000	-1.30467100
H	-5.97847100	-0.35703700	-1.32310500
C	-6.72295300	-0.97259200	0.61836700
H	-6.89877400	-1.89048100	1.18650500
H	-7.68985300	-0.48556900	0.45313900
H	-6.10850000	-0.30735400	1.23163700
C	-4.64465400	-3.35112200	-0.71640000
H	-3.78074900	-3.62777100	-1.33128700
H	-5.52589800	-3.69298800	-1.26594800
C	-4.57745900	-4.07183100	0.63676300
H	-4.48555300	-5.15184800	0.48049600
H	-3.71745300	-3.74055300	1.22561400
C	1.18178100	-0.93255800	0.03003800
C	1.23451100	0.45933900	0.15994600
C	2.51837500	1.02711200	0.21824200
H	2.61143900	2.10466200	0.31621700
C	3.67358400	0.26998200	0.14841100
H	4.62737700	0.77940200	0.17959600
C	3.61195500	-1.14667000	0.01719100

C	2.32593500	-1.72504200	-0.04118200
H	2.18095200	-2.79341400	-0.12743300
C	6.08760600	-1.33428000	0.11177600
H	6.73253500	-2.11735100	0.52254100
H	6.05021900	-0.55016900	0.87375000
C	6.69850900	-0.79404200	-1.18664200
H	6.78207000	-1.58668500	-1.93701100
H	7.70176400	-0.39790700	-0.99818400
H	6.08747900	0.00864900	-1.60952000
C	4.69846700	-3.35434800	-0.31162700
H	5.62354500	-3.63009600	-0.82769000
H	3.88895200	-3.56755600	-1.01651100
C	4.54504300	-4.20405900	0.95548600
H	5.37872200	-4.03129800	1.64355400
H	4.53239000	-5.26841800	0.69867800
H	3.61653900	-3.96928000	1.48402000
N	-4.72638000	-1.89113300	-0.63600300
N	4.75383100	-1.91424900	-0.05752600
O	-0.16882200	3.66594500	2.92630200
O	-0.00341700	-1.62412100	-0.04115300
O	-0.10097100	1.73887100	1.75508700
H	-5.48123300	-3.88991000	1.22497900

RhB-TS

C	0.05705500	3.08536500	-1.74704200
H	0.10852500	2.37007700	-2.56249300
C	0.05309300	4.45697900	-2.01264100
H	0.10192100	4.80304900	-3.04068700
C	-0.01380100	5.38378900	-0.96619200
H	-0.01686000	6.44743100	-1.18487200
C	-0.07601000	4.93874900	0.35412700
H	-0.12867300	5.63256800	1.18722900
C	-0.07157600	3.56969700	0.62130200
C	-0.00619100	2.64228000	-0.42122300
C	-0.00919300	1.18509900	-0.06775800
C	-0.13427300	2.97106000	2.00374200
C	-1.21580800	0.42210500	-0.23646500
C	-2.50393000	0.99543000	-0.36081800
H	-2.59309200	2.07628100	-0.36442600
C	-3.64145700	0.23146300	-0.46934700
H	-4.59384700	0.73627200	-0.55188200
C	-3.57876700	-1.19966600	-0.46541300
C	-2.29860900	-1.78516900	-0.32641300
H	-2.15426500	-2.85597200	-0.30386200

