Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Supporting Information for

Synthesis, Spectroscopic Properties of fluorescent 5-benzimidazolyl-2'-deoxyuridines from o-phenylenediamine derivatives as 5-fdU Probes

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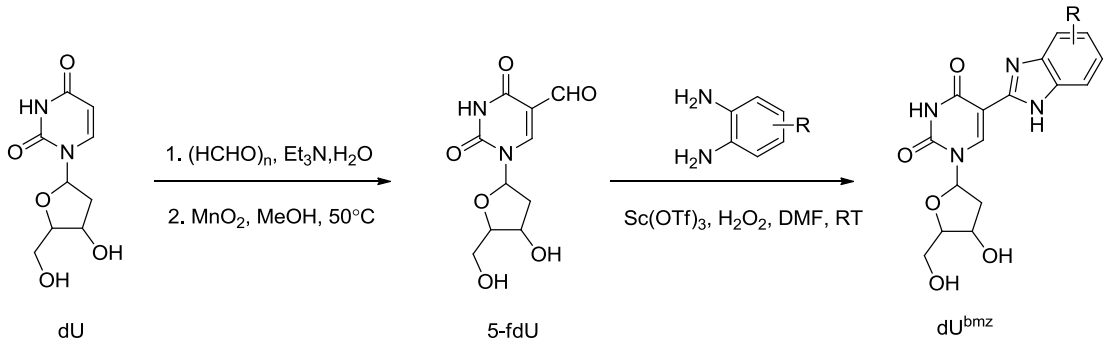
Materials, methods and instrumentation.

The following solvent, compounds and reagents were commercially available: 2'-deoxyuridine, 3, 4-dinitrobenzoic acid, o-phenylenediamine derivatives, Scandium trifluoromethanesulfonate, dithiothreitol (DTT) were bought from Sigma-Aldrich. 30% Hydrogen Peroxide, Dimethyl Formamide, ammonium acetate, glacial acetic acid, Paraformalclehyde were bought from SCRC (Shanghai, China).

^{1}H and ^{13}C NMR spectra were recorded on Varian Mercury 300 spectrometers, respectively. HRMS were recorded on a Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS and Varian ProMALDI. API-ES were recorded on Agilent LC/MSD. Fluorescent emission spectra were collected on PerkinElmer LS 55. UV absorption spectra were collected on SHIMADZU UV-2550. Quartz cuvettes with 2mL volume were used for emission measurements. Unless otherwise specified, all spectra were taken at an ambient temperature.

General procedure for the synthesis of dU^{bmz}



Scheme S1. Synthesis of dU^{bmz}

Synthesis of 5-fdU: (1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbaldehyde)[1]:

5.25g (23.0 mmol) 2'- deoxyuridine and 3.11g (103.5mmol) paraformalclehyde were added into 250mL bottle with two necks and dissolved by 80mL 0.5mol/L triethylamine aqueous solution. The mixture was stirred at 60°C for 4 days. In the process, more paraformalclehyde (4.49g, 149.5mmol), triethylamine (1mL) and water

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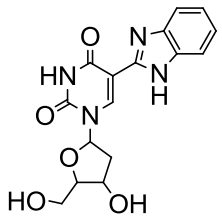
(10mL) was added into reaction mixture each day. After reaction finished, the mixture was concentrated *in vacuo*, the residue was recrystallized in MeOH to obtain 4.11g white solid, yield= 62%. ^{1}H NMR(300 MHz, DMSO-d_6) δ(ppm): 11.34(s, 1H), 7.71 (s,1H), 6,17 (t, J=6.8 Hz,1H), 5.26 (s,1H), 4.97 (s,2H), 4.20 (q, J=3.2 Hz, 1H), 4.10 (s, 2H), 3.75 (q, J=3.2 Hz, 1H), 3.57~3.47 (m, 2H), 2.09~1.99 (m, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.5, 150.2, 136.7, 114.1, 87.1, 83.7, 70.4, 61.3, 55.9, 35.2.
The 0.70g (2.7mmol) compound from last step was added into 25mL bottle with two necks and dissolved in 10mL MeOH following with 0.94g (10.9mmol) MnO_2. The mixture was stirred at 50°C for 6h. After cooling to room temperature, the mixture was filtered through celatom to collect filtrate. The filtrate was concentrated *in vacuo*, the residue was recrystallized in MeOH to obtain 0.56g (2.19mmol) 5-fdU, yield=55%. ^{1}H NMR(300 MHz, DMSO-d_6) δ(ppm): 11.76 (s, 1H), 9.73 (s, 1H), 8.71 (s, 1H), 6.07 (t, J=6.2 Hz, 1H), 5.28 (s, 1H), 5.13 (s, 1H), 4.21 (q, J=4 Hz,1H), 3.83 (q, J=3.2 Hz, 1H), 3.61 (q, J=4 Hz), 3.54 (q, J=4 Hz, 1H), 2.22 (q, J=8 Hz, 1H), 2.15 (q, J=8 Hz, 1H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 186.1, 161.6, 149.4, 147.0, 110.5, 87.7, 85.7, 69.6, 60.5, 40.5.

General procedure for Synthesis of dU^{bmz} [2]

A solution of 5-fdU (50mg, 0.2mmol) and 0.21mmol o-phenylenediamine derivatives in DMF (4mL) was stirred at room temperature for 5 min. $Sc(OTf)_3$ (10mg, 0.020mmol) and aqueous H_2O_2 (30%, 20μL) were added successively to the mixture, which was further stirred under air at room temperature for 4h. After removing the solvent *in vacuo*, the residue was purified by column chromatography (SiO_2, MeOH in $CHCl_3$, 5%-8%) to give dU^{bmz}.

5-(1H-benzo[d]imidazol-2-yl)-1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3a):



Yield= 83%, ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.19(s, 1H), 11.93(s, 1H), 8.80(s, 1H), 7.56(d, J= 3.3 Hz, 2H), 7.12(d, J= 3.3 Hz, 2H), 6.19(t, J= 6.6 Hz, 1H), 5.33(d, J=4.2 Hz, 1H), 5.05(d, J=4.8 Hz, 1H), 4.27(s, 1H), 3.86(d, J=2.4 Hz, 1H), 3.59(s, 2H), 2.22(t, J=5.4 Hz, 2H);^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.5, 150.2, 146.7, 143.2, 141.6, 135.0, 122.2, 118.6, 112.9, 104.6, 88.5, 86.0, 71.2, 62.0, 56.7. HRMS (MALDI) calcd for $C_{16}H_{17}N_4O_5$ $[M+H]^+$: 345.1194; found: 345.1196.

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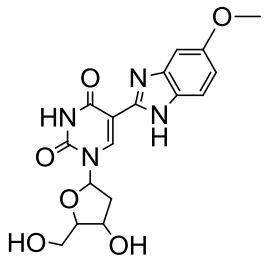
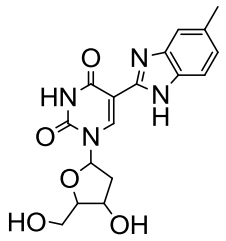
1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(5-methoxy-1H-benzo[d]imidazol-2-yl)pyrimidine-2,4(1H,3H)-dione (3b):



Yield= 77%, the product is a mixture of two tautomers in the ratio: 4:6. ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.02(s, 1H), 11.91(br, 1H), 8.72(s, 1H), 7.44(t, J= 8.1 Hz, 1H), 7.13(s, 1H), 6.77(s, 1H), 6.20(t, J=6.3 Hz, 1H), 5.33(s, 1H), 5.06(s, 1H), 4.27(s, 1H), 3.86(s, 1H), 3.74(s, 3H), 3.60(s, 2H), 2.21(s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.6, 156.1, 150.2, 145.8, 144.0, 140.7, 137.7, 135.6, 129.5, 119.1, 112.1, 111.7, 88.5, 85.8, 71.2, 62.1, 56.0. HRMS (MALDI) calcd for $C_{17}H_{18}Na_1N_4O_6$ $[M+Na]^+$: 397.1119; found: 397.1114.

1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(5-methyl-1H-benzo[d]imidazol-2-yl)pyrimidine-2,4(1H,3H)-dione (3c):



Yield= 93%, ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.06(br, 1H), 11.92(s, 1H), 8.77(s, 1H), 7.44(d, J= 6.0 Hz, 1H), 7.36(s, 1H), 6.95(d, J=8.1 Hz, 1H), 6.20(t, J=6.6 Hz, 1H), 5.33(d, J=3.0 Hz, 1H), 5.07(s, 1H), 4.27(s, 1H), 3.86(s, 1H), 3.60(s, 2H), 2.38(s, 3H), 2.22 (s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 161.8, 149.4, 145.6, 140.6, 140.4, 130.6, 123.1, 118.3, 104.0, 87.7, 85.1, 70.4, 61.3, 56.0, 21.3. HRMS (ESI) calcd for $C_{17}H_{17}N_4O_5$ $[M-H]^-$: 357.1204; found: 357.1204.

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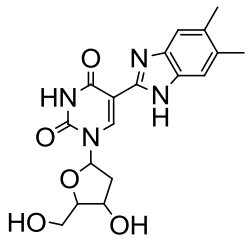
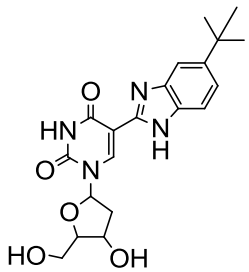
5-(5,6-dimethyl-1H-benzo[d]imidazol-2-yl)-1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3d):



Yield= 87%, ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 11.96(br, 1H), 11.90(s, 1H), 8.74(s, 1H), 7.33(s, 2H), 6.20(s, 1H), 5.32(s, 1H), 5.06(s, 1H), 4.27(s, 1H), 3.85(s, 1H), 3.60(s, 2H), 2.27(s, 6H), 2.21 (s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 161.8, 149.4, 145.0, 140.3, 130.0, 129.9, 104.1, 87.7, 85.1, 79.1, 70.5, 61.3, 56.0,20.0.

HRMS (ESI) calcd for $C_{18}H_{19}N_4O_5$ $[M-H]^-$: 371.1361; found: 371.1360.

5-(5-(tert-butyl)-1H-benzo[d]imidazol-2-yl)-1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3e):



Yield= 84%, the product is a mixture of two tautomers in the ratio: 3:7. ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 11.96(s, 1H), 11.84(s, 1H), 8.70(s, 1H), 7.40(s, 2H), 7.14(d, J=8.4 Hz, 1H), 6.12(s, 1H), 5.26(s, 1H), 5.01(s, 1H), 4.20(s, 1H), 3.78(s, 1H), 3.53(s, 2H), 2.14 (s, 2H), 1.24(s, 9H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.4, 162.0, 149.6, 145.8, 144.5, 142.6, 141.7, 140.8, 119.7, 104.2, 87.9, 85.3, 70.6, 61.4, 55.9, 35.9, 31.8.

HRMS (ESI) calcd for $C_{20}H_{23}N_4O_5$ $[M-H]^-$: 399.1674; found: 399.1664.

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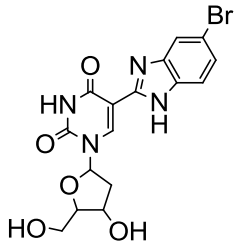
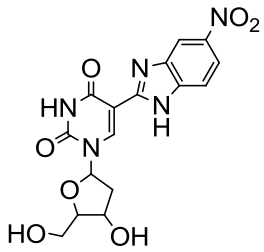
5-(5-bromo-1H-benzo[d]imidazol-2-yl)-1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3f):



Yield= 83%, the product is a mixture of two tautomers in the ratio: 5:5. ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.36(s, 1H), 11.96(br, 1H), 8.85(s, 1H), 7.77(s, 1H), 7.55(d, J=8.1 Hz, 1H), 7.27(s, 1H), 6.18(s, 1H), 5.32(s, 1H), 5.04(s, 1H), 4.27(s, 1H), 3.87(s, 1H), 3.60 (s, 2H), 2.23(s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.6, 150.2, 148.2, 144.7, 142.3, 136.3, 134.2, 125.2, 120.9, 115.6, 104.1, 88.6, 86.1, 71.2, 62.0, 56.7. HRMS (ESI) calcd for $C_{16}H_{14}Br_1N_4O_5$ [M-H]$^-$: 421.0153; found: 421.0146.

1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(5-nitro-1H-benzo[d]imidazol-2-yl)pyrimidine-2,4(1H,3H)-dione (3g):



Yield= 92%, the product is a mixture of two tautomers in the ratio: 5.8:4.2. ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.80(s, 1H), 12.05(br, 1H), 9.02(s, 1H), 8.53(s, 1H), 8.07(s, 1H), 7.77(d, J=9.0 Hz, 1H), 6.19(t, J=6.3 Hz, 1H), 5.34(s, 1H), 5.09(s, 1H), 4.30(s, 1H), 3.91(s, 1H), 3.64 (s, 2H), 2.27(s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 162.7, 152.5, 150.3, 148.2, 143.6, 140.1, 134.6, 118.5, 114.7, 109.8, 103.5, 88.8, 86.6, 71.3, 62.1, 56.9. HRMS (ESI) calcd for $C_{16}H_{14}N_5O_7$ [M-H]$^-$: 388.0899; found: 388.0881.

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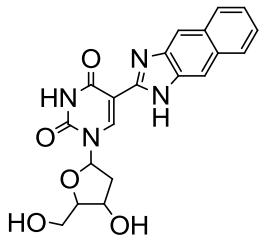
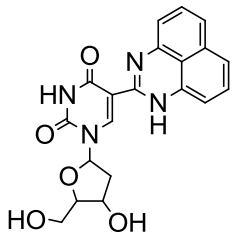
1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(1H-naphtho[2,3-d]imidazol-2-yl)pyrimidine-2,4(1H,3H)-dione (3h):



Yield= 80%, ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 12.32(s, 1H), 12.08(s, 1H), 9.05(s, 1H), 8.12(d, J= 12.3 Hz, 2H), 8.01(s, 2H), 7.41(d, J= 4.2 Hz, 2H), 6.28(s, 1H), 5.42(d, J=3.0 Hz, 1H), 5.17(s, 1H), 4.37(s, 1H), 3.97(s, 1H), 3.71(s, 2H), 2.33(s, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 161.9, 150.6, 149.6, 143.1, 142.5, 135.3, 129.9, 129.8, 128.0, 127.5, 123.5, 123.0, 114.0, 107.6, 103.5, 88.0, 85.6, 70.6, 61.4, 56.1.

HRMS (ESI) calcd for $C_{20}H_{17}N_4O_5$ $[M-H]^-$:393.1204; found: 393.1199.

1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(1H-perimidin-2-yl)pyrimidine-2,4(1H,3H)-dione (3i):



Yield= 79%, ^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 11.97(s, 1H), 10.68(s, 1H), 8.84(s, 1H), 7.07(d, J= 8.1 Hz, 1H), 6.99(d, J=7.2 Hz, 1H), 6.93(d, J= 7.2 Hz, 2H), 6.52(d, J=7.5 Hz, 1H), 6.35(d, J=6.3 Hz, 1H), 6.09(s, 1H), 5.27(d, J=3.9 Hz, 1H), 4.98(s, 1H), 4.20(s, 1H), 3.82(s, 1H), 3.56(s, 2H), 2.16(d, J=4.5 Hz, 2H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 163.2, 149.3, 149.1, 144.7, 143.9, 137.0, 135.1, 128.9, 128.9, 127.9, 121.8, 118.5, 117.9, 104.1, 102.7, 97.9, 85.8, 70.2, 61.1, 56.0. HRMS (ESI) calcd for $C_{20}H_{17}N_4O_5$ $[M-H]^-$:393.1204; found: 393.1199.

