Supporting information

Long conjugated 2-nitrobenzyl derivatives caged anticancer prodrugs with visible light regulated release: preparation and functionalizations

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Experimental Section for the intermediate compounds

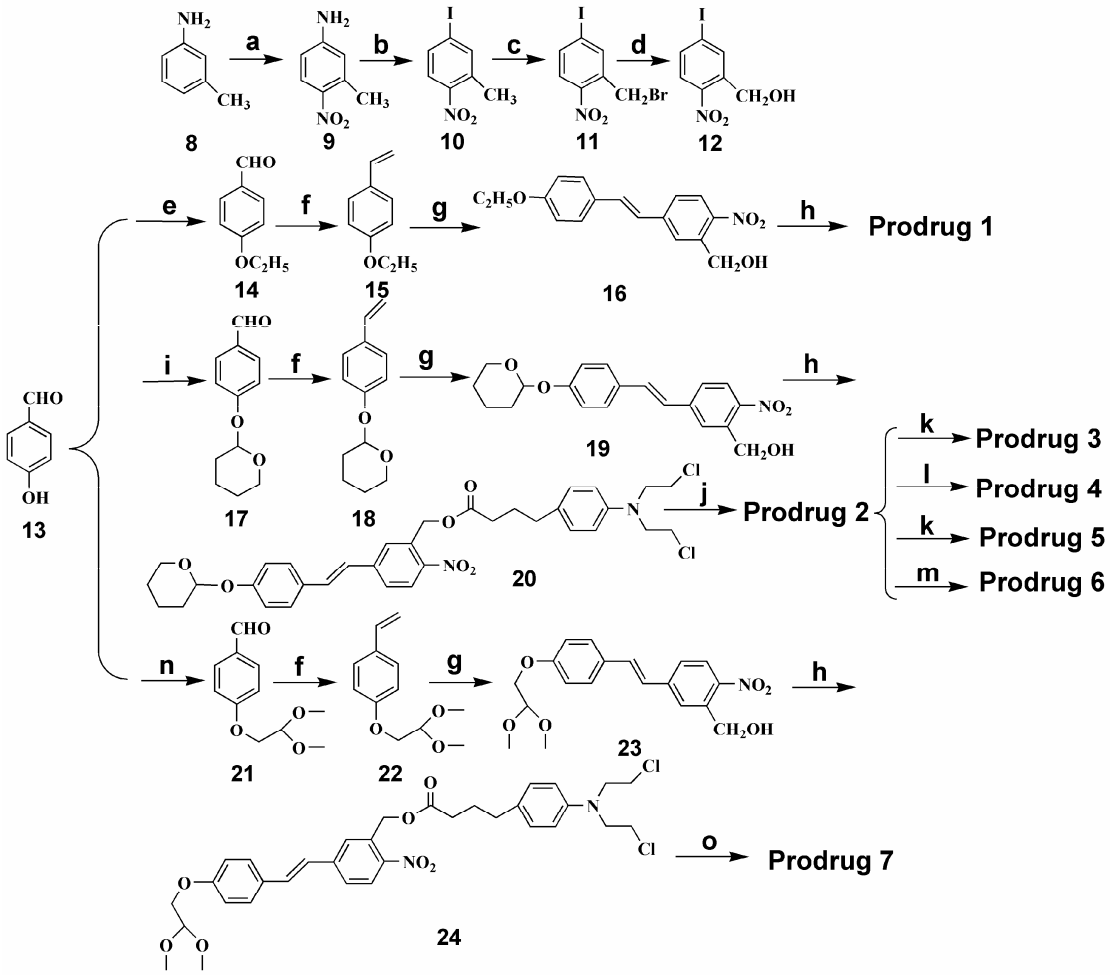


Figure S1 The synthesis procedures for **Prodrug 1-7**.

3-methyl-4-nitroaniline (**compound 9**): To a well-stirred mixture of m-toluidine (10.7 g, 100 mmol) and sulfuric acid (85%, 150 mL), guanidinium nitrate (12.2 g, 100 mmol) was added slowly at 0–5 °C. After the addition, the mixture was stirred for an additional 1h at the same temperature. Then, the reaction mixture was poured into an ice-cold NaOH solution (25%, 1000 mL). The obtained solid was filtered, washed thoroughly with water and dried under vacuum. A brown crude was purified by column chromatography on silica gel (hexane/CH_2Cl_2 = 1/2) to afford 8.2 g **9** as a bright yellow solid (54.0 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 8.02 (d,

J =8.7 Hz, 1H), 6.49 (d, J =8.7 Hz, 1H), 6.46 (s, 1H), 4.23 (s, 2H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): δ= 154.3, 137.2, 136.1, 128.2, 115.2, 111.0, 22.0. EI-MS (m/z): calcd for $C_7H_8N_2O_2$, 152.1 $[M]^+$; found, 152.1.