C	-1.16843400	-0.98885200	-0.21891700
C	-6.03520400	-1.34993100	-0.73909700
H	-6.67504800	-2.07912600	-1.24201400
H	-5.96840600	-0.49166300	-1.41444600
C	-6.67803500	-0.93257100	0.58900600
H	-7.65112200	-0.46824100	0.39911300
H	-6.05639000	-0.21084600	1.12642800
H	-6.83552800	-1.79654100	1.24033800
C	-4.63646700	-3.43001600	-0.57133300
H	-3.78191500	-3.76060200	-1.17076900
H	-5.52623200	-3.80677300	-1.08133500
C	-4.55992200	-4.02932400	0.83824500
H	-4.47908400	-5.11907700	0.77224700
H	-3.69029900	-3.65718900	1.38683800
C	1.19702300	-0.96800400	-0.09452700
C	1.22085700	0.44438000	-0.10978900
C	2.50485600	1.04150800	-0.10382900
H	2.57376900	2.12379000	-0.11752300
C	3.66076900	0.29866700	-0.08771100
H	4.60906800	0.81823000	-0.10572600
C	3.62226500	-1.13328500	-0.06402900
C	2.34599600	-1.74348200	-0.07391300
H	2.22177000	-2.81719500	-0.05084300
C	6.09768400	-1.25857300	0.07784600
H	6.73800000	-1.97692100	0.59803800
H	6.03533400	-0.38531300	0.73194700
C	6.72478900	-0.88558600	-1.26914700
H	6.82539200	-1.76653900	-1.91061900
H	7.72224400	-0.46214700	-1.11467300
H	6.11753900	-0.14703700	-1.80033500
C	4.74657500	-3.33985400	-0.11665400
H	5.68564700	-3.65407100	-0.58131900
H	3.95281900	-3.65354800	-0.80020400
C	4.58944500	-4.01942500	1.24778100
H	5.40877200	-3.74207100	1.91812900
H	4.60085300	-5.10742900	1.12894100
H	3.64833300	-3.73690000	1.72776600
N	-4.70640900	-1.96369800	-0.61133300
N	4.77058300	-1.87474900	-0.04275300
O	-0.19110000	3.69150800	3.01466500
O	0.01777400	-1.65944400	-0.10722300
O	-0.12034200	1.68410400	1.97791400
H	-5.45546300	-3.78971500	1.41799900

RhB-O

C	0.05296600	3.10741600	-1.75684600
H	0.10740100	2.40571400	-2.58413500
C	0.04656000	4.48100600	-2.00541300
H	0.09621100	4.84166800	-3.02844200
C	-0.02409200	5.38588300	-0.94232700
H	-0.02968800	6.45435700	-1.13740300
C	-0.08680300	4.91081100	0.36682600
H	-0.14209700	5.58680400	1.21413700
C	-0.08053700	3.53814500	0.62770200
C	-0.01119100	2.63072400	-0.43948400
C	-0.00621600	1.15457800	-0.19530200
C	-0.14705900	2.98809100	2.04623900
C	-1.20981600	0.40566800	-0.31422200
C	-2.50250900	0.98209300	-0.41649300
H	-2.58792000	2.06280400	-0.42734500
C	-3.63944000	0.21864500	-0.49305700
H	-4.59364800	0.72221400	-0.55837800
C	-3.57857200	-1.21555400	-0.47819700
C	-2.29625900	-1.80471700	-0.36218700
H	-2.15470500	-2.87546700	-0.33008500
C	-1.16541000	-1.01016300	-0.28655600
C	-6.04021500	-1.35874700	-0.69413100
H	-6.69163900	-2.09279700	-1.17388300
H	-5.98620900	-0.50906000	-1.38081300
C	-6.64996900	-0.92594400	0.64424200
H	-7.62622400	-0.46201700	0.47118100
H	-6.01478400	-0.19944300	1.15881400
H	-6.79399800	-1.78228700	1.30844700
C	-4.64314400	-3.44250500	-0.53800300
H	-3.80316600	-3.78025500	-1.15314700
H	-5.54527000	-3.81919500	-1.02515900
C	-4.53842700	-4.02728200	0.87558300
H	-4.46368400	-5.11778300	0.81768200
H	-3.65551700	-3.65387600	1.40145400
C	1.20085000	-0.98518400	-0.16019100
C	1.21792500	0.43233500	-0.18481100
C	2.50228800	1.03693200	-0.15345800
H	2.56506500	2.11907600	-0.17380700
C	3.65659700	0.29861500	-0.10452000
H	4.60374100	0.82027500	-0.10228400
C	3.62311900	-1.13645000	-0.07306300
C	2.34954500	-1.75477000	-0.10766100
H	2.23055200	-2.82865100	-0.07626800