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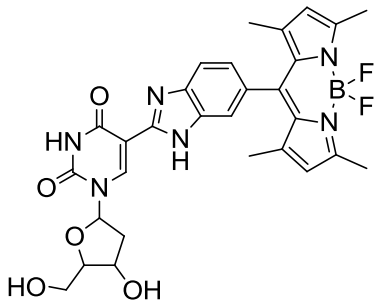
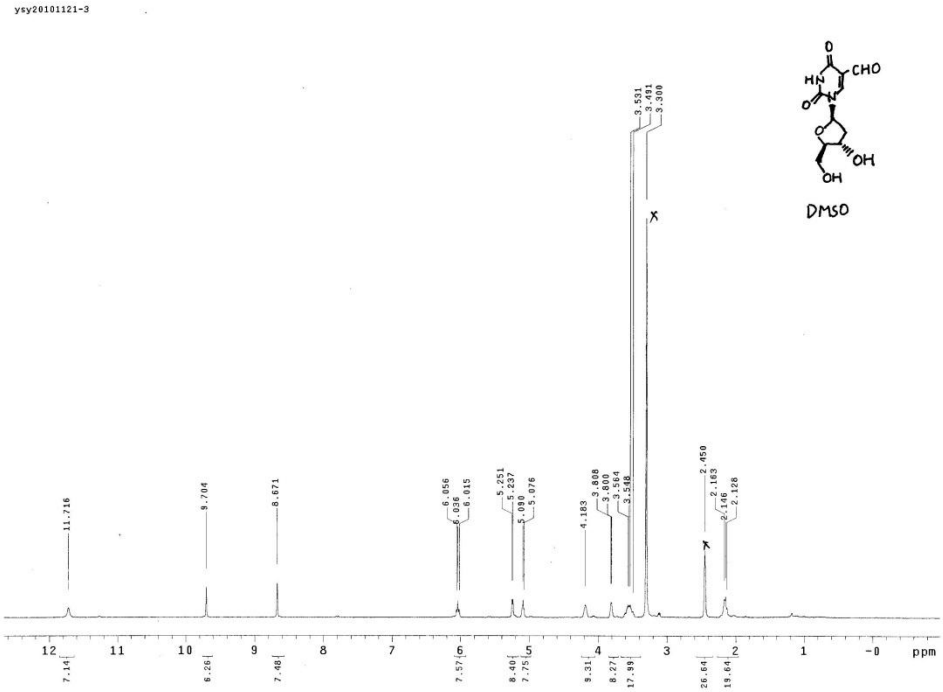
5,5-difluoro-10-(2-(1-(4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-1H-benzo[d]imidazol-6-yl)-1,3,7,9-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide (3j):



Yield= 77%, the product is a mixture of two tautomers in the ratio: 5:5. ^{1}H NMR (400 MHz, DMSO-d_6) δ(ppm): 12.46(s, 1H), 12.00(s, 1H), 8.89(s, 1H), 7.78(d, J= 7.8 Hz, 1H), 7.52(s, 1H), 7.08(s, 1H), 6.20(s, 1H), 6.16(s, 2H), 5.33(s, 1H), 5.05(s, 1H), 4.36(s, 1H), 3.88(s, 1H), 3.61(s, 2H), 2.45(s, 6H), 2.23(s, 2H), 1.26(s, 6H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ: 163.6, 162.6, 155.3, 150.2, 148.3, 148.1, 143.6, 142.2, 135.5, 132.0, 127.9, 121.9, 119.6, 117.8, 114.1, 112.3, 104.3, 88.5, 86.1, 73.2, 71.1, 62.0, 56.7, 14.9, 14.7. HRMS (ESI) calcd for $C_{29}H_{28}{}^{*}B_1F_2N_6O_5$ $[M-H]^-$:588.2224; found: 588.2239.

Compound 2j was prepared by the literature methods. [3]
^{1}H NMR (300 MHz, DMSO-d_6) δ(ppm): 6.79 (d, 1H, J = 8.4 Hz); 6.59 (s, 1H); 6.58 (d, 1H, J = 8.4 Hz); 5.96 (s, 2H); 3.52 (s, 2H); 3.44 (s, 2H); 2.54 (s, 6H); 1.53 (s, 6H).
^{13}C NMR (DMSO-d_6, 75 MHz) δ: 154.9, 143.3, 142.7, 135.4, 135.4, 131.9, 126.5, 120.8, 119.8, 117.0, 116.0, 14.6,14.6.



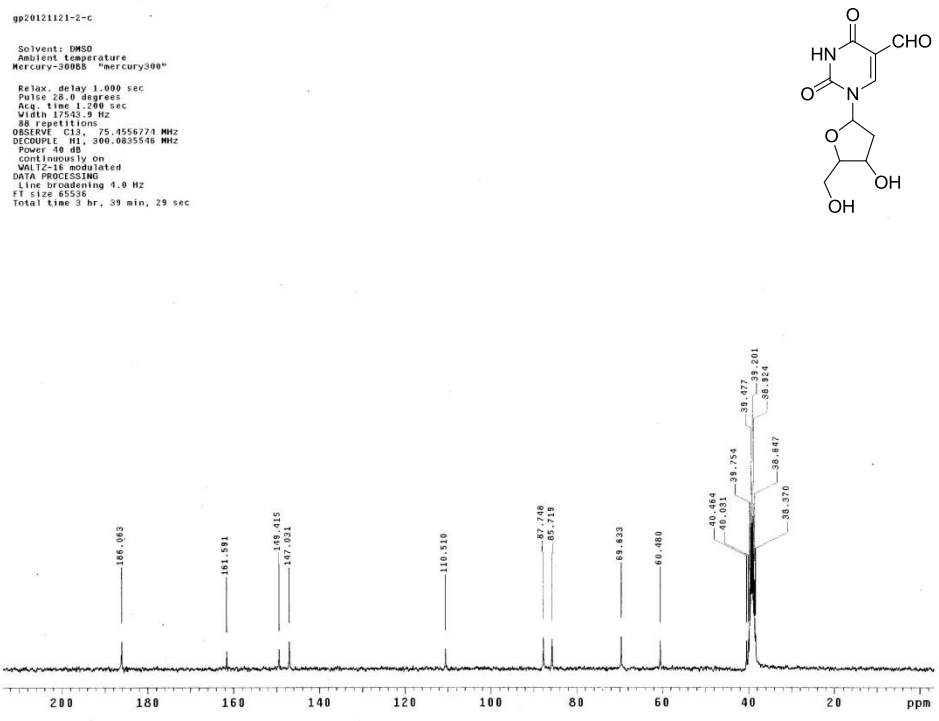


Figure S1. The ^{1}H NMR, ^{13}C NMR spectra of 5-fdU

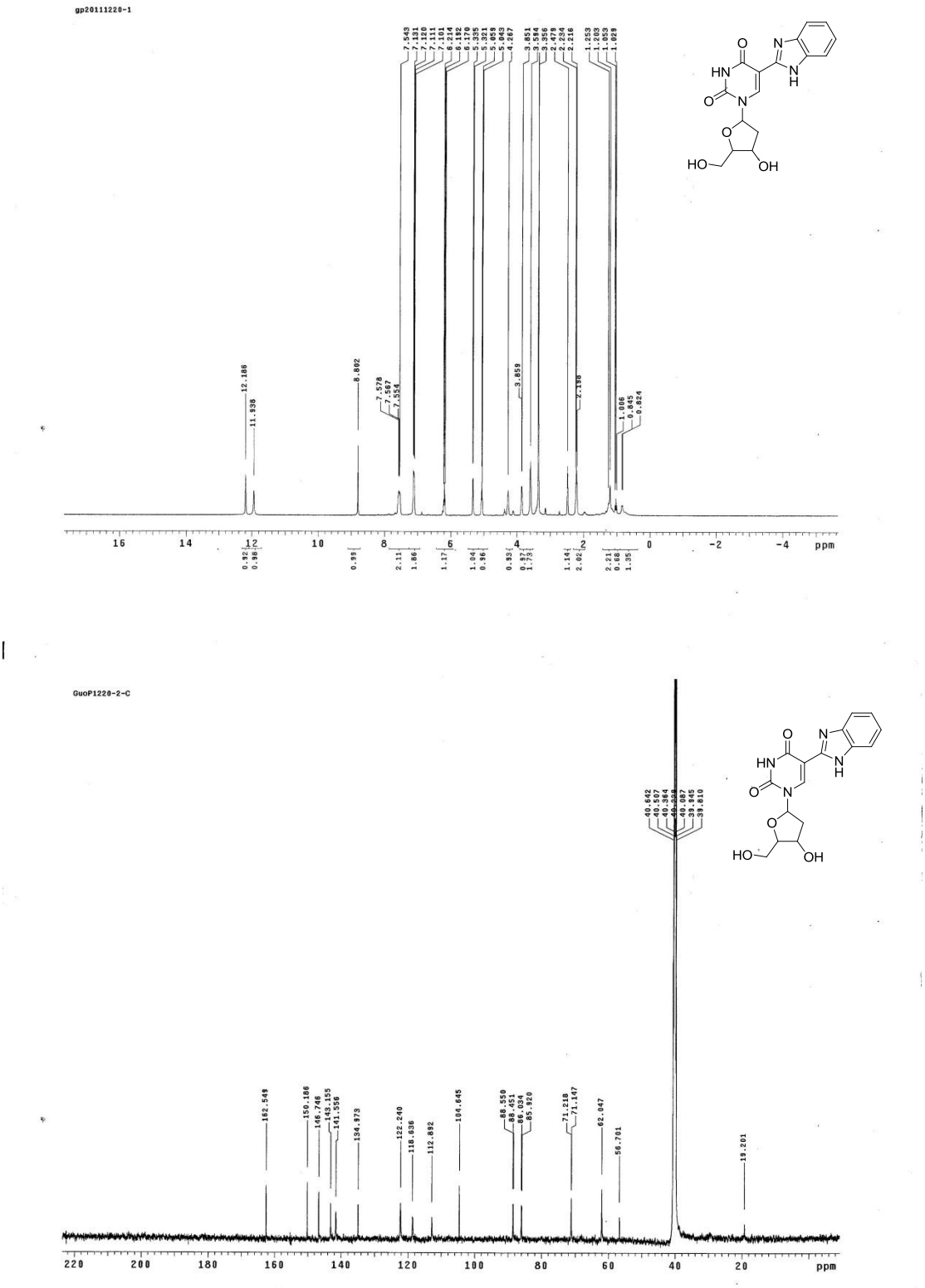


Figure S2. The ^{1}H NMR, ^{13}C NMR spectra of 3a

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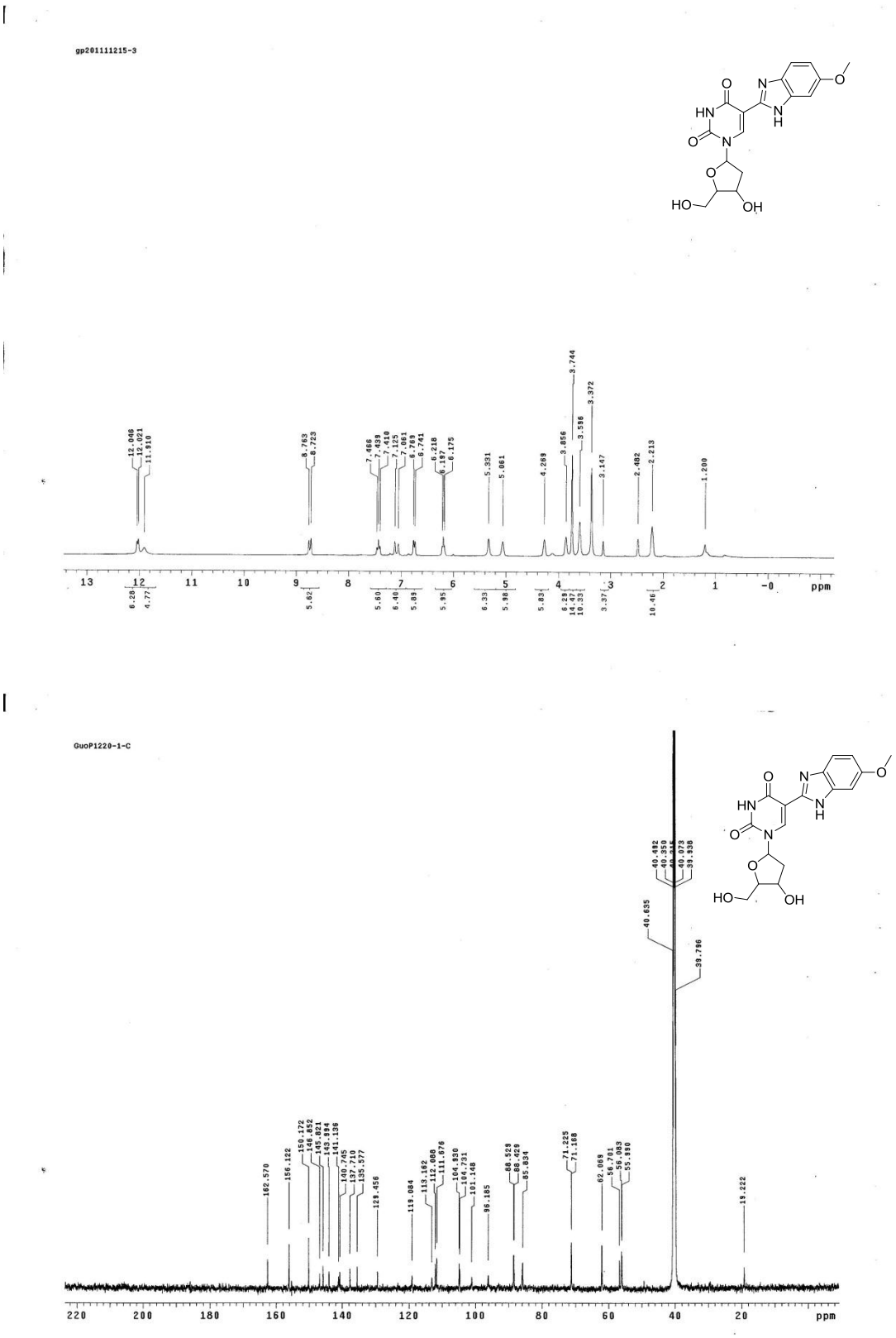