4-iodo-2-methyl-1-nitrobenzene (**compound 10**): Mechanical stirring is essential for this reaction! To a cooled solution of bright yellow powder **9** (6.1 g, 40 mmol) at 0 °C in H_2SO_4/H_2O (12.2 mL/150 mL), an aqueous solution (15 mL) of sodium nitrite (2.9 g, 42 mmol) was added dropwise. The diazotization process was completed in 10 minutes with occasional grinding. Then potassium iodide (9.3 g, 56 mmol) aqueous solution (30 mL) was added into the above solution at 0 °C within 10 minutes. After the addition, the mixture was stirred and kept at this temperature for another 30 minutes, and then warmed up to room temperature for 3h, which was followed by extraction with ethyl acetate. The combined organic layer was washed with dilute sodium thiosulfate aqueous solution, brine and water, dried over anhydrous Na2SO4, and concentrated in vacuum. The crude was purified by recrystallization in ethanol to afford 8.6 g **10** as a white solid with 81.6 % yield. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 7.74 (d, J = 8.7Hz, 1H), 7.69 (s, 1H), 7.68 (d, J = 8.7 Hz, 1H), 2.56 (s, 3H). 13C NMR (100 MHz, CDCl3), δ (ppm): δ= 148.6, 141.6, 136.1, 130.0, 126.0, 100.6, 20.3. EI-MS (m/z): calcd for $C_7H_6INO_2$, 263.0 $[M]^+$; found, 263.0.

2-(bromomethyl)-4-iodo-1-nitrobenzene (**compound 11**): A suspension of **10** (5.3 g, 20 mmol), BPO (97 mg, 0.4 mmol) and NBS (3.9 g, 22 mmol) in carbon tetrachloride (150 mL) was heated under reflux for 36 hours. The solids were removed by filtration then washed with dichloromethane, and the filtrate was

concentrated in vacuum. The dark brown residue was purified by silica gel column chromatography (hexane/CH_2Cl_2 = 4/1) to afford a yellowish solid **11** (3.0 g, 43.5 % yield). 1H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 7.94 (s, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.76 (d, J = 8.5 Hz, 1H), 4.76 (s, 2H). 13C NMR (100 MHz, $CDCl_3$), δ (ppm): δ= 147.4, 141.3, 138.8, 134.4, 126.8, 101.1, 28.0. EI-MS (m/z): calcd for $C_7H_5BrINO_2$, 340.9 $[M]^+$; found, 340.9.

(5-iodo-2-nitrophenyl) methanol (**compound 12**): Yellowish solid **11** (1.5 g, 4.4 mmol) and Na_2CO_3 (466 mg, 4.4 mmol) was dissolved in acetone/water (160 mL, 3:1 ratio) and heated to reflux for 48 hours, then the mixture was extracted with ethyl acetate. The combined organic phase was washed with brine, water, dried over anhydrous Na_2SO_4, and evaporated in vacuum The brown residue was purified by silica gel column chromatography (hexane/ethyl acetate, 3/1) to afford 0.8 g **12** as a pale solid with 65.4 % yield. ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm): δ= 8.18 (s, 1H), 7.91 (d, J = 8.5Hz, 1H), 7.81 (d, J = 8.5Hz, 1H), 5.64 (t, J = 5.6, 1H), 4.79 (d, J = 5.6Hz, 2H). 13C NMR (100 MHz, DMSO-d_6), δ (ppm): δ= 146.6, 140.7, 137.2, 129.7, 126.5, 103.3, 59.9. EI-MS (m/z): calcd for $C_7H_5INO_3$, 278.9 $[M]^+$; found, 278.9.

4-ethoxybenzaldehyde (**compound 14**): Under the protection of argon, p-hydroxybenzaldehyde **13** (4.9 g, 40 mmol), potassium carbonate (8.3 g, 60 mmol), potassium iodide (166 mg, 1 mmol), bromoethane (5.45 g, 50 mmol) was suspended in 100 mL acetone in a 250 mL three-necked flask. The mixture was stirred and refluxed overnight. After cooling to room temperature, the mixture was filtered and evaporated in vacuum. The crude product was purified by silica gel column

chromatography (hexanes/ ethyl acetate, 8/1). 5.1 g **14** was obtained as colorless oil with 85 % yield. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 9.87 (s, 1H), 7.82 (d, J = 8.4Hz, 2H), 6.98 (d, J = 8.4Hz, 2H), 4.13 (q, J = 6.9Hz, 2H), 1.45 (t, J = 6.9Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ= 190.8, 164.0, 131.9, 129.6, 114.6, 63.8, 14.6. EI-MS (m/z): calcd for $C_9H_{10}O_2$, 150.1 $[M]^+$; found, 150.1.