C	6.09515700	-1.24725500	0.12209600
H	6.72465000	-1.95899500	0.66362800
H	6.01679800	-0.36729700	0.76470100
C	6.74731800	-0.88986900	-1.21672000
H	6.86041200	-1.77788100	-1.84608100
H	7.74140200	-0.46489300	-1.04667900
H	6.15085100	-0.15707600	-1.76761900
C	4.75691600	-3.33668900	-0.07839200
H	5.70738300	-3.64872100	-0.52009800
H	3.97927900	-3.66152400	-0.77457100
C	4.57566300	-3.99940300	1.29100200
H	5.37957000	-3.70958000	1.97443100
H	4.59544200	-5.08843400	1.18485100
H	3.62330600	-3.71640400	1.74774700
N	-4.70870200	-1.97479300	-0.58871500
N	4.77118100	-1.86930300	-0.01954200
O	-0.20082400	3.79687100	2.99914500
O	0.02319700	-1.67420600	-0.18956000
O	-0.14013600	1.71824900	2.10903800
H	-5.42022500	-3.77837600	1.47201000

NO₂-RhB

C	-0.10608400	2.12197100	2.02370700
H	-0.09027200	1.23488300	2.64784000
C	-0.14575800	3.39391100	2.59162500
H	-0.16336200	3.50672000	3.67010500
C	-0.16631100	4.53873000	1.78538900
H	-0.20138200	5.52804000	2.22450200
C	-0.16707800	4.40497300	0.40144400
C	-0.10996300	3.13609100	-0.18806500
C	-0.07525900	2.01551400	0.63379000
C	0.00541800	0.74745000	-0.19975100
C	0.03267600	2.67639800	-1.60227100
C	1.26064700	-0.04904000	0.02953700
C	2.52737900	0.55466700	0.10296500
H	2.60118100	1.63606400	0.03286100
C	3.69334600	-0.17315800	0.25283500
H	4.63205100	0.36249500	0.28963800
C	3.66169900	-1.59410000	0.35083000
C	2.39349000	-2.20747700	0.26403400
H	2.26881900	-3.28024600	0.31555100
C	1.23741900	-1.44506100	0.11004900
C	6.12240300	-1.68400200	0.62829400
H	6.78110800	-2.36224300	1.17775400

H	6.03726100	-0.78341300	1.24547200
C	6.76146300	-1.33655800	-0.72266500
H	6.94710800	-2.23696600	-1.31505400
H	7.72009800	-0.83163000	-0.56337300
H	6.12109300	-0.67141200	-1.30898700
C	4.76687500	-3.79575200	0.59025600
H	3.92441400	-4.10894600	1.21719800
H	5.66850200	-4.12857300	1.11130400
C	4.68668400	-4.48348800	-0.77904600
H	4.62563400	-5.56901700	-0.64827600
H	3.80529900	-4.15989900	-1.33984400
C	-1.12941900	-1.51023300	-0.00799000
C	-1.22143800	-0.11717000	-0.09836200
C	-2.52048600	0.41642600	-0.15532600
H	-2.64524300	1.49316700	-0.22311900
C	-3.65375700	-0.37452200	-0.12193800
H	-4.62135400	0.10829100	-0.14986900
C	-3.55278800	-1.79255100	-0.03158100
C	-2.25135200	-2.33558500	0.02686800
H	-2.07674900	-3.40151100	0.08166800
C	-6.01976900	-2.05010400	-0.17389600
H	-6.63042800	-2.83740400	-0.62690200
H	-5.99140200	-1.23781800	-0.90587700
C	-6.67399800	-1.57794600	1.12972500
H	-6.74668400	-2.39990300	1.84894900
H	-7.68570900	-1.20775400	0.93412300
H	-6.09851700	-0.77208000	1.59450300
C	-4.57720900	-4.03896900	0.21811900
H	-5.50381300	-4.35712000	0.70604500
H	-3.77611200	-4.24738300	0.93402500
C	-4.37115300	-4.84608000	-1.06919900
H	-5.19635800	-4.68055000	-1.76910000
H	-4.32830800	-5.91638600	-0.84233700
H	-3.44077300	-4.56561100	-1.57131600
N	4.81098600	-2.33222100	0.54482300
N	-4.67170000	-2.59418400	0.00353000
O	0.14326500	3.31823800	-2.62311100
O	0.07291400	-2.17082300	0.05474000
O	0.06508100	1.32264800	-1.59536900
N	-0.27561000	5.63334000	-0.39586600
O	-0.99881800	5.61187100	-1.38753000
O	0.34259800	6.62247200	0.00268700
H	5.57178900	-4.26361400	-1.38248500