Figure S3. The ^{1}H NMR, ^{13}C NMR spectra of 3b

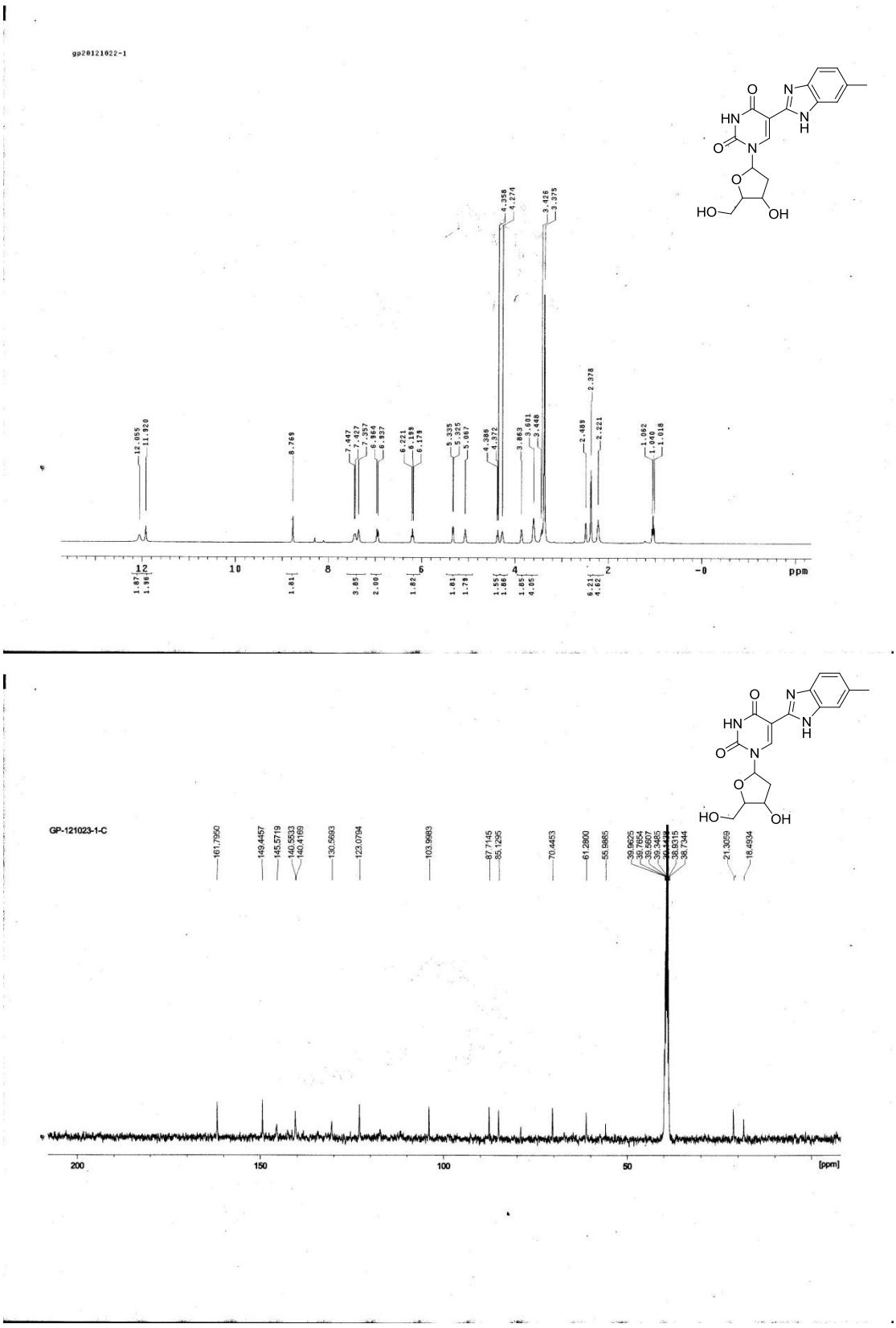

Figure S4. The ^{1}H NMR, ^{13}C NMR spectra of 3c

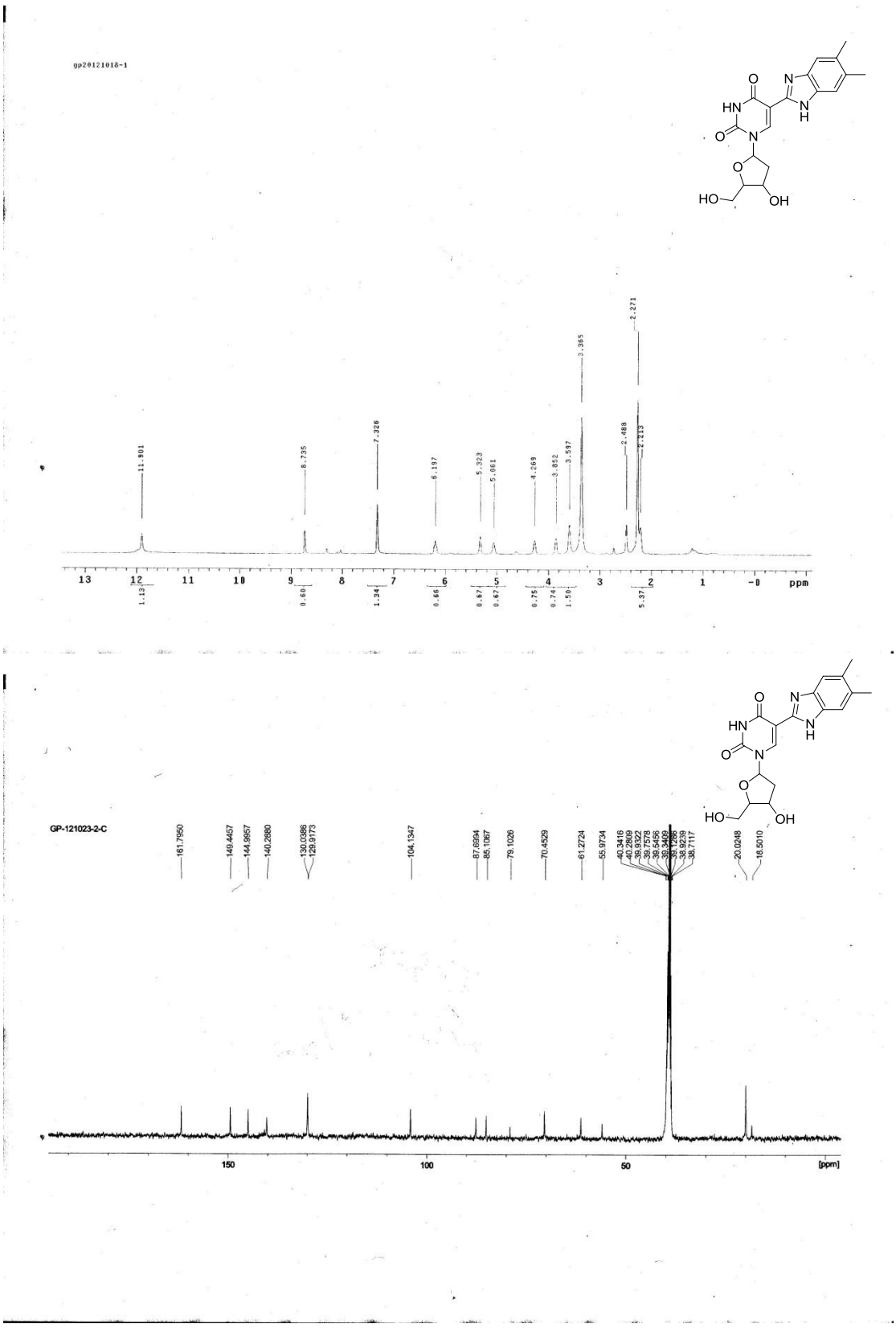

Figure S5. The ^{1}H NMR, ^{13}C NMR spectra of 3d

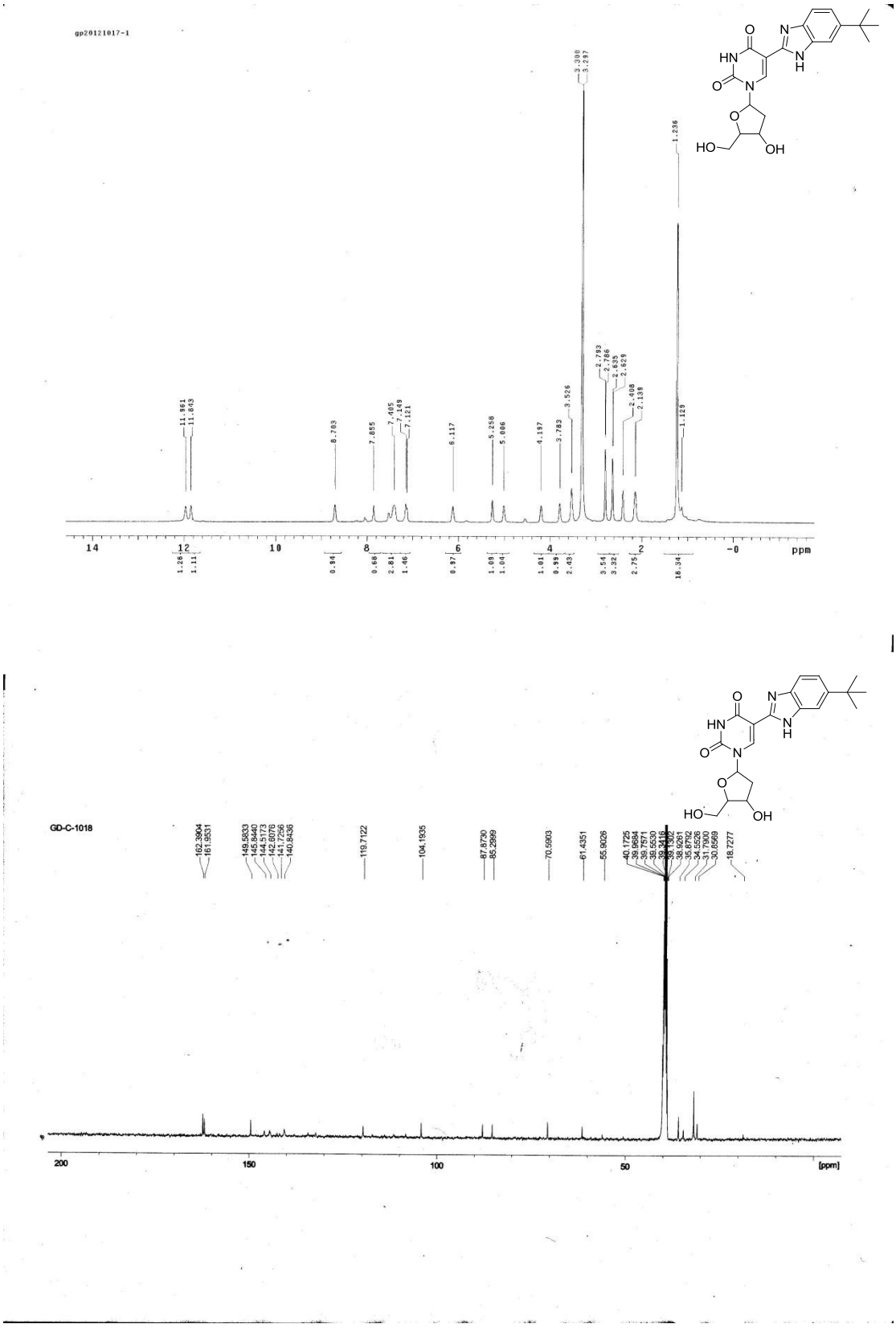

Figure S6. The ^{1}H NMR, ^{13}C NMR spectra of 3e

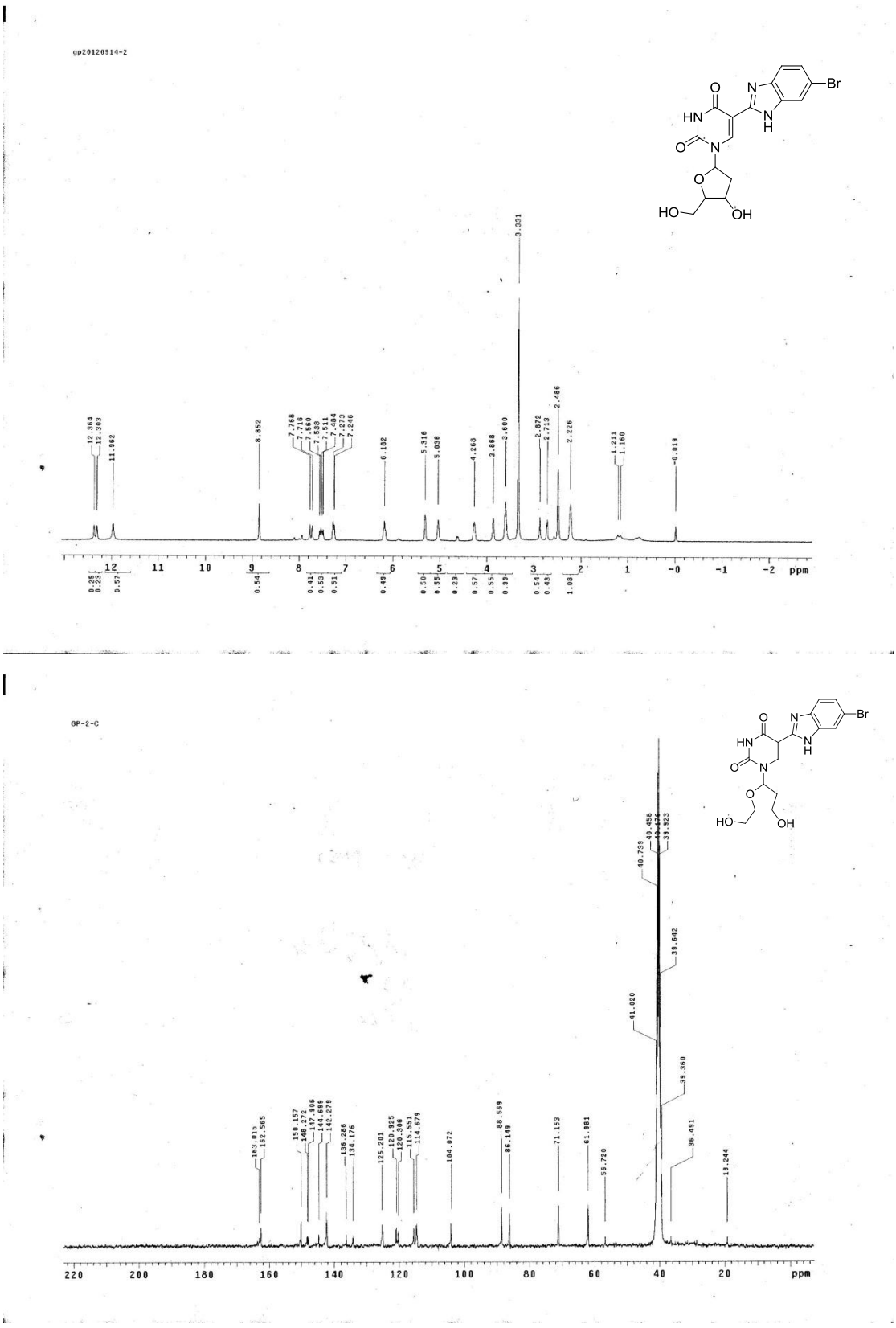

Figure S7. The ^{1}H NMR, ^{13}C NMR spectra of 3f

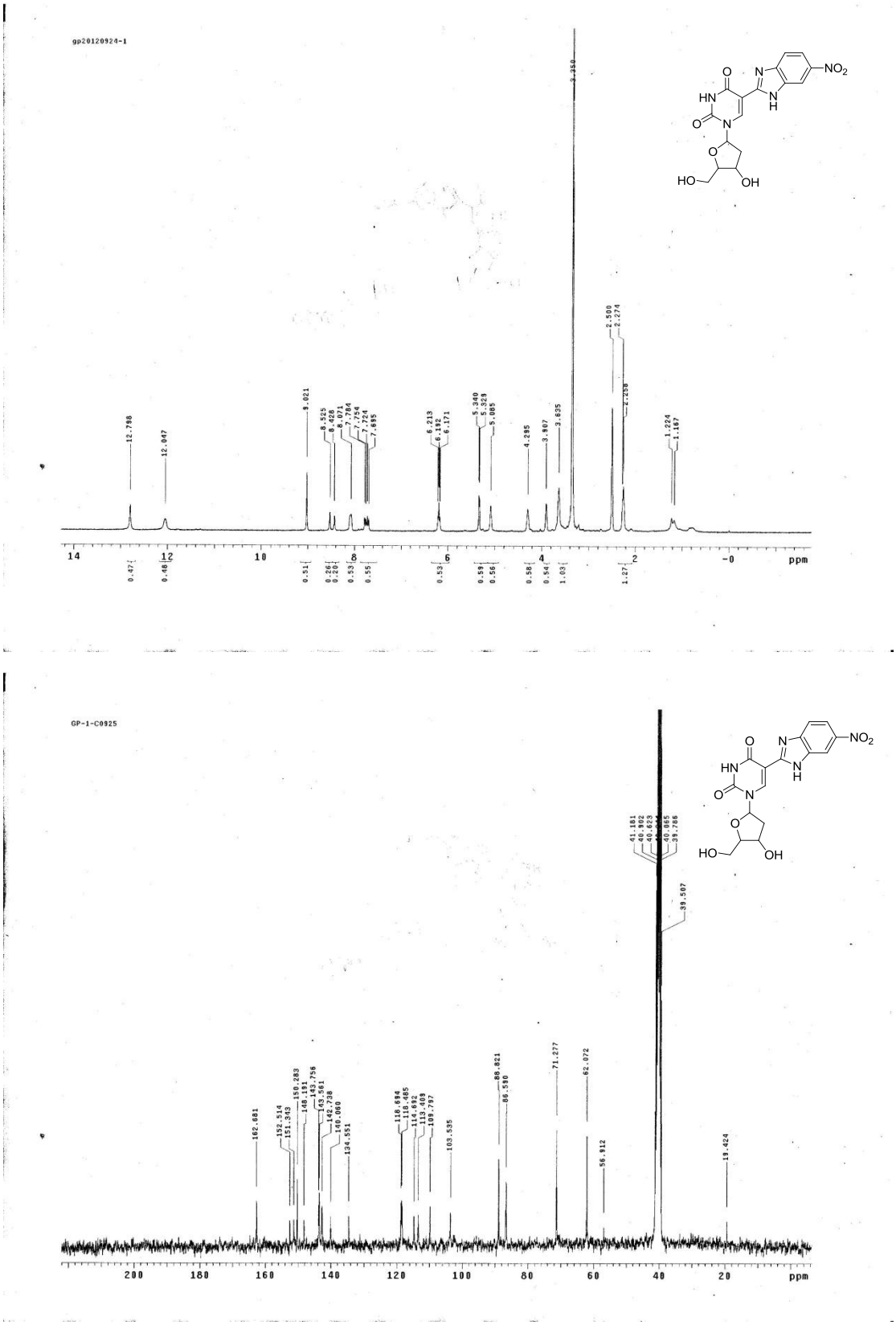

Figure S8. The ^{1}H NMR, ^{13}C NMR spectra of 3g

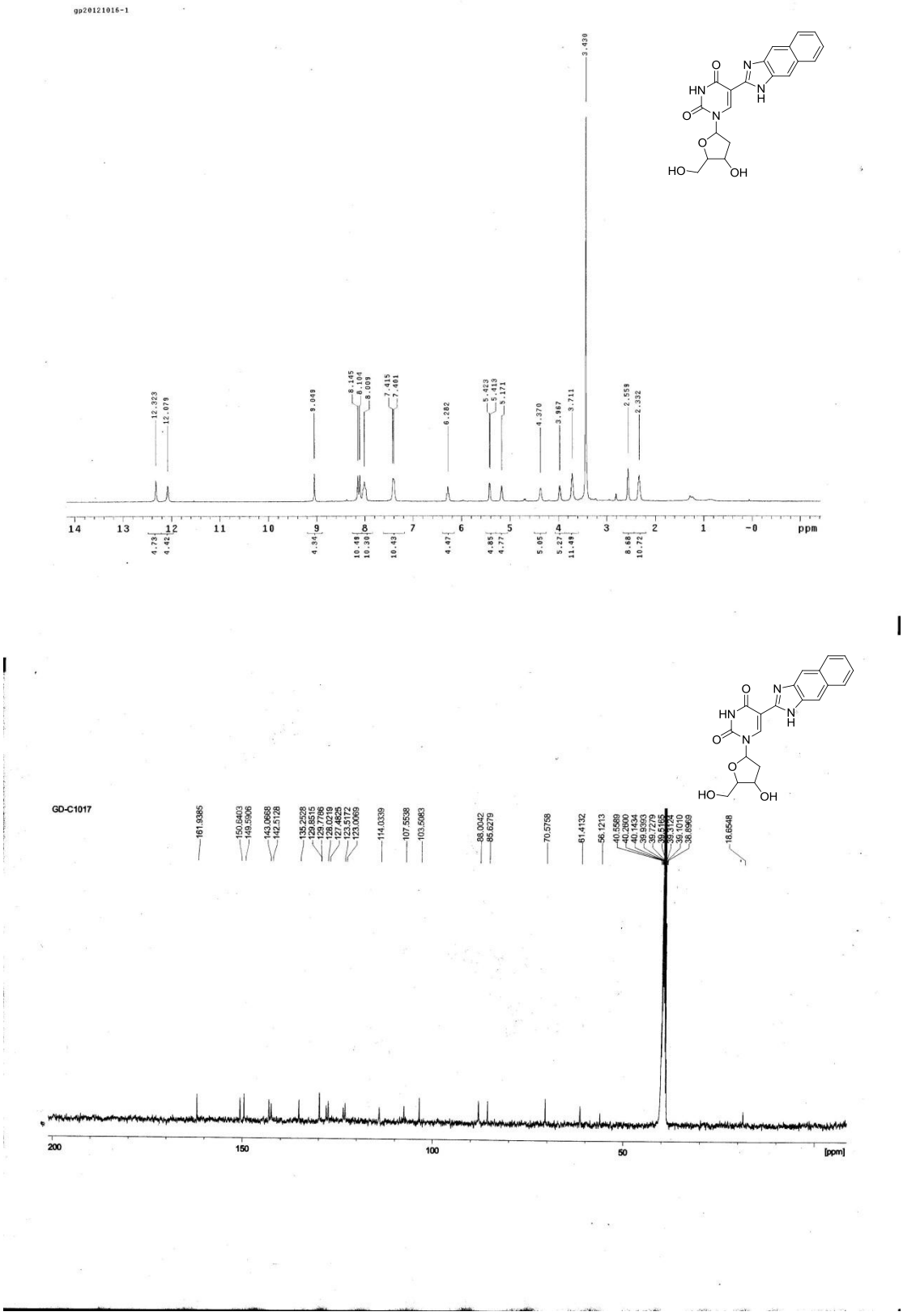

Figure S9. The ^{1}H NMR, ^{13}C NMR spectra of 3h

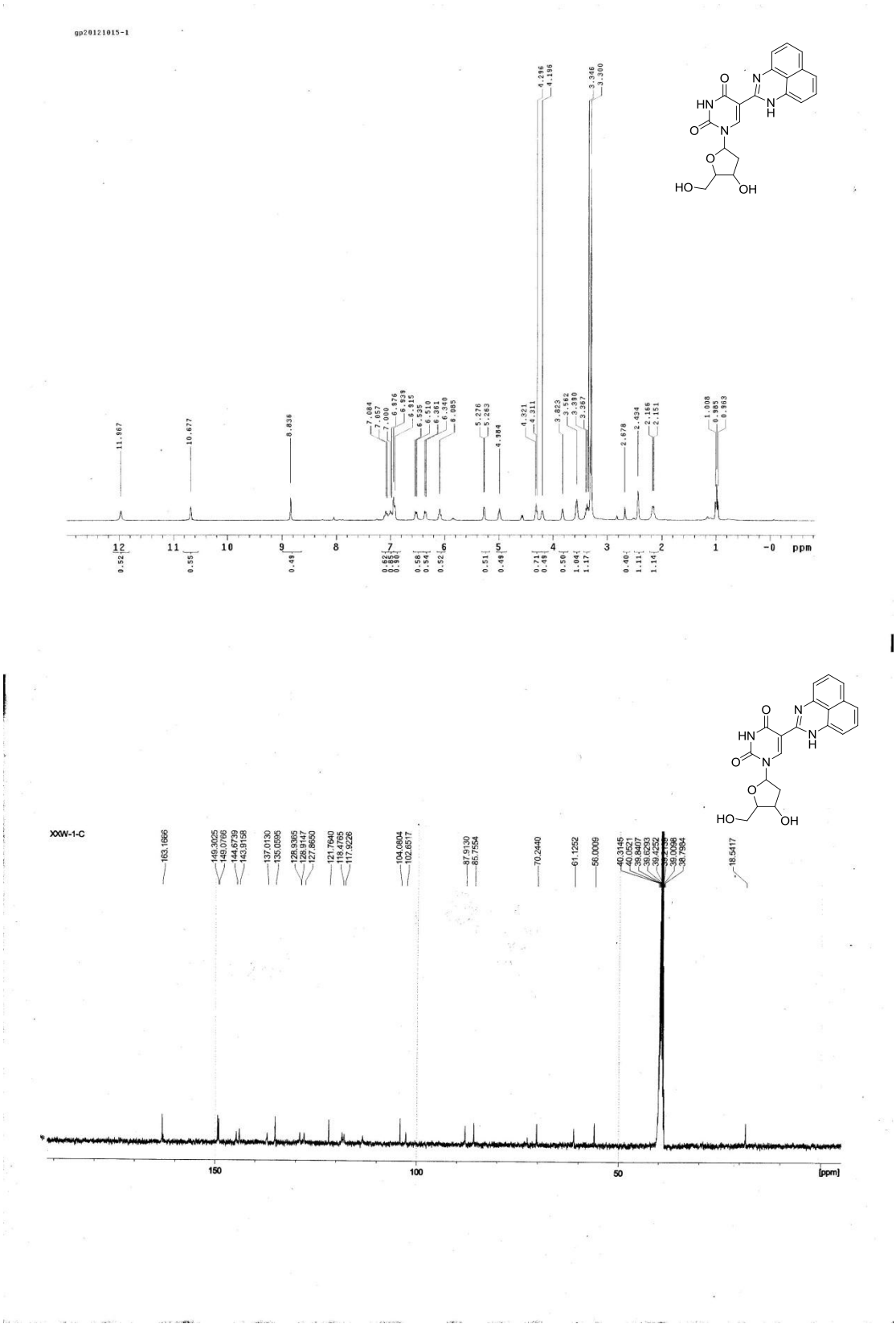

Figure S10. The ^{1}H NMR, ^{13}C NMR spectra of 3i