1-ethoxy-4-vinylbenzene (**compound 15**): To a stirred suspension of **14** (1.5 g, 10 mmol) and methyltriphenylphosphonium bromide (4.28 g, 12 mmol) in THF (50 mL) was added potassium tert-butoxide (2.25 g, 20 mmol) under argon at room temperature. After the mixture was stirred at room temperature overnight, the organic layer was washed three times with brine, dried over Na_2SO_4, filtered, and concentrated. The crude product was purified by silica gel column chromatography (hexanes/CH_2Cl_2, 20/1) to afford a colorless oil **15** (1.05 g, 71 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 7.31(d, J = 8.7Hz, 2H), 6.82(d, J = 8.7Hz, 2H), 6.63(dd, J1 = 17.6Hz, J2 = 10.8Hz, 1H), 5.58(d, J = 17.6Hz, 1H), 5.09(d, J = 10.8Hz, 1H), 4.0(q, J = 7.0Hz, 2H), 1.38(t, J = 7.0Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ= 158.7, 136.2, 130.2, 127.4, 114.4, 111.4, 63.4, 14.8. EI-MS (m/z): calcd for $C_{10}H_{12}O$, 148.1 $[M]^+$; found, 148.1.

(E)-(5-(4-ethoxystyryl)-2-nitrophenyl)methanol (**compound 16**): Under the protection of argon, an overdried two-necked round-bottom flask containing a stirring bar was charged with **12** (1.2 g, 4.3 mmol), compound **15** (0.7 g, 4.7 mmol), palladium acetate (25 mg, 0.1 mmol) and triethanolamine (20 mL). The mixture was heated and stirred at 110 °C for 12 hours. After cooling to room temperature, diethyl

ether was added to extract the product. The combined diethyl ether layers were washed with brine and water, dried with anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (ethyl acetate /hexane, 1/3) on silica gel to afford a yellow powder **16** (470 mg, 36.5 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 8.13 (d, J = 8.6Hz, 1H), 7.80 (s, 1H), 7.53 (d, J = 8.6Hz, 1H), 7.48 (d, J = 8.7Hz, 2H), 7.25 (d, J = 16.2Hz, 1H), 6.99 (d, J = 16.2Hz, 1H), 6.91 (d, J = 8.7Hz, 2H), 5.01 (d, J = 6.6Hz, 2H), 4.07 (q, J = 7.0Hz, 2H), 2.58 (t, J = 6.6Hz, 1H), 1.43 (t, J = 7.0Hz, 3H). ^{13}C NMR (100 MHz, CDCl3), δ (ppm): δ = 159.6, 145.2, 143.9, 137.7, 133.1, 128.7, 128.4, 127.0, 126.0, 125.4, 123.8, 114.8, 63.6, 62.8, 14.8. EI-HRMS (m/z): calcd for $C_{17}H_{17}NO_4$, 299.1158 $[M]^+$; found, 299.1161.

4-((tetrahydro-2H-pyran-2-yl)oxy)benzaldehyde (**compound 17**): p-hydroxybenzal dehyde **13** (12.2 g, 100 mmol), PPTS (2.51 g, 10 mmol) and dichloromethane (50 mL) were added into a 250 mL three-necked flask. And then, 25 mL dichloromethane solution of 3,4-2H-dihydropyran (12.6 g, 150 mmol) was added by constant pressure dropping funnel in 30 minutes at rt. The reaction was monitored by TLC on SiO_2 (UV detection). The reaction mixture was washed with saturated sodium bicarbonate solution, brine, and water and dried over anhydrous Na_2SO_4. After evaporated in vacuum, the residue was purified by silica gel column chromatography (hexane/ ethyl acetate, 6:1) to afford a colorless oil **17** (16.6 g, 80.5% yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 9.88 (s, 1H), 7.82 (d, J = 8.7Hz, 2H), 7.15 (d, J = 8.7Hz, 2H), 5.53 (t, J = 3.1Hz, 1H), 3.83 (dt, J1 = 3.0Hz, J2 =

11.4Hz, 1H), 3.62 (dt, J1 = 3.0Hz, J2 = 11.4Hz, 1H), 2.03-1.95 (m, 1H), 1.90-1.86 (m, 2H), 1.76-1.57 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 190.9, 162.1, 131.7, 130.3, 116.4, 96.0, 61.9, 29.9, 24.9, 18.4. ES-MS (m/z): calcd for $C_{12}H_{13}O_3$, 205.1 $[M-H]^-$; found, 205.1.