NO₂-RhB-TS

C	-0.03288800	2.33282100	2.12004600
H	-0.07250900	1.52682700	2.84535500
C	-0.01403800	3.66152300	2.54589000
H	-0.03855500	3.89164700	3.60556900
C	0.03423100	4.70365400	1.61739200
H	0.04328200	5.73882400	1.93921400
C	0.04679000	4.39295200	0.26145800
C	0.05492600	3.07444700	-0.19226500
C	0.01088200	2.04788200	0.75166400
C	0.01388400	0.64038400	0.22288000
C	0.21281200	2.58904000	-1.61589500
C	1.21545300	-0.14716900	0.34513400
C	2.50706200	0.40297600	0.52052400
H	2.60856500	1.47862600	0.61734300
C	3.63878600	-0.37645500	0.56494400
H	4.59438500	0.11202100	0.69399200
C	3.56507500	-1.80076300	0.43556300
C	2.27994600	-2.36180600	0.25113600
H	2.12696800	-3.42561600	0.13771600
C	1.15579700	-1.55051700	0.21049100
C	6.02348900	-1.99061700	0.65985200
H	6.66990100	-2.76697300	1.07613400
H	5.98069700	-1.19885600	1.41412500
C	6.63622800	-1.45445600	-0.63959900
H	6.77128900	-2.25484700	-1.37220000
H	7.61696000	-1.01447100	-0.43196700
H	6.00676300	-0.68280000	-1.09162700
C	4.60507600	-4.04057200	0.35056700
H	3.74631700	-4.41073700	0.91977500
H	5.49022900	-4.46503000	0.83052500
C	4.52706700	-4.52376700	-1.10288200
H	4.44432700	-5.61515400	-1.12558100
H	3.65813600	-4.10696600	-1.61967500
C	-1.20886800	-1.50191300	0.08521400
C	-1.22505800	-0.09618200	0.21190300
C	-2.50466300	0.50758200	0.24804600
H	-2.57051100	1.58596200	0.34418800
C	-3.66564900	-0.22422700	0.16985200
H	-4.61042400	0.29924800	0.22424300
C	-3.63566900	-1.64979600	0.03548700
C	-2.36301800	-2.26598900	0.00257000
H	-2.24473200	-3.33529700	-0.10345700
C	-6.11029800	-1.74955700	-0.13326500