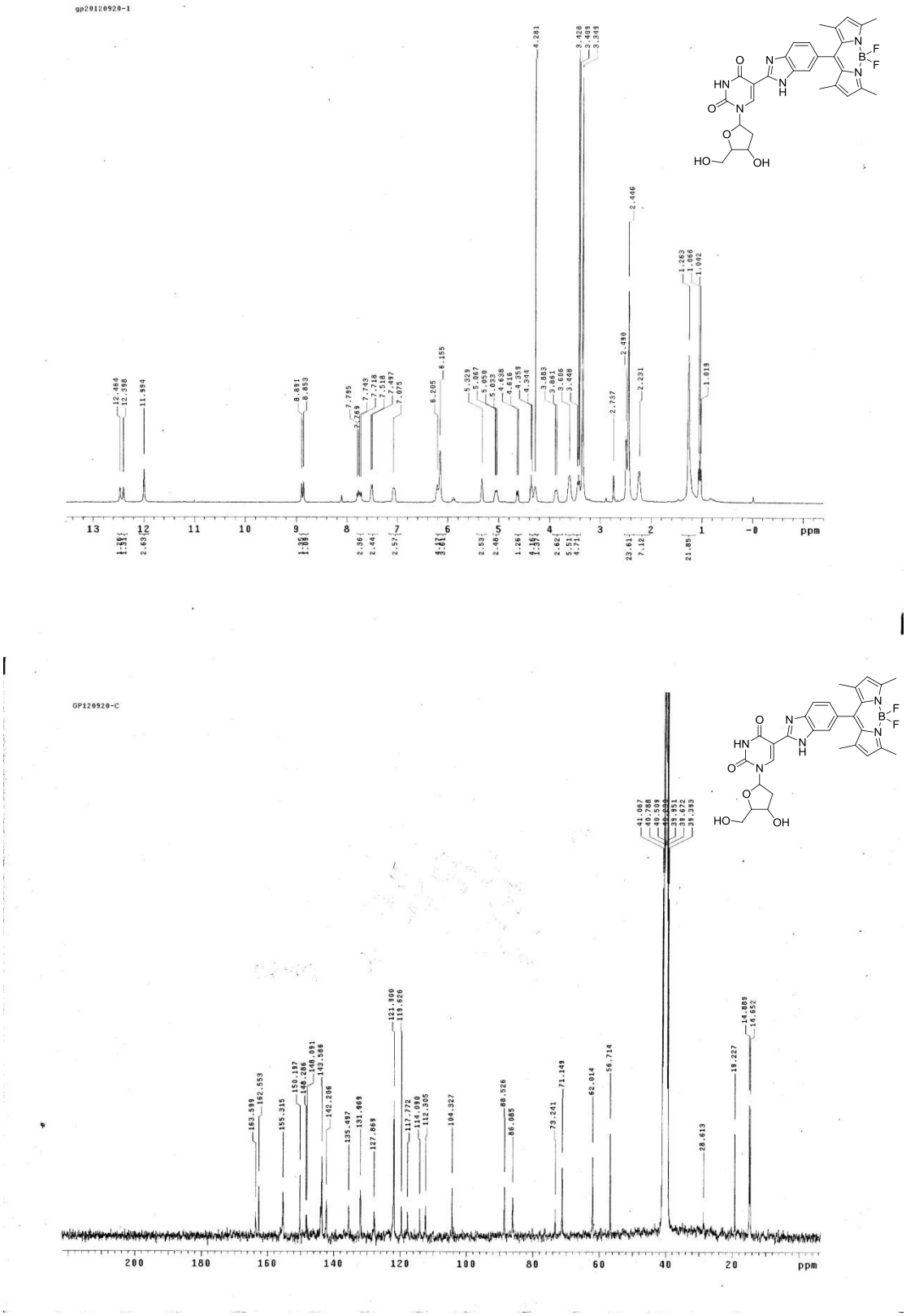

Figure S11. The ^{1}H NMR, ^{13}C NMR spectra of 3j

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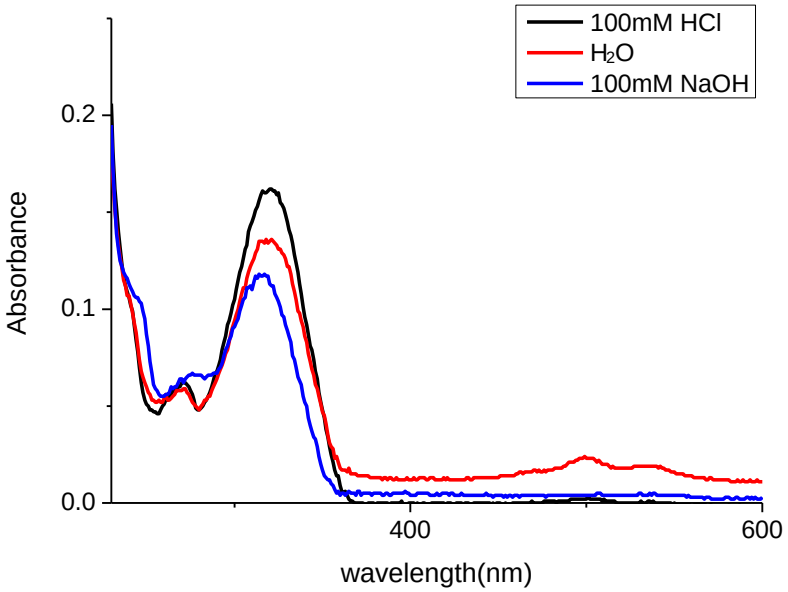

Figure S12. UV absorption spectra of 1μM 3a in aqueous solution

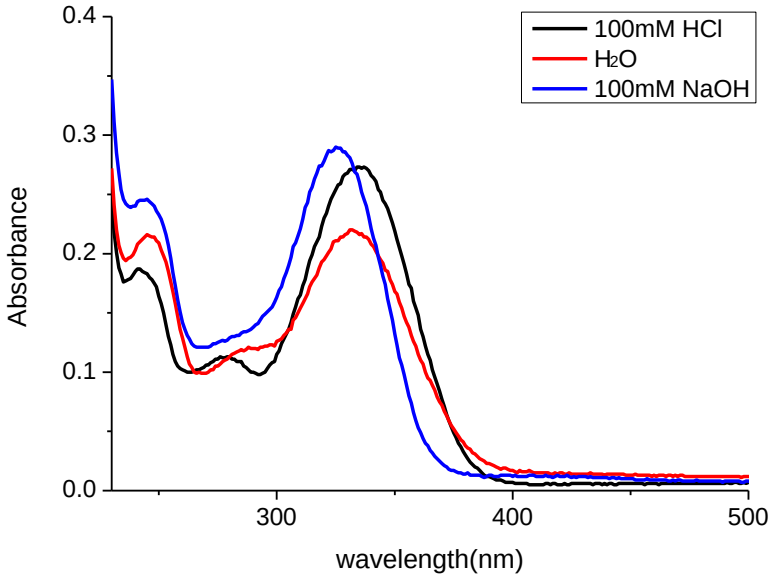

Figure S13. UV absorption spectra of 1μM 3b in aqueous solution

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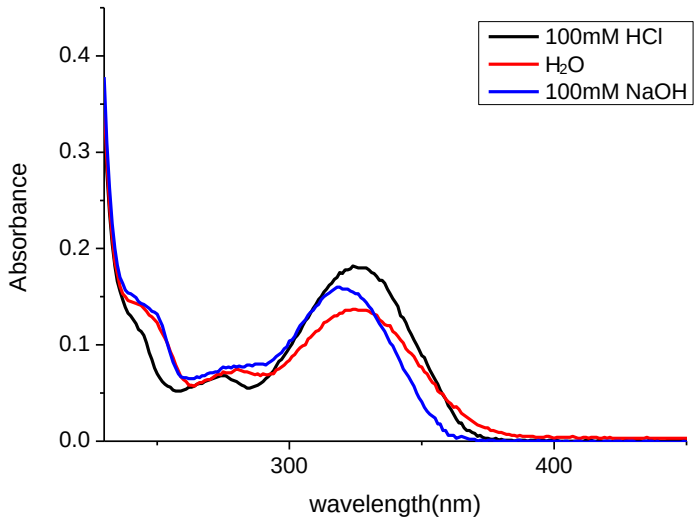

Figure S14. UV absorption spectra of 1μM 3c in aqueous solution

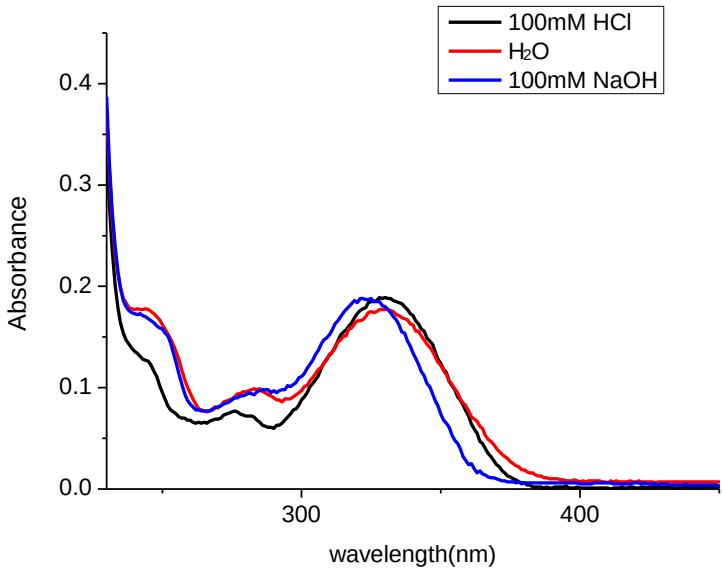

Figure S15. UV absorption spectra of 1μM 3d in aqueous solution

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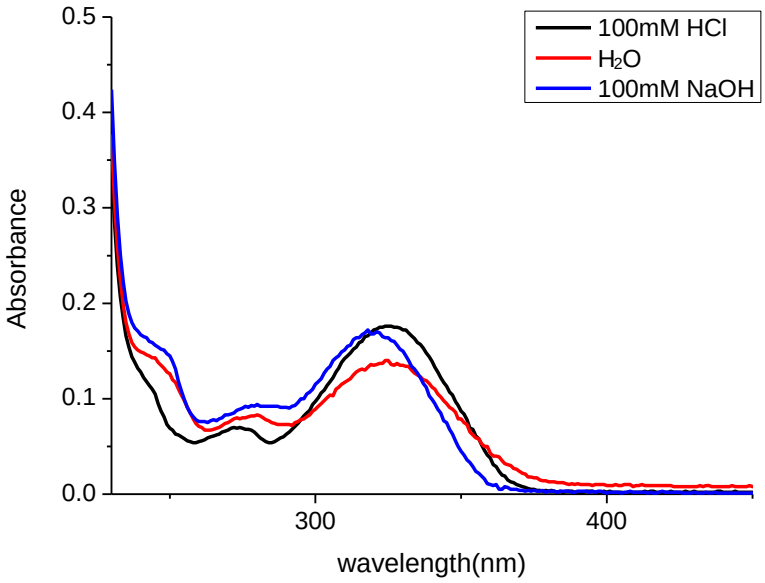