2-(4-vinylphenoxy)tetrahydro-2H-pyran (**compound 18**): To a stirred suspension of **17** (8.2 g, 40 mmol) and methyltriphenylphosphonium bromide (21.4 g, 60 mmol) in THF (150 mL) was added potassium tert-butoxide (9.0 g, 80 mmol) under argon purge at room temperature. After the mixture was stirred at room temperature overnight, the organic layer was washed three times with brine (150 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified by silica gel column chromatography (hexane/CH_2Cl_2, 10:1) to afford a colorless oil **18** (6.1 g, 75.2% yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ= 7.34(d, J = 8.7Hz, 2H), 7.02(d, J = 8.7Hz, 2H), 6.67(dd, J1 = 10.9Hz, J2 = 17.6 Hz, 1H), 5.62(d, J =17.6Hz, 1H), 5.43(t, J = 3.2Hz, 1H), 5.13(d, J = 10.9Hz,1H), 3.94-3.88(m, 1H), 3.63-3.58(m, 1H), 2.07-1.95(m, 1H), 1.89-1.85(m, 2H), 1.75-1.57(m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ= 156.9, 136.4, 131.3, 127.3, 116.5, 111.8, 96.3, 62.0, 30.4, 25.3, 18.8. EI-MS (m/z): calcd for $C_{13}H_{16}O_2$, 204.1 $[M]^+$; found, 204.1.

(E)-(2-nitro-5-(4-((tetrahydro-2H-pyran-2-l)oxy)styryl)phenyl)methanol (**compound 19**): Under the protection of argon, an overdried two-necked round-bottom flask containing a stirring bar was charged with **12** (1.1 g, 4 mmol), colorless oil **18** (900 mg, 4.4 mmol), palladium acetate (23 mg, 0.1 mmol), DMF (5 mL) and triethanolamine (20 mL). The mixture was heated and stirred at 110 °C for

12 h. After cooling to room temperature, diethyl ether was added to extract the product. The combined organic layers were washed with water and brine, dried with anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (CH_2Cl_2) on silica gel to afford **compound 19** as an orange yellow powder (385 mg, 27.1 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 8.12 (d, J = 8.5Hz, 1H), 7.80 (s, 1H), 7.52 (d, J = 8.5Hz, 1H), 7.47 (d, J = 8.7Hz, 2H), 7.23 (d, J = 16.2Hz, 1H), 7.07 (d, J = 8.7Hz, 2H), 7.00 (d, J = 16.2 Hz, 1H), 5.46 (t, J = 3.1Hz, 1H), 5.01 (s, 2H), 3.93-3.87 (m, 1H), 3.65-3.60 (m, 1H), 2.68 (s, 1H), 2.07-1.97 (m, 1H), 1.90-1.86 (m, 2H), 1.73-1.59 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ= 157.1, 145.2, 143.5, 135.7, 132.8, 128.7, 128.6, 126.4, 125.6, 124.0, 115.9, 99.2, 66.5, 62.9, 30.6, 25.3, 19.7. EI-MS (m/z): calcd for $C_{20}H_{21}NO_5$, 355.2 $[M]^+$; found, 355.1.

(E)-2-nitro-5-(4-((tetrahydro-2H-pyran-2-yl)oxy)styryl)ben zyl-4-(4-(bis(2-chloro ethyl)amino)phenyl)butanoate (**compound 20**): In the dark, yellow powder **19** (400 mg, 1.12 mmol) with chloroambucil (377 mg, 1.24 mmol) in the presence of DCC (277 mg, 1.34 mmol) and DMAP (12 mg, 0.1 mmol) was dissolved and stirred in dry dichloromethane (20 mL) at room temperature for 12 hours. The mixture was filtered and the solvent was evaporated. The residual was purified by silica gel chromatography (hexane/ethyl acetate, 6:1) to afford **20** as a yellow solid (520 mg, 72.4 % yield).^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 8.11 (d, J = 8.5Hz, 1H), 7.61 (s, 1H), 7.54 (d, J = 8.5Hz, 1H), 7.46 (d, J = 8.7Hz, 2H), 7.20 (d, J = 16.3Hz, 1H), 7.08 (d, J = 8.6Hz, 2H), 7.06 (d, J = 8.7Hz, 2H), 6.98 (d, J = 16.3 Hz, 1H), 6.61 (d, J =