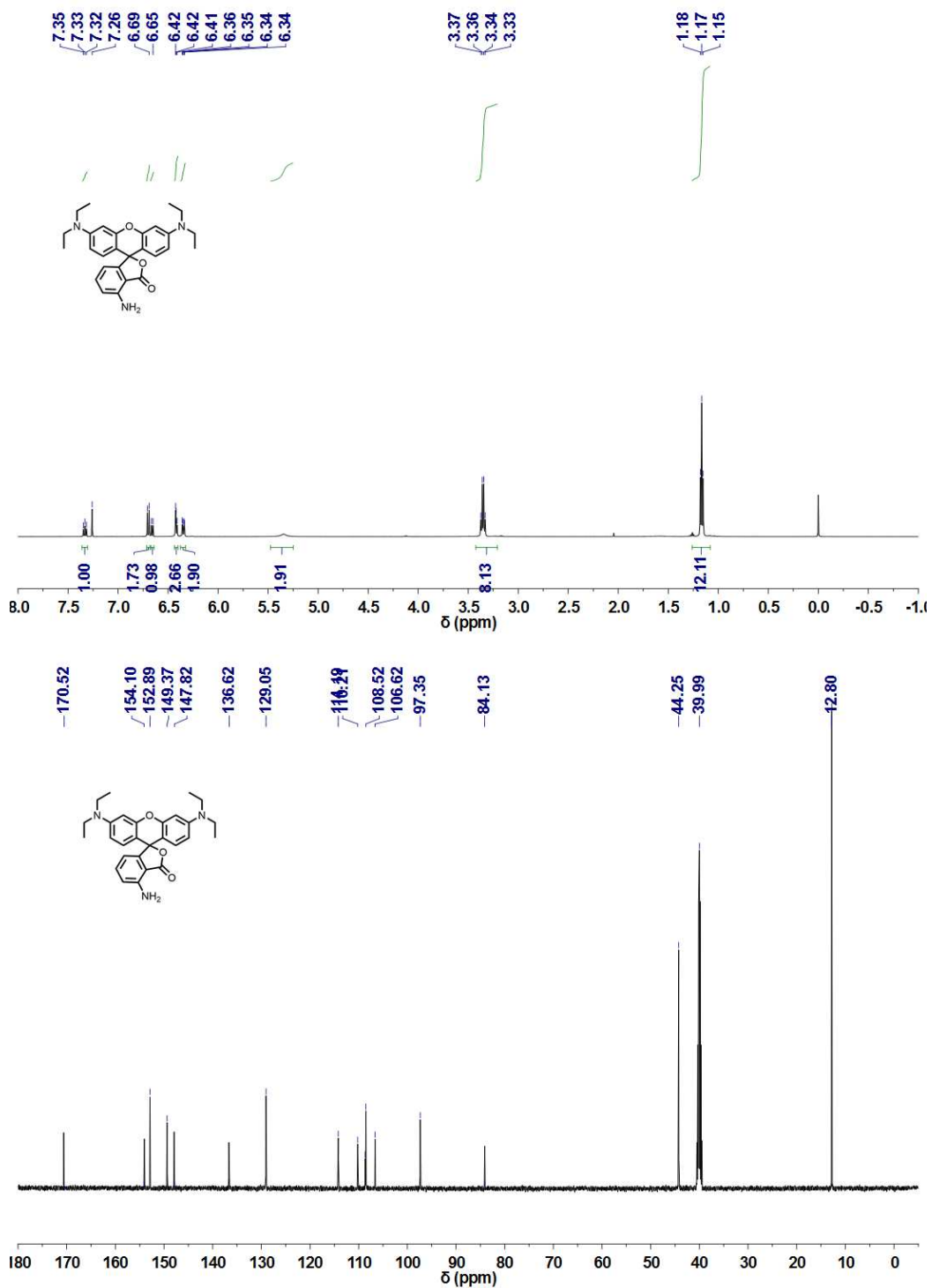
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H	-6.03754400	-0.83216900	-0.72285900
C	-6.74674900	-1.46927800	1.23171100
H	-6.86005400	-2.39292200	1.80780800
H	-7.73958900	-1.02783300	1.09938300
H	-6.13926800	-0.77558900	1.81999500
C	-4.77219200	-3.84770000	-0.07935500
H	-5.71531100	-4.18897400	0.35715700
H	-3.98361300	-4.21398700	0.58379800
C	-4.61124600	-4.43004000	-1.48782000
H	-5.42767700	-4.10556900	-2.14031700
H	-4.62458000	-5.52367200	-1.44539600
H	-3.66802100	-4.11627200	-1.94359000
N	4.68728700	-2.58304900	0.50934800
N	-4.78796700	-2.38110700	-0.04770200
O	0.42192400	3.36711700	-2.55298100
O	-0.03481700	-2.20144500	0.04360000
O	0.14088400	1.30316800	-1.67689200
N	0.01439600	5.52183800	-0.68703600
O	-0.98360100	5.64754000	-1.38836200
O	0.96599700	6.30188300	-0.66534700
H	5.42319700	-4.23942500	-1.66110300