Figure S16. UV absorption spectra of 1μM 3e in aqueous solution

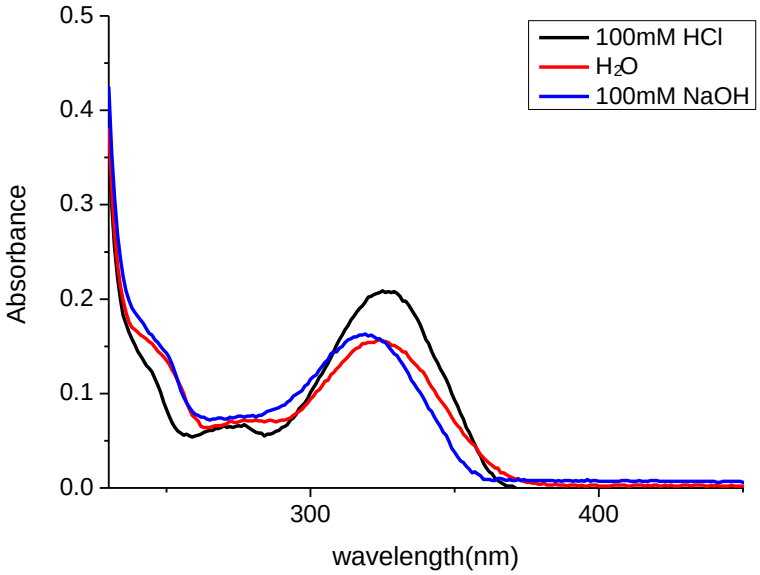

Figure S17. UV absorption spectra of 1μM 3f in aqueous solution

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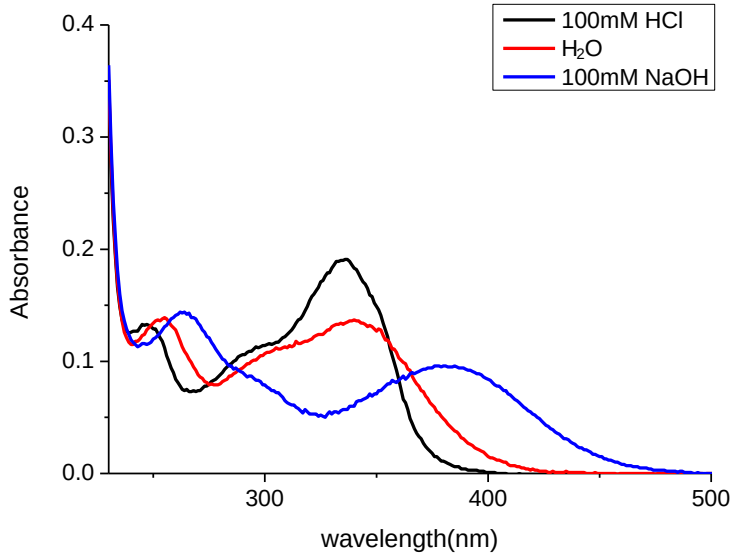

Figure S18. UV absorption spectra of 1μM 3g in aqueous solution

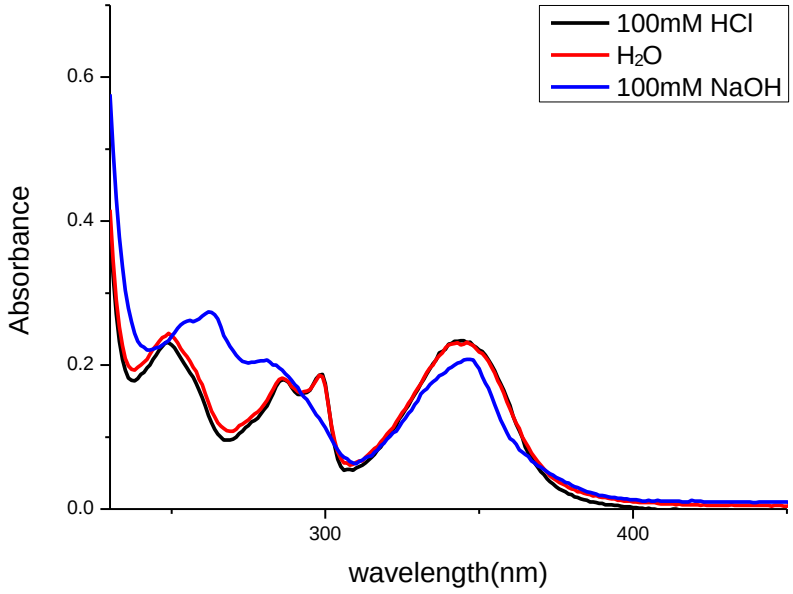

Figure S19. UV absorption spectra of 1μM 3h in aqueous solution

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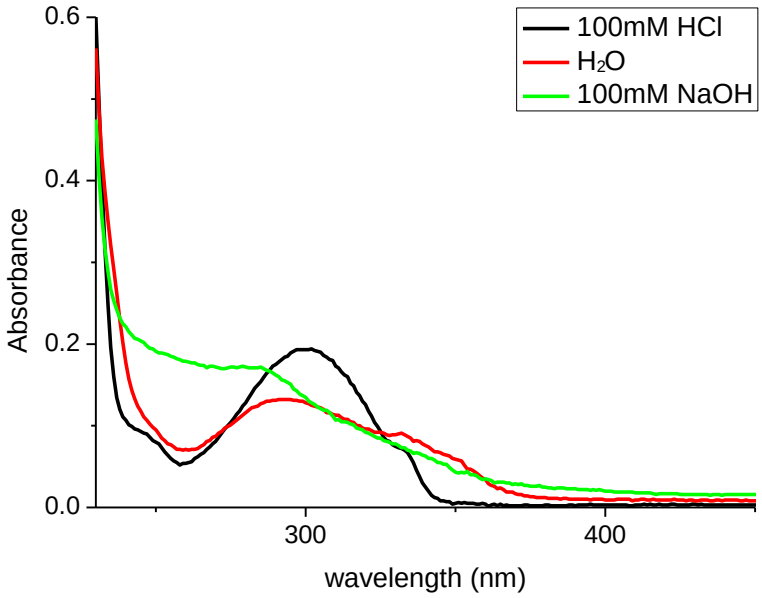

Figure S20. UV absorption spectra of 1μM 3i in aqueous solution

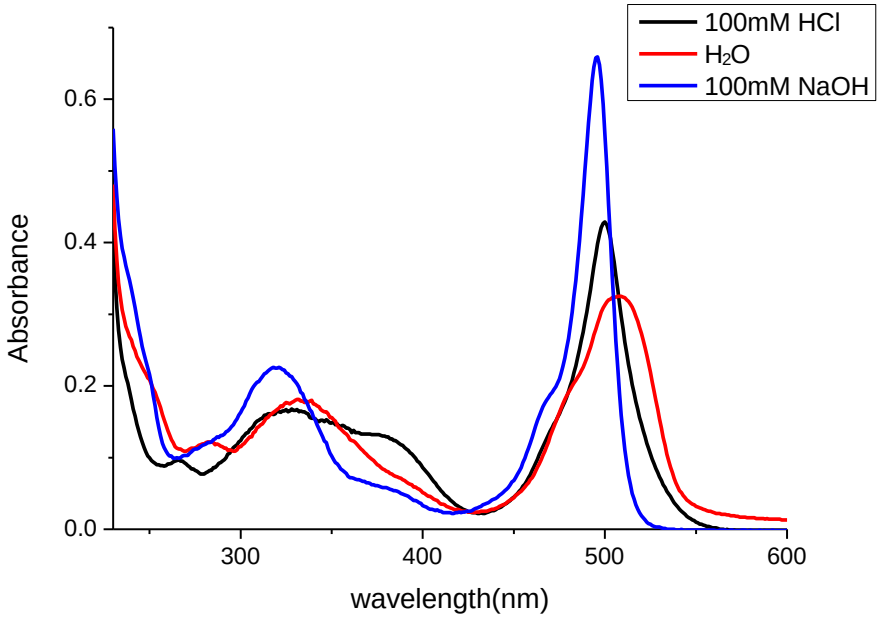

Figure S21. UV absorption spectra of 1μM 3j in aqueous solution

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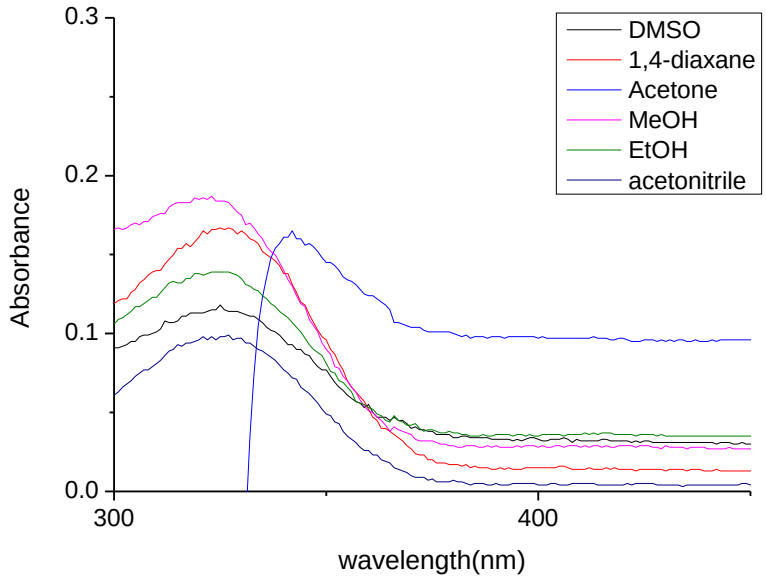

Figure S22. UV absorption spectra of 1μM 3a in organic solvents

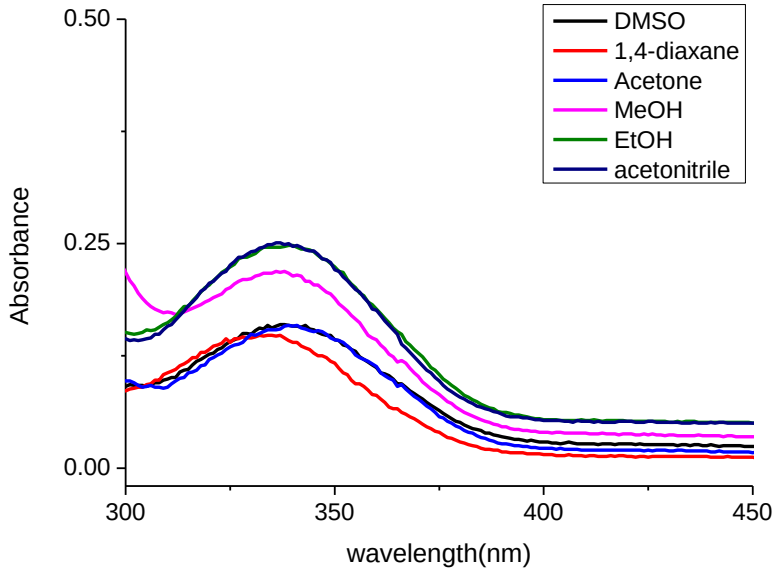

Figure S23. UV absorption spectra of 1μM 3b in organic solvents

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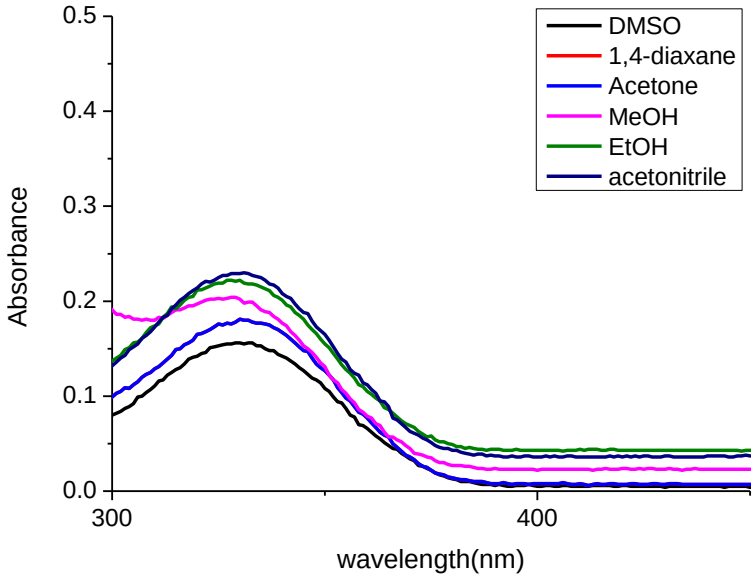

Figure S24. UV absorption spectra of 1μM 3c in organic solvents

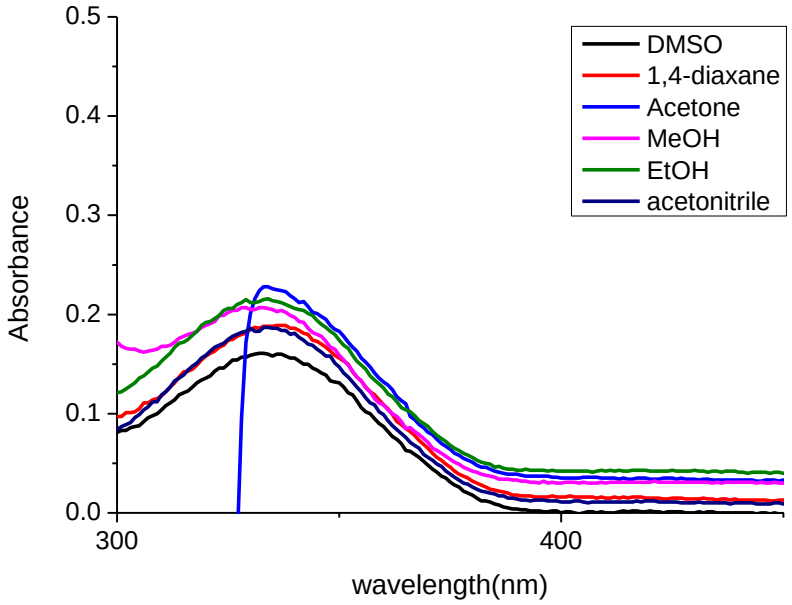

Figure S25. UV absorption spectra of 1μM 3d in organic solvents

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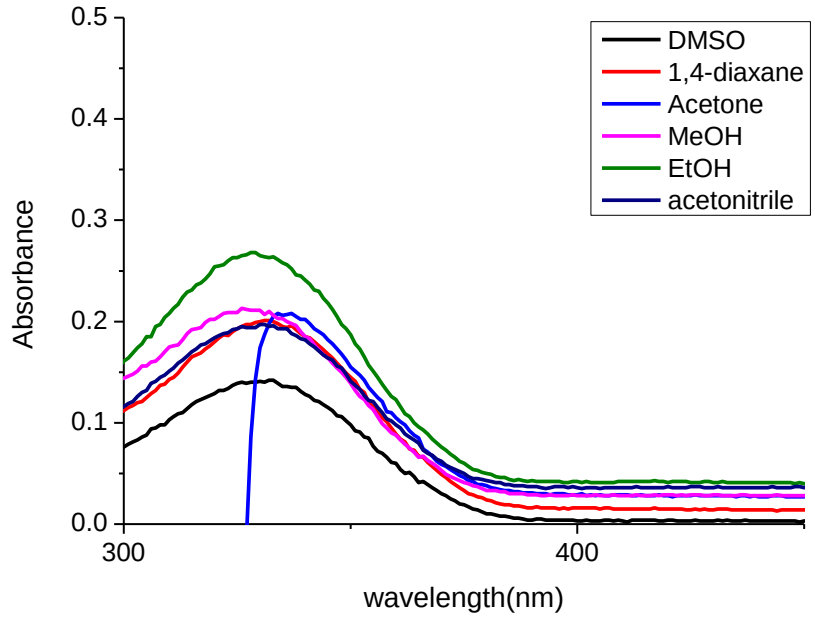