8.6Hz, 2H), 5.54(s, 2H), 5.48 (t, J = 3.1Hz, 1H), 3.94-3.88 (m, 1H), 3.67 (t, J = 7.0Hz, 4H), 3.65-3.60 (m, 1H), 3.60 (t, J = 7.0Hz, 4H), 2.62 (t, J = 7.4Hz, 2H), 2.48 (t, J = 7.4Hz, 2H), 2.05-1.96 (m, 3H), 1.91-1.87 (m, 2H), 1.77-1.59 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 166.6, 161.4, 156.1, 153.3, 153.3, 150.7, 148.2, 124.5, 108.9, 107.5, 98.4, 82.6, 63.2, 62.8, 48.8, 45.8, 27.7, 25.0, 11.9. ES-HRMS (m/z): calcd for $C_{34}H_{39}Cl_2N_2O_6$, 641.2185 $[M+H]^+$; found, 641.2185.

4-(2,2-dimethoxyethoxy)benzaldehyde (**compound 21**): p-hydroxybenzaldehyde (6.1 g, 50 mmol), potassium carbonate (10.4 g, 75 mmol), potassium iodide (33 mg, 2 mmol), 2-bromo-1,1-dimethoxyethane (12.7 g, 75 mmol) and DMF(50 mL), were mixed in a 250 mL three-necked flask. The mixture was stirred under argon in 100 °C overnight. After the solution cooled to room temperature, it was filtered to remove the inorganic solids. The excess of DMF was distilled off under reduced pressure. The residual was purified by silica gel column chromatography (hexane/ ethyl acetate, 8:1) to afford **compound 21** as colorless oil (8.2 g, 78.0 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 9.89 (s, 1H), 7.83 (d, J = 8.7Hz, 2H), 7.03 (d, J = 8.7Hz, 2H), 4.74 (t, J = 5.1Hz, 1H), 4.09 (d, J = 5.1Hz, 2H), 3.47 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 190.7, 163.4, 131.9, 130.2, 114.8, 101.9, 67.7, 54.3. EI-MS (m/z): calcd for $C_{11}H_{14}O_4$, 210.09 $[M]^+$; found, 210.1.

1-(2,2-dimethoxyethoxy)-4-vinylbenzene (**compound 22**): To a stirred suspension of **21** (6 g, 28.5 mmol) and methyltriphenylphosphonium bromide (15.2 g, 42.5 mmol) in THF (150 mL) was slowly added potassium tert-butoxide (6.4 g, 57 mmol) under argon purge at room temperature. After the mixture was stirred at room

temperature overnight, the organic layer was washed three times with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified by silica gel column chromatography (hexane/CH_2Cl_2, 15:1) to give **compound 22** as colorless oil (4.2 g, 70.8 % yield). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 7.34 (d, J = 8.5Hz, 2H), 6.90 (d, J = 8.5Hz, 2H), 6.66 (dd, J1 = 10.9Hz, J2 = 17.6Hz, 1H), 5.62 (d, J = 17.6Hz, 1H), 5.13 (d, J = 10.9Hz, 1H), 4.72 (t, J = 5.2Hz, 1H), 4.01 (d, J = 5.2Hz, 2H), 3.46 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 158.3, 136.2, 130.9, 127.4, 114.6, 111.8, 102.1, 67.6, 54.1. EI-MS (m/z): calcd for $C_{12}H_{16}O_3$, 218.1 $[M]^+$; found, 208.1.

(E)-(5-(4-(2,2-dimethoxyethoxy)styryl)-2-nitrophenyl) methanol (**compound 23**): Under the protection of argon, an overdried two-necked round-bottom flask containing a stirring bar was charged with **compound 12** (2.2 g, 7.4 mmol), **compound 22** (2.0g, 9.6 mmol), palladium diacetate (35 mg, 0.15 mmol), DMF(15 mL) and triethanolamine (30 mL). The mixture was heated and stirred at 110 °C for 12 h. After cooling to room temperature, diethyl ether was added to extract the product. The combined organic layers were washed with brine and water, dried with anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (hexane/ ethyl acetate, 6:1) on silica gel to afford a orange yellow powder **23** (900 mg) with 31.7 % yield. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 8.01 (d, J = 8.5Hz, 1H), 7.79 (s, 1H), 7.48 (d, J = 8.5Hz, 1H), 7.46 (d, J = 8.7Hz, 2H), 7.21 (d, J = 16.3Hz, 1H), 6.96 (d, J = 16.3Hz, 1H), 6.93 (d, J = 8.7Hz, 2H), 5.00 (s, 2H), 4.73 (t, J = 5.0Hz, 1H), 4.02 (d, J = 5.0Hz, 2H), 3.47 (s, 6H), 2.82 (s, 1H). ^{13}C

NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 159.1, 145.4, 143.8, 137.8, 132.9, 129.4, 128.4, 127.0, 125.9, 125.4, 124.2, 115.0, 102.1, 67.6, 62.7 54.3. EI-MS (m/z): calcd for $C_{19}H_{21}NO_6$, 359.1 $[M]^+$; found, 359.1.