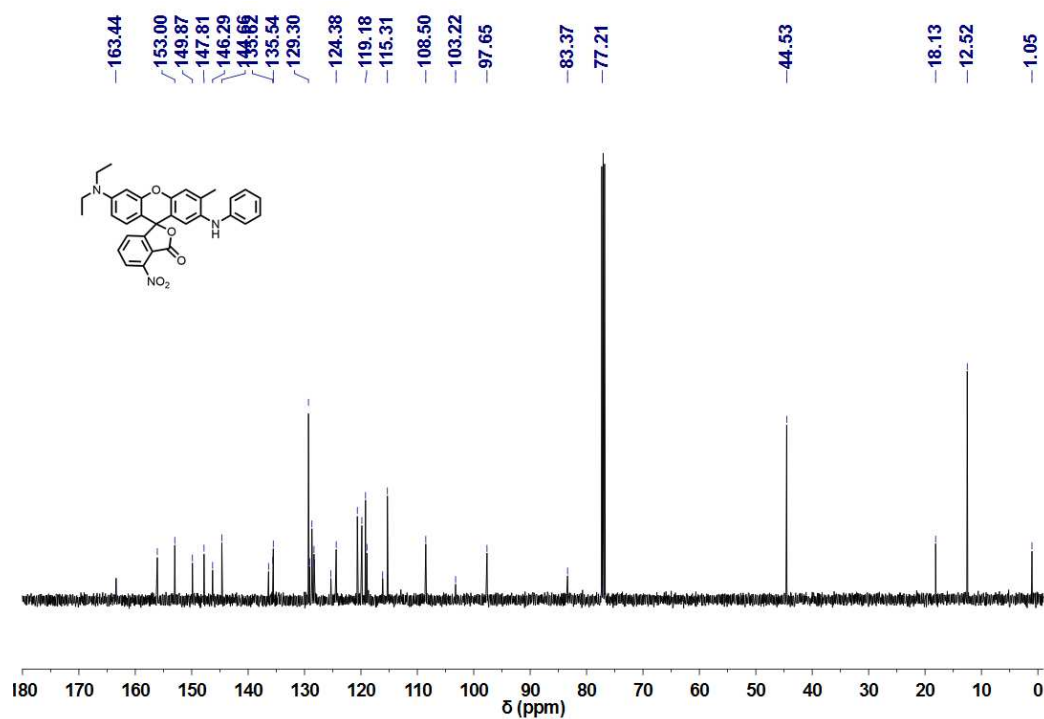
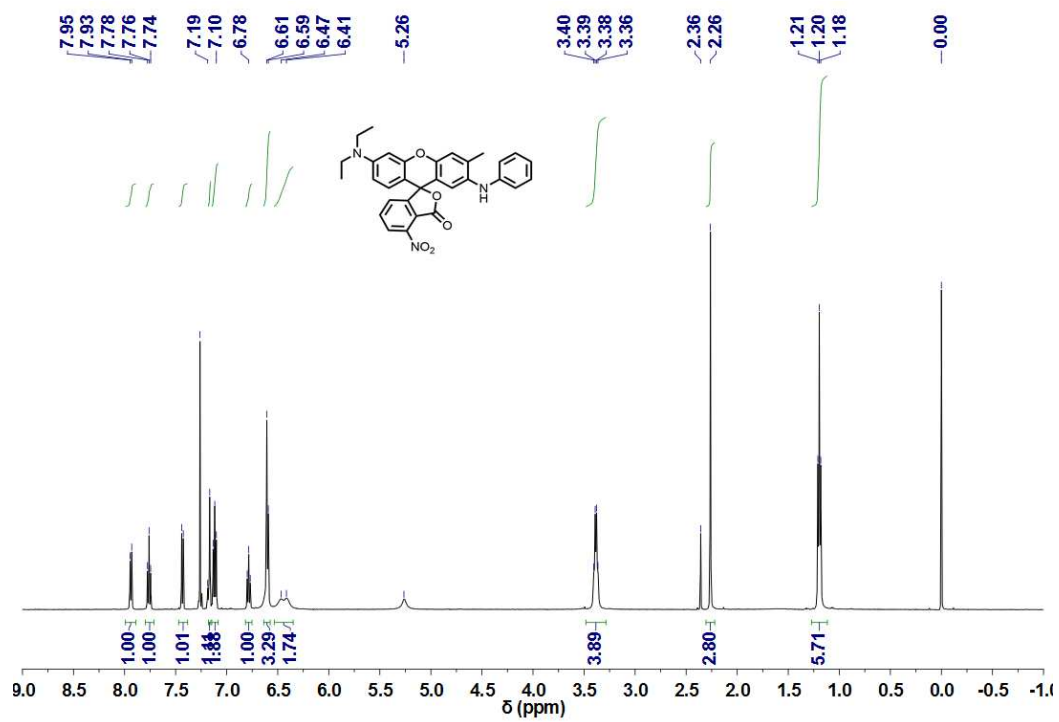
NO₂-RhB-O