Figure S26. UV absorption spectra of 1μM 3e in organic solvents

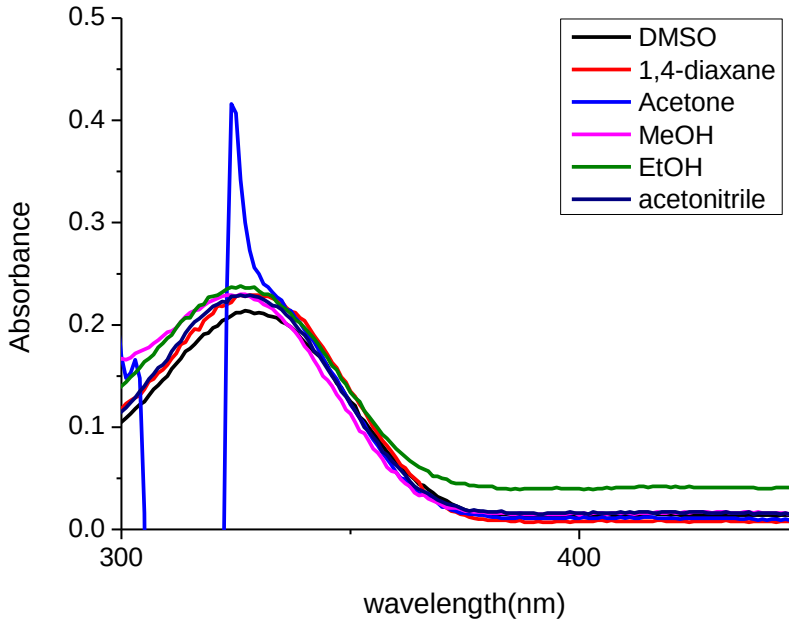

Figure S27. UV absorption spectra of 1μM 3f in organic solvents

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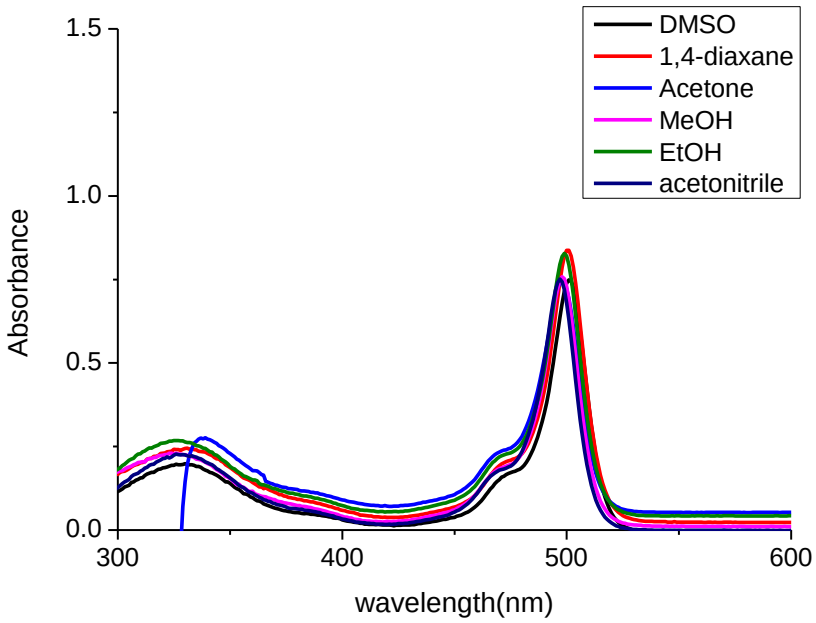

Figure S28. UV absorption spectra of 1μM 3j in organic solvents

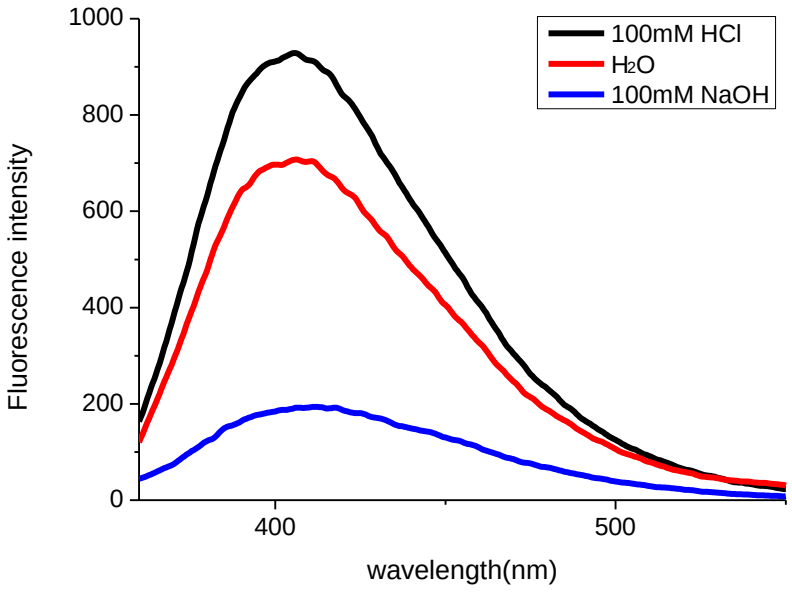

Figure S29. Fluorescence emission spectra of 1μM 3a in aqueous solution

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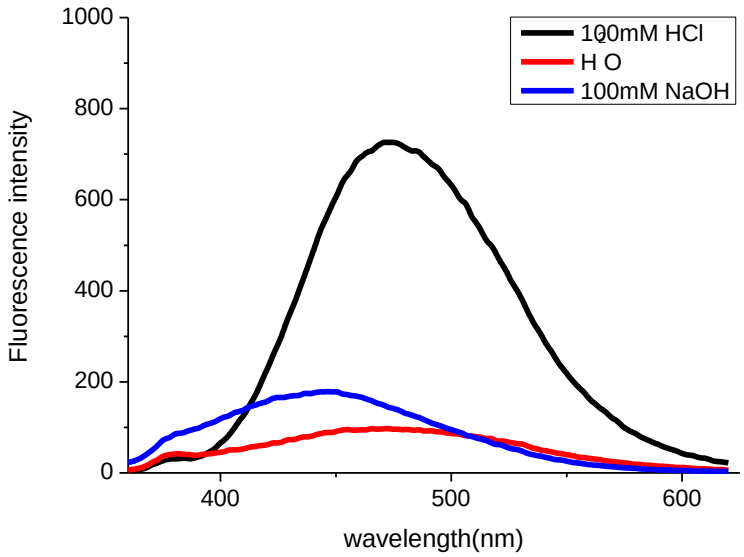

Figure S30. Fluorescence emission spectra of 1μM 3b in aqueous solution

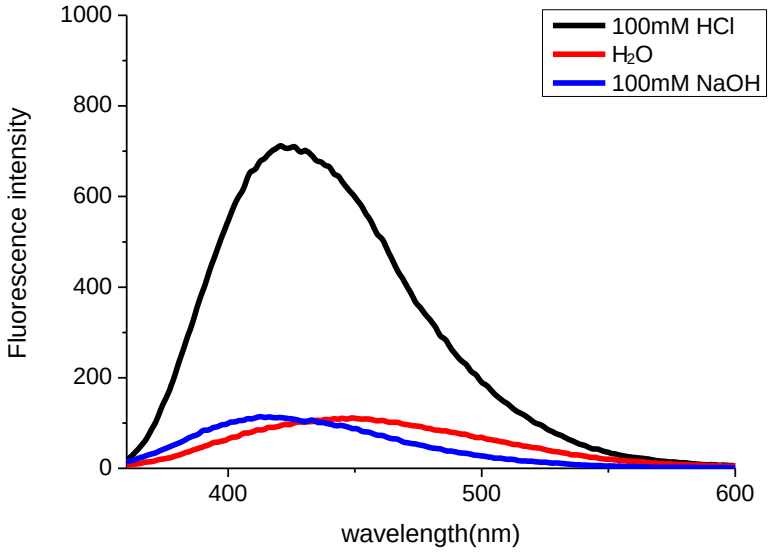

Figure S31. Fluorescence emission spectra of 1μM 3c in aqueous solution

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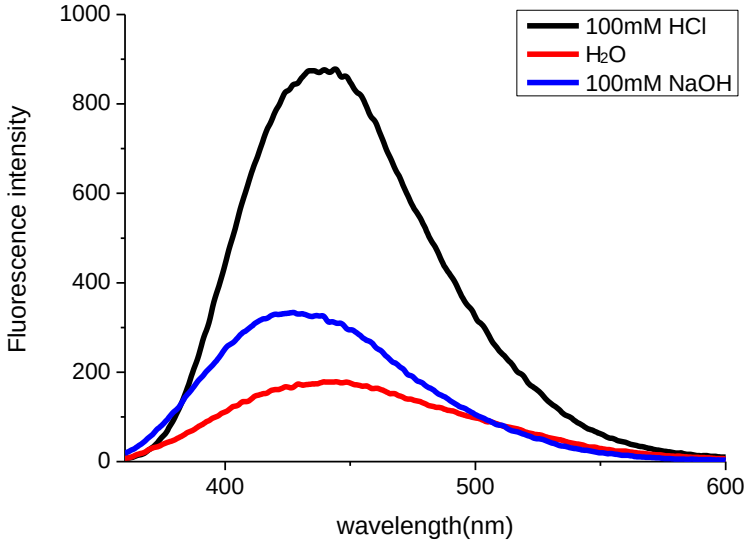

Figure S32. Fluorescence emission spectra of 1μM 3d in aqueous solution

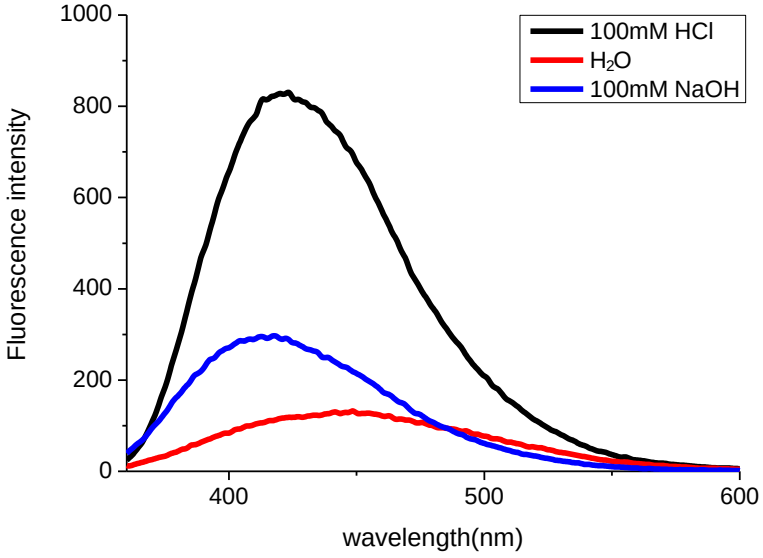

Figure S33. Fluorescence emission spectra of 1μM 3e in aqueous solution

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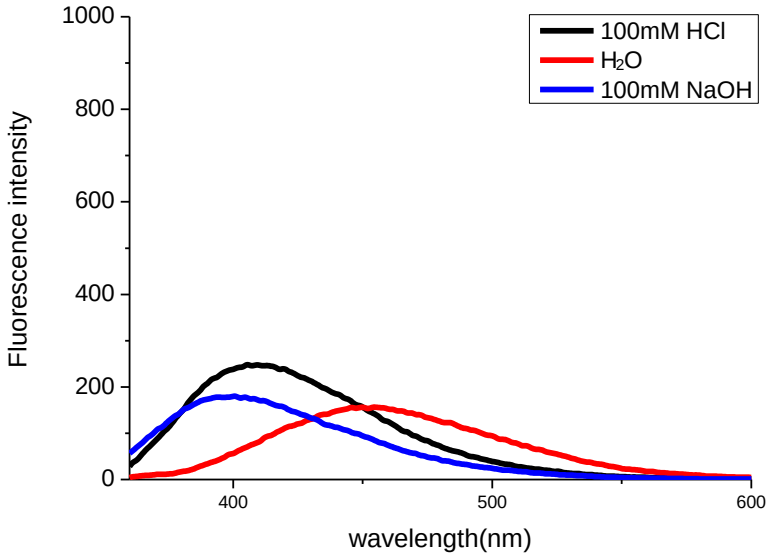

Figure S34. Fluorescence emission spectra of 1μM 3f in aqueous solution

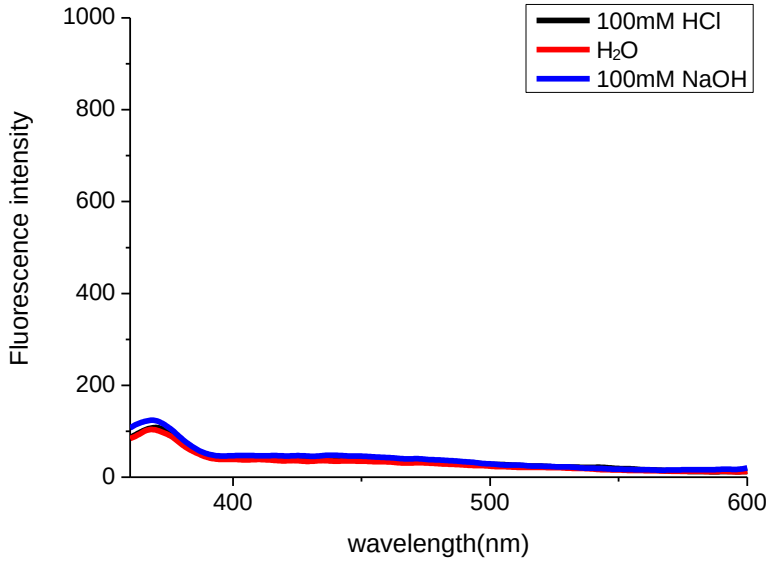

Figure S35. Fluorescence emission spectra of 1μM 3g in aqueous solution

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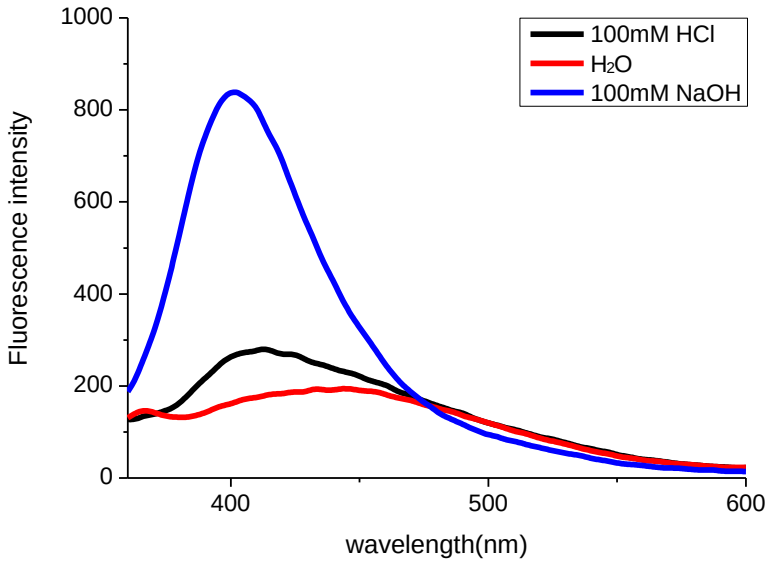