(E)-5-(4-(2,2-dimethoxyethoxy)styryl)-2-nitrobenzyl-4-(4-(bis(2-chloroethyl)amino)phenyl)butanoate (**compound 24**): In the dark, a mixture of yellow powder **23** (200 mg, 0.56 mmol), chloroambucil (186 mg, 0.61 mmol) in the presence of DCC (172 g, 0.83 mmol) and DMAP (8 mg, 0.06mmol) in dichloromethane (20 mL) were reacted at room temperature for 12 hours. The reaction mixture was filtered and the solvent was removed in vacuum. The residue was purified by silica gel chromatography (hexane/ethyl acetate, 8:1) to afford 280 mg **compound 24** as a yellow solid with 78.0 % yield. ^1H NMR (400 MHz, $CDCl_3$), δ (ppm): δ = 8.12 (d, J = 8.5Hz, 1H), 7.60 (s, 1H), 7.56 (d, J = 8.5Hz, 1H), 7.46 (d, J = 8.5Hz, 2H), 7.19 (d, J = 16.3Hz, 1H), 7.08 (d, J = 8.3Hz, 2H), 6.98 (d, J = 16.3 Hz, 1H), 6.92 (d, J = 8.5Hz, 2H), 6.65 (d, J = 8.3Hz, 2H), 5.53 (s, 2H), 4.74 (t, J = 5.1Hz, 2H), 4.04 (d, J = 5.1Hz, 2H), 3.67 (t, J = 6.7Hz, 4H), 3.60 (t, J = 6.7Hz, 4H), 3.48 (s, 6H), 2.60 (t, J = 7.5Hz, 2H), 2.46 (t, J = 7.5Hz, 2H), 2.02-1.94 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): δ = 172.9, 159.1, 145.6, 143.5, 133.0, 132.9, 129.8, 129.3, 128.5, 126.8, 126.0, 125.6, 124.1, 115.0, 112.7, 102.1, 67.6, 63.2, 54.3, 53.9, 40.2, 34.0, 33.5, 26.7. ES-HRMS (m/z): calcd for $C_{33}H_{39}Cl_2N_2O_7$， 645.2134 $[M+H]^+$; found, 645.2131.