C	0.08238000	2.59345300	-2.02127700
H	0.55753700	1.95545200	-2.76003500
C	-0.18240100	3.92852700	-2.32869500
H	0.09418200	4.33231400	-3.29628900
C	-0.79436200	4.73964200	-1.38055800
H	-1.00176200	5.78417500	-1.57796600
C	-1.12553400	4.19428100	-0.13965200
C	-0.89293800	2.85593400	0.20647900
C	-0.26705800	2.05761000	-0.77325900
C	0.03135800	0.61546700	-0.51848400
C	-1.36329200	2.21054000	1.52853200
C	-0.99831300	-0.34942200	-0.51738300
C	-2.38464500	-0.06057900	-0.67981800
H	-2.69490000	0.97252700	-0.76973300
C	-3.33367600	-1.04598300	-0.68817700
H	-4.36948200	-0.75853400	-0.79956300
C	-2.98094200	-2.43342200	-0.54585100
C	-1.60652900	-2.73717400	-0.37010400
H	-1.25164600	-3.74912800	-0.23930600
C	-0.66710800	-1.72681200	-0.36359900
C	-5.35421700	-3.09600300	-0.76854100

H	-5.82136700	-3.98526100	-1.19714200
H	-5.45400000	-2.30967600	-1.52118500
C	-6.08010800	-2.70060300	0.52162300
H	-6.06772200	-3.51586500	1.24965400
H	-7.12436200	-2.46393200	0.29506600
H	-5.62535800	-1.82135900	0.98638000
C	-3.56211800	-4.82694800	-0.42001400
H	-2.65825200	-5.03159600	-1.00148500
H	-4.35827600	-5.41681600	-0.87866100
C	-3.37217900	-5.25998800	1.03815300
H	-3.08079300	-6.31437700	1.07049500
H	-2.59219800	-4.67673300	1.53482900
C	1.64019700	-1.20419700	-0.19807500
C	1.36564000	0.18454400	-0.35833300
C	2.49763900	1.04880200	-0.30698800
H	2.34228900	2.11586300	-0.41080700
C	3.76777200	0.57276600	-0.13111600
H	4.58582800	1.27923400	-0.11653400
C	4.02800300	-0.83466100	0.01793100
C	2.91191700	-1.70893200	-0.01957000
H	3.01345500	-2.77673700	0.11151700
C	6.45096900	-0.40638600	0.33322800
H	7.18025100	-0.93397500	0.95367600
H	6.15756800	0.47892300	0.90148800
C	7.08703000	-0.01589800	-1.00366100
H	7.41197300	-0.90208000	-1.55694200
H	7.96334300	0.61512100	-0.82711800
H	6.38559000	0.53972100	-1.63250000
C	5.58628000	-2.74077000	0.24840300
H	6.60308900	-2.87320400	-0.13066900
H	4.93176600	-3.27072100	-0.44773100
C	5.47487600	-3.32399000	1.66024000
H	6.15980600	-2.81827500	2.34740700
H	5.73314700	-4.38710000	1.64352700
H	4.46040600	-3.22347900	2.05579400
N	-3.92563200	-3.41046700	-0.59240900
N	5.29128200	-1.30126900	0.18802100
O	-2.60443400	2.22312000	1.69856400
O	0.62906800	-2.11595900	-0.20869400
O	-0.45611300	1.69840800	2.22288700
N	-1.71622000	5.11405500	0.83949000
O	-1.45096600	4.95406400	2.03019000
O	-2.42759100	6.02864200	0.41096600
H	-4.29768300	-5.14571500	1.60822200

23. ^1H NMR and ^{13}C NMR of $\text{NH}_2\text{-RhB}$ and $\text{NO}_2\text{-ODB}$





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