Figure S36. Fluorescence emission spectra of 1μM 3h in aqueous solution

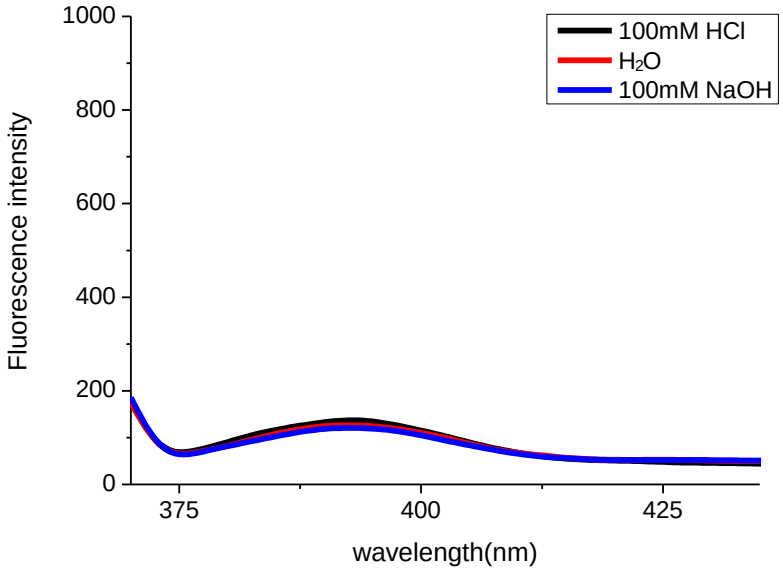

Figure S37. Fluorescence emission spectra of 1μM 3i in aqueous solution

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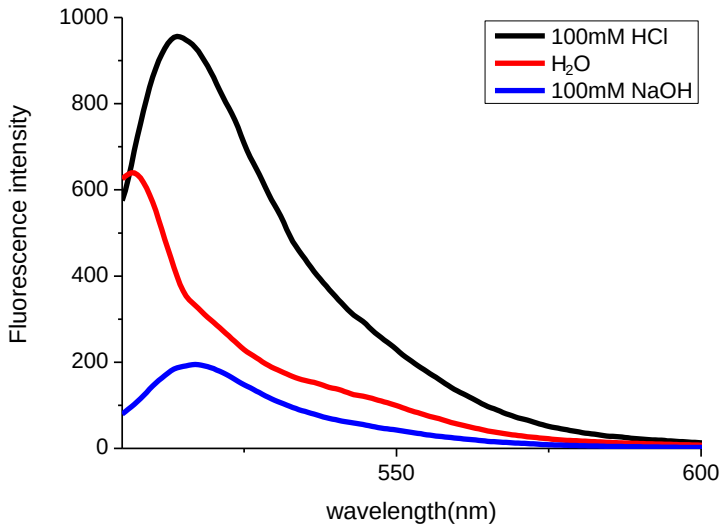

Figure S38. Fluorescence emission spectra of 1μM 3j in aqueous solution

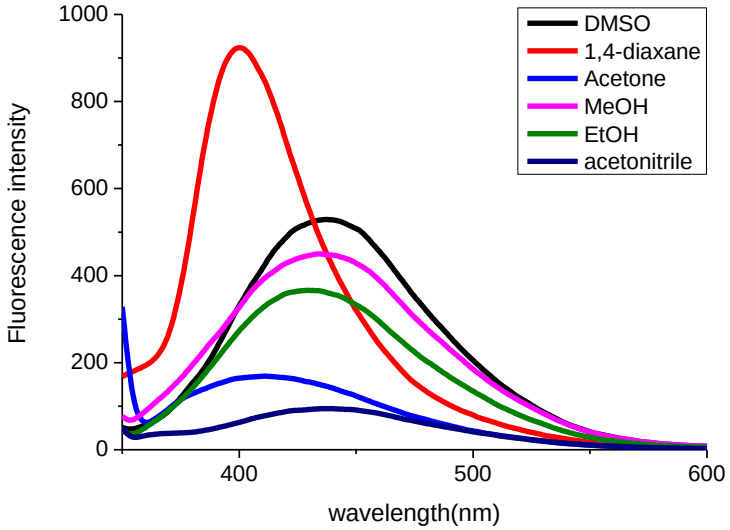

Figure S39. Fluorescence emission spectra of 1μM 3a in organic solvents

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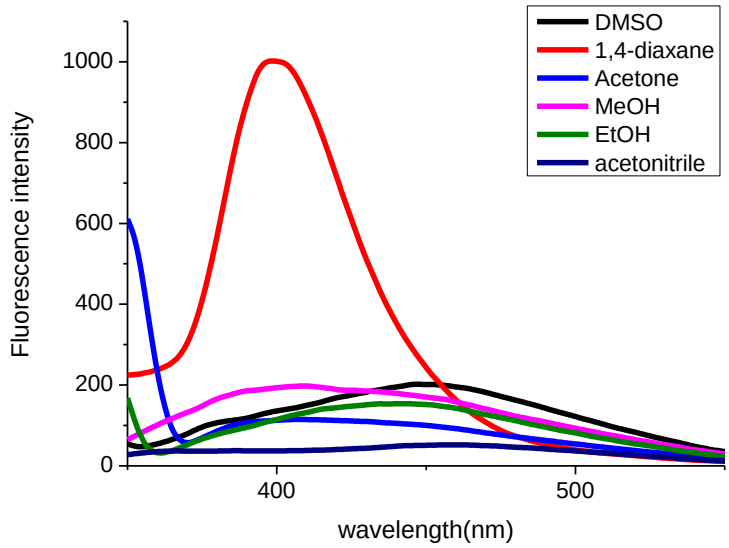

Figure S40. Fluorescence emission spectra of 1μM 3b in organic solvents

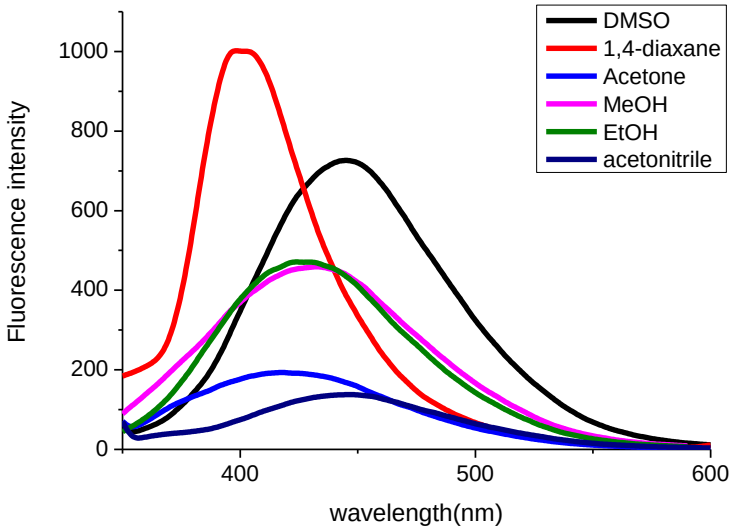

Figure S41. Fluorescence emission spectra of 1μM 3c in organic solvents

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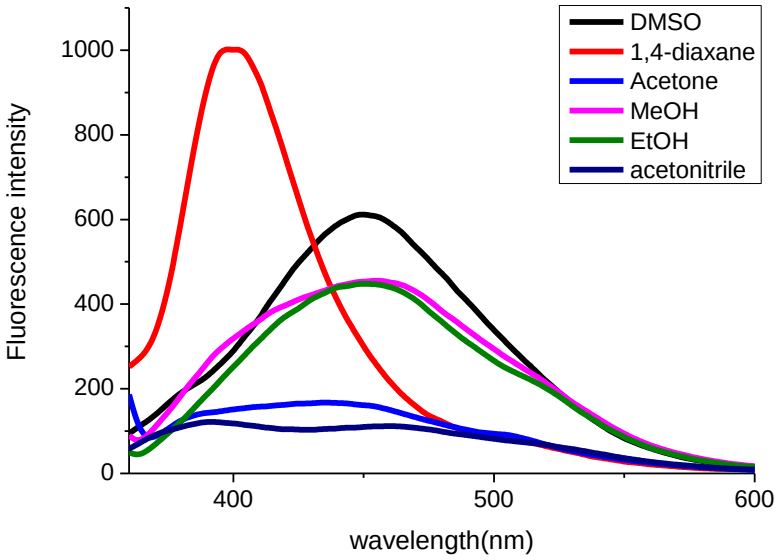

Figure S42. Fluorescence emission spectra of 1μM 3d in organic solvents

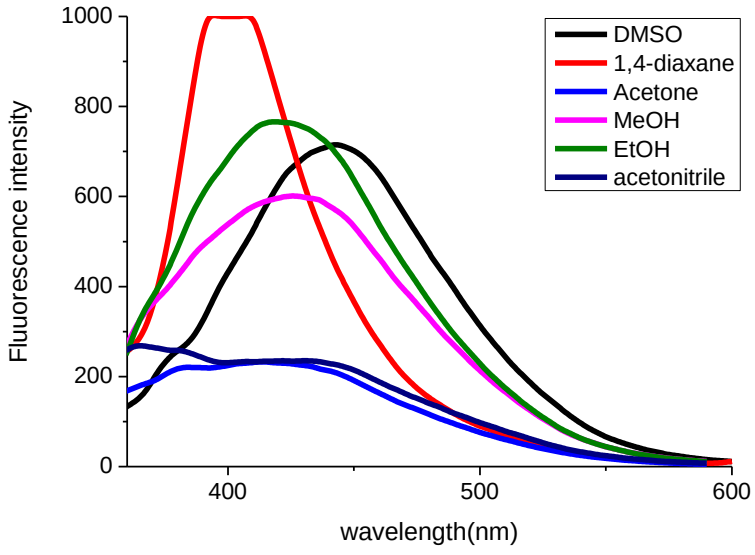

Figure S43. Fluorescence emission spectra of 1μM 3e in organic solvents

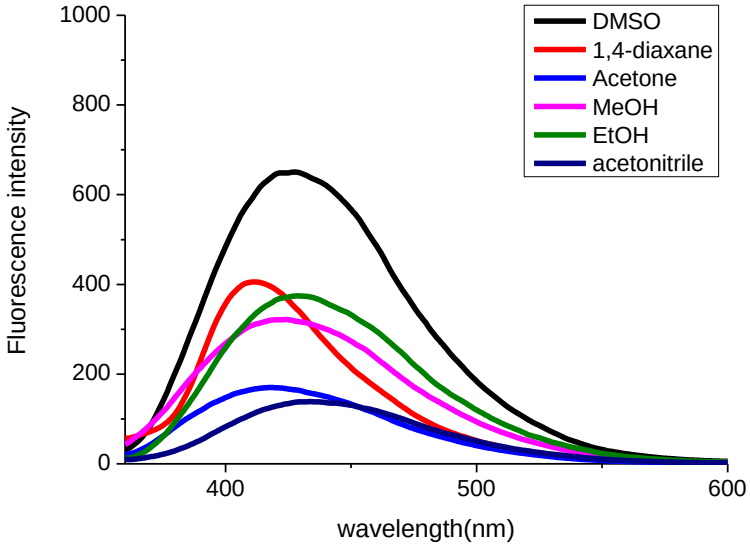

Figure S44. Fluorescence emission spectra of 1μM 3f in organic solvents

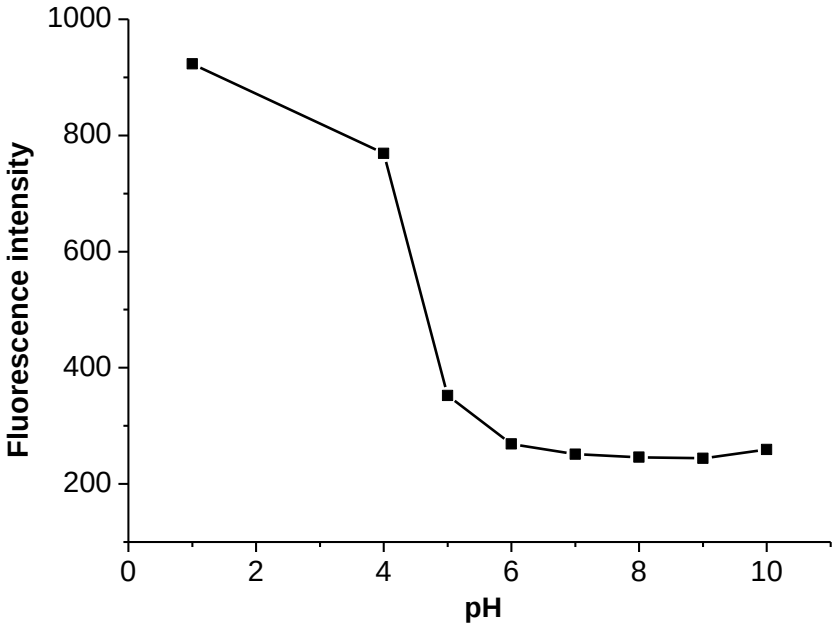

Figure S45. Effect of pH on fluorescence intensity of 1μM 3a

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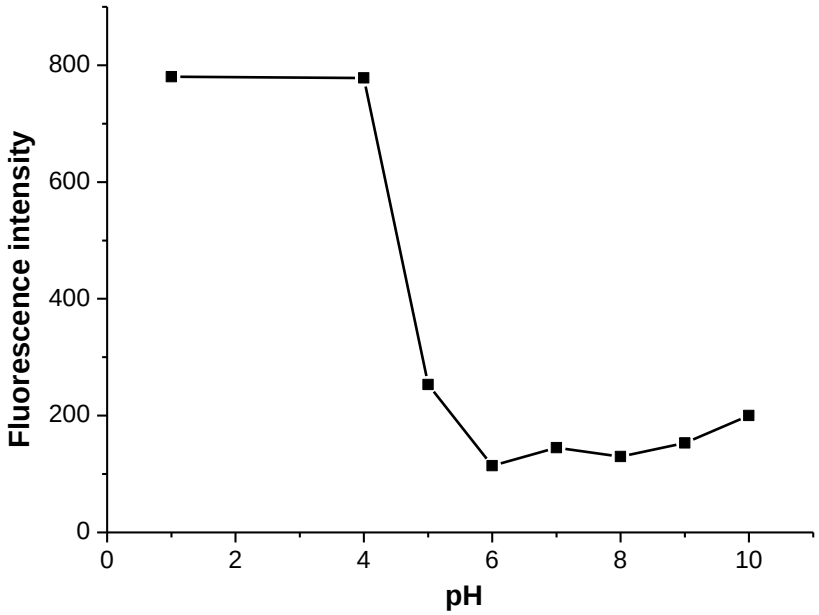

Figure S46. Effect of pH on fluorescence intensity of 1μM 3b

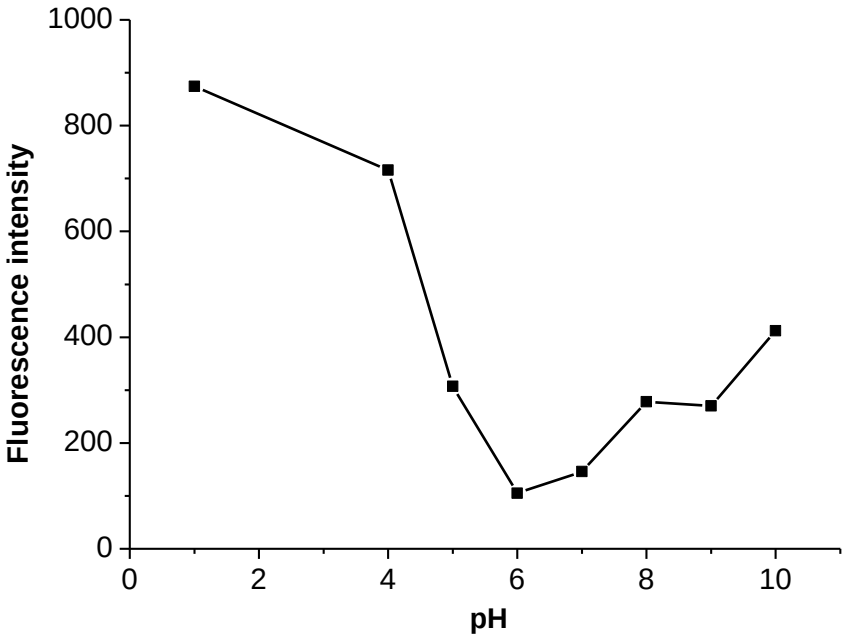

Figure S47. Effect of pH on fluorescence intensity of 1μM 3d

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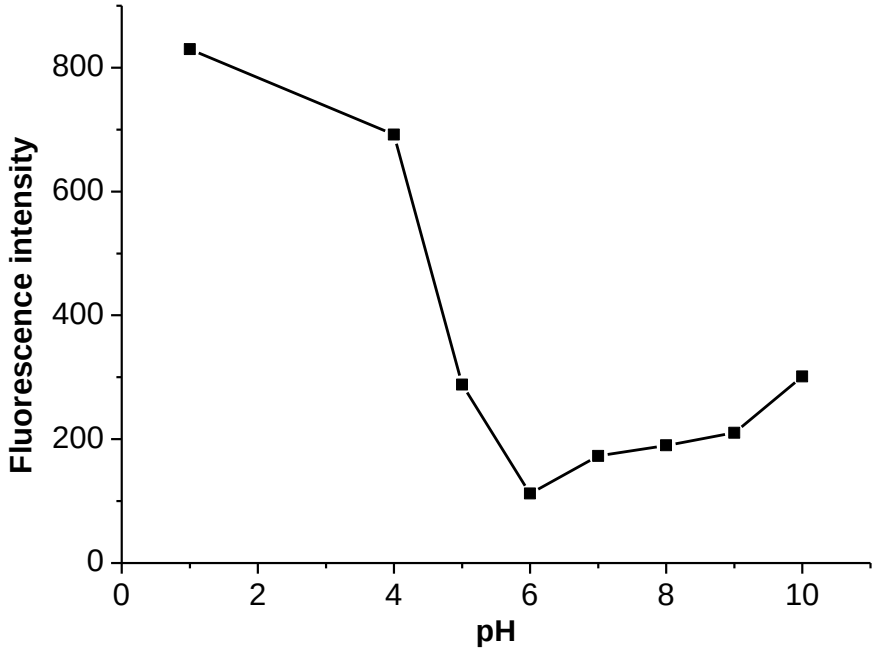