UV-vis spectra for Prodrug 1-7

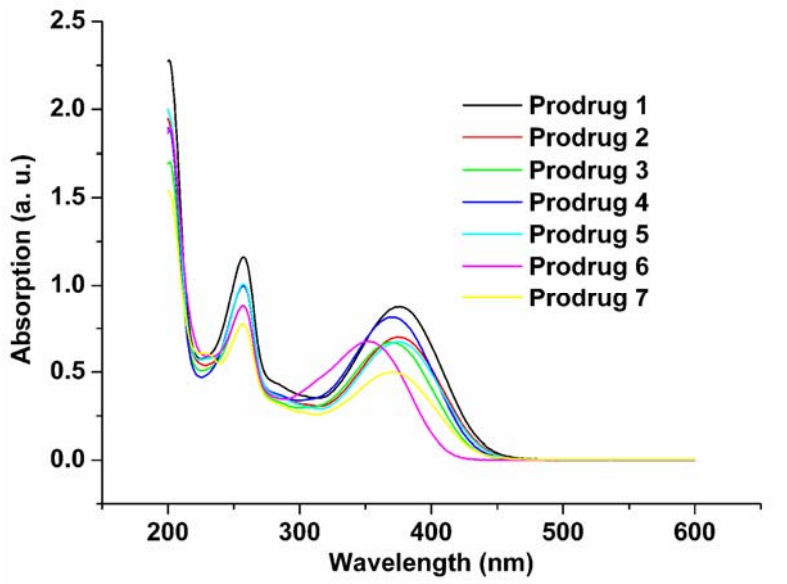
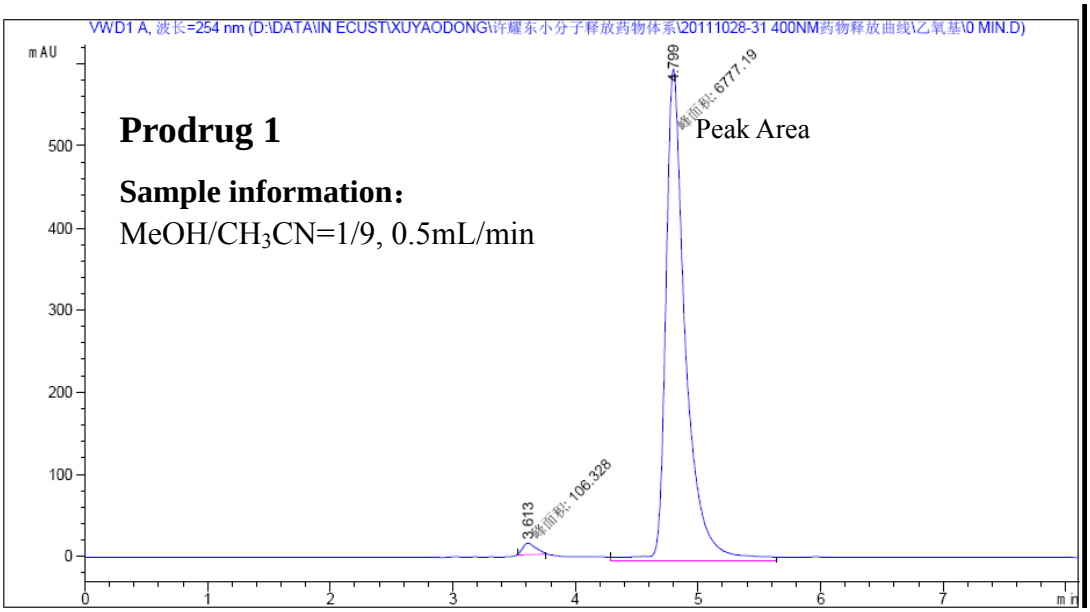


Figure S2 UV-vis spectra of **Prodrug 1-7** in acetonitrile solution.

Scanned HPLC spectra for Prodrug 1-7



信号 1: VWD1 A, 波长=254 nm

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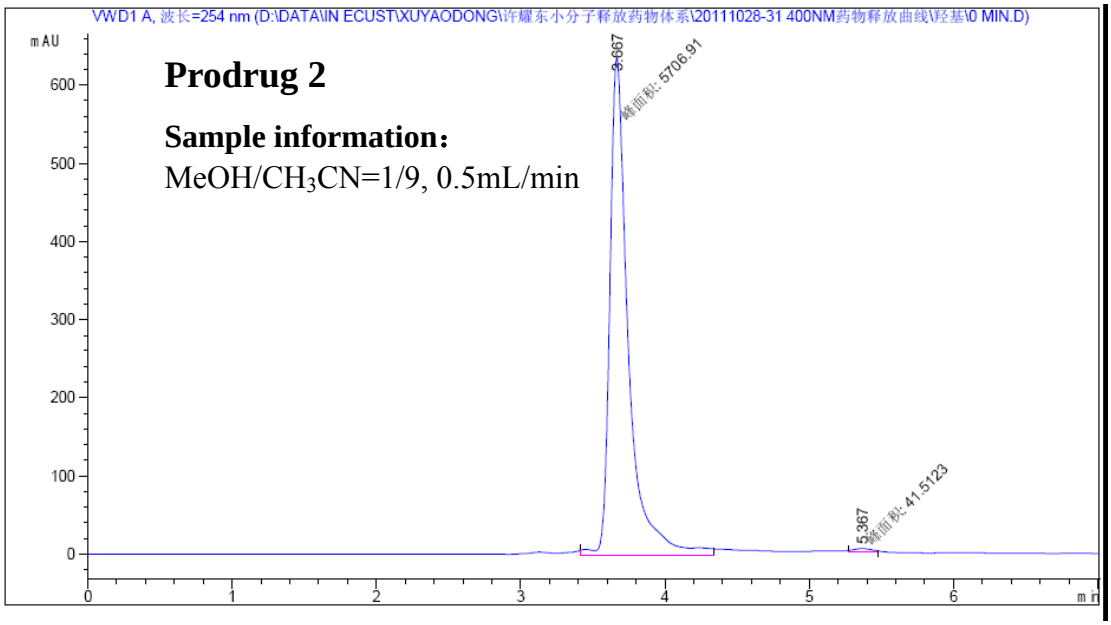