Figure S48. Effect of pH on fluorescence intensity of 1μM 3e

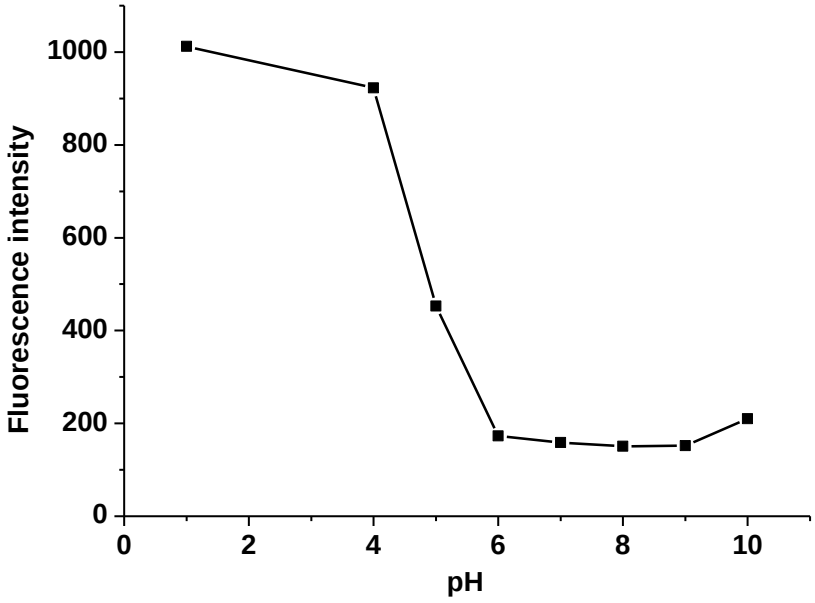

Figure S49. Effect of pH on fluorescence intensity of 1μM 3c

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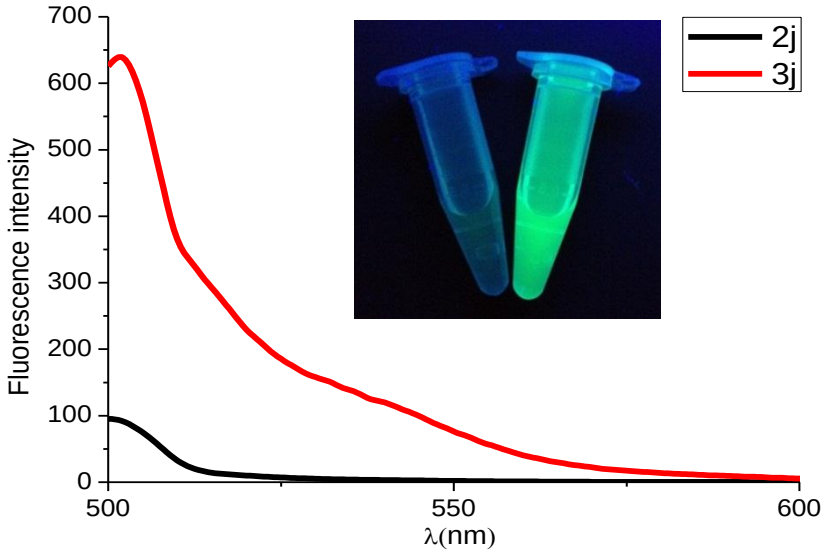

Figure S50. Fluorescence emission spectra of 2j (black) and 3j (red) in water with concentration of 10μM, and the photographs of 2j (left) and 3j (right).

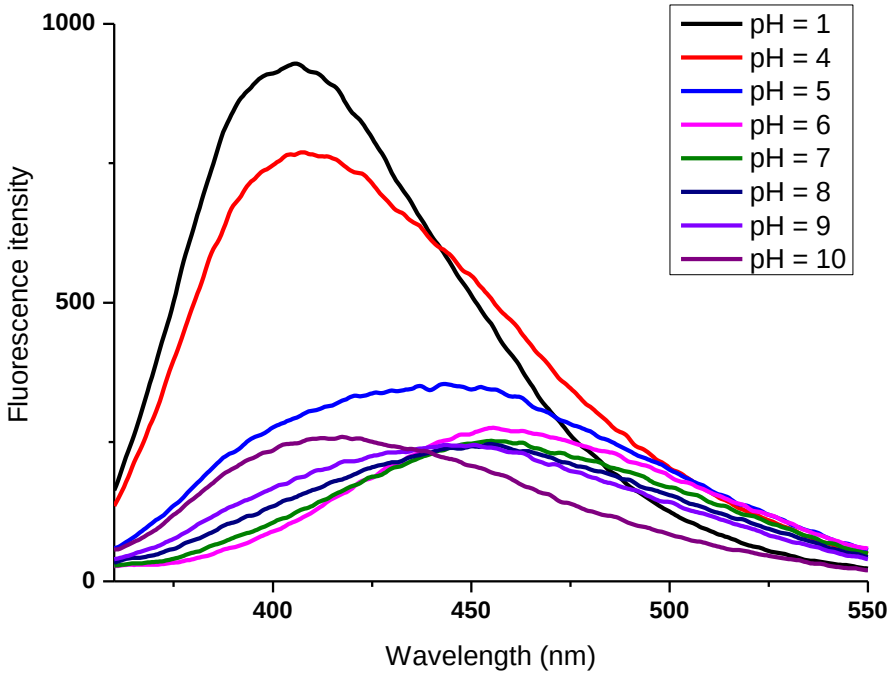

Figure S51. Fluorescence spectrum of changing fluorescence intensity during the pH titration of 1μM 3a

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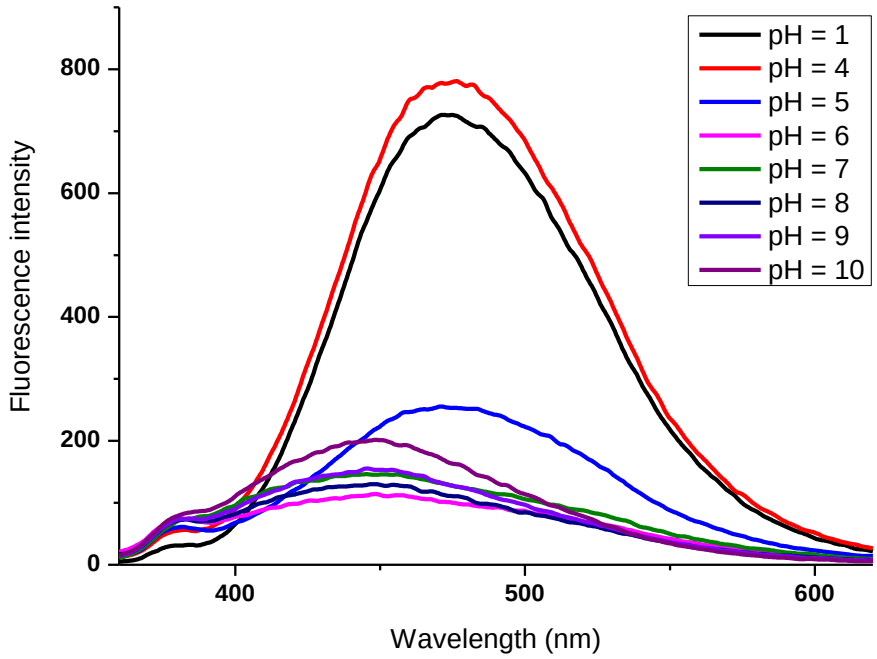

Figure S52. Fluorescence spectrum of changing fluorescence intensity during the pH titration of 1μM 3b

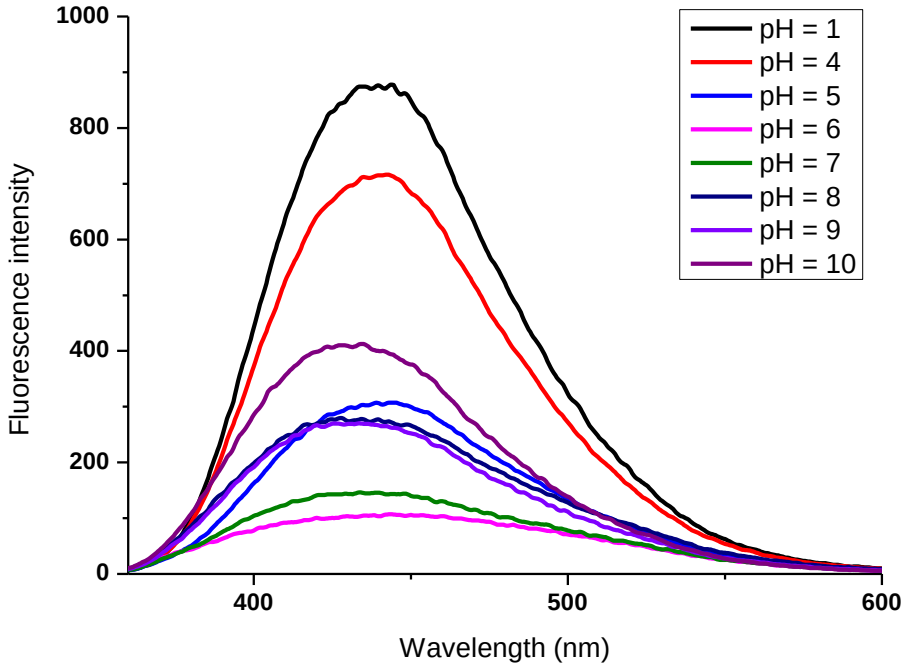

Figure S53. Fluorescence spectrum of changing fluorescence intensity during the pH titration of 1μM 3d

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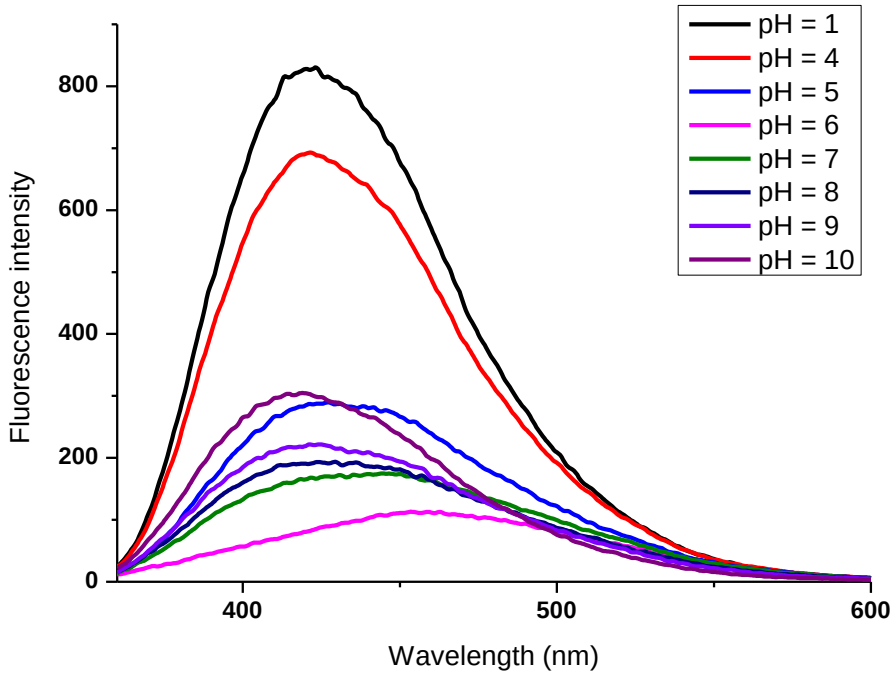

Figure S54. Fluorescence spectrum of changing fluorescence intensity during the pH titration of 1μM 3e

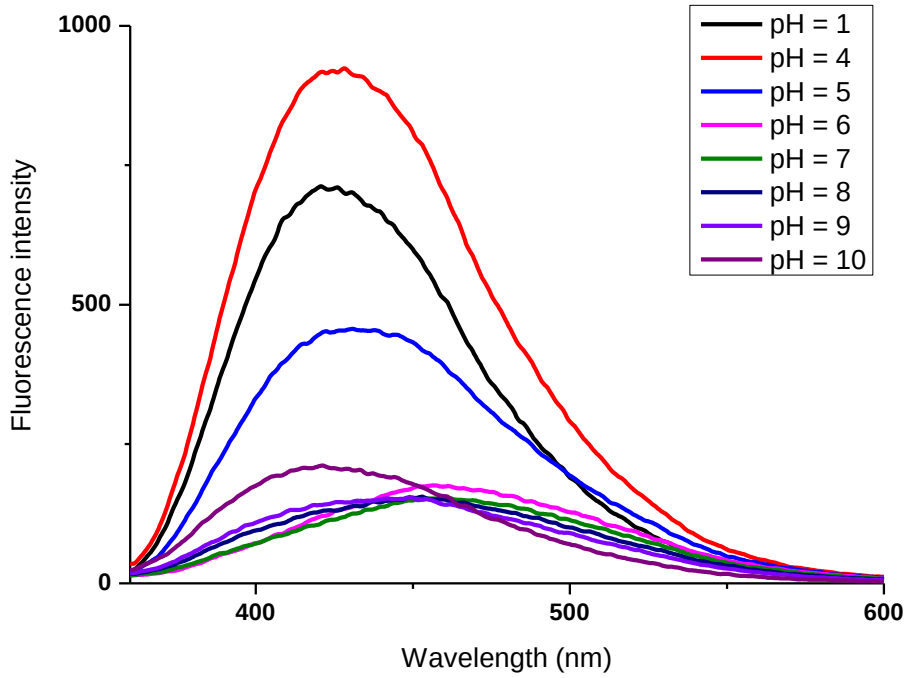

Figure S55. Fluorescence spectrum of changing fluorescence intensity during the pH titration of 1μM 3c

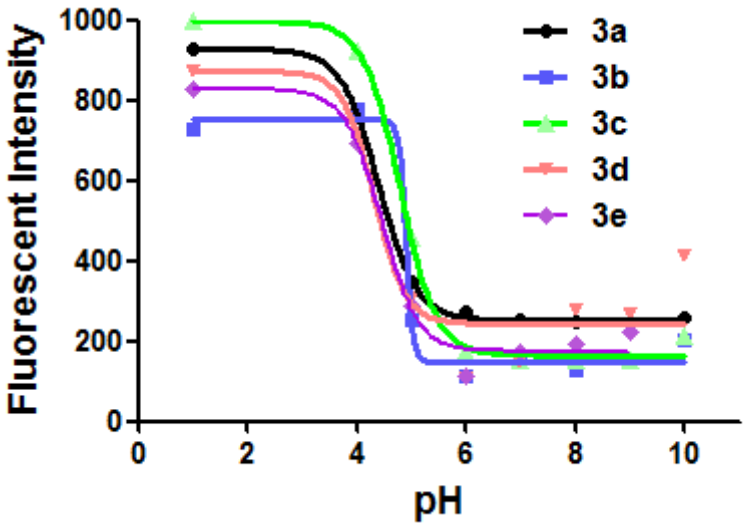

Figure S56. Effect of pH on fluorescence intensity of 1μM 3a (pKa=4.4), 1μM 3b (pKa=4.9), 1μM 3c (pKa=4.8), 1μM 3d (pKa=4.3), 1μM 3e (pKa=4.5).

References:

1. Chunjuan, Wang; Fang, Xie; Wanbin, Zhang; *Chinese Journal of Organic Chemistry*, **2008**, 28(3), 503-505.

2. Wataru, Hirose; Kousuke, Sato; Akira, Matsuda; *Angew. Chem. Int. Ed.* **2010**, 49, 8392 –8394.

3. Yu, Gabe; Yasuteru, Urano; Kazuya, Kikuchi; Hirotatsu, Kojima; Tetsuo, Nagano; *J. Am. Chem. Soc.*, **2004**, 126, 3357-3367.