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	3.667	MM	0.1494	5706.91260	636.60352	99.2778
2	5.367	MM	0.1521	41.51233	4.54777	0.7222
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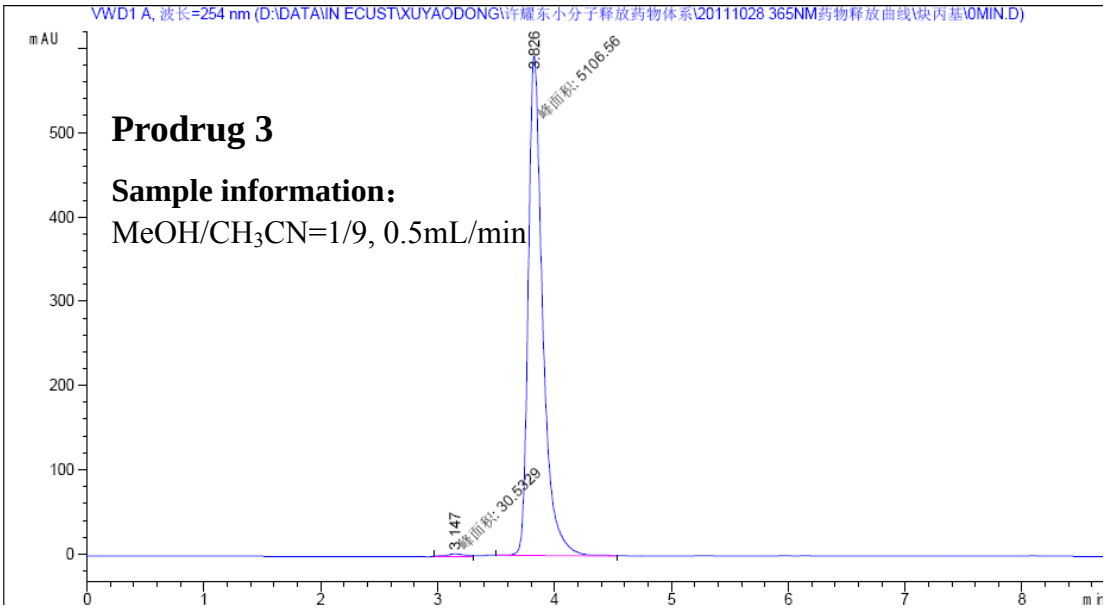
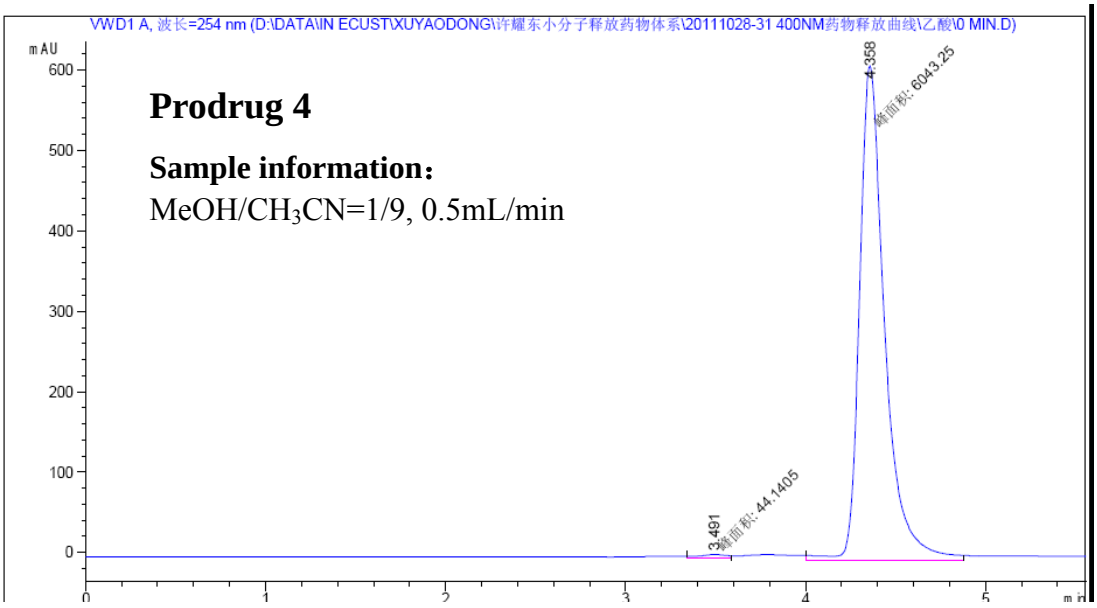


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	3.147	MM	0.1703	30.53295	2.98849	0.5944
2	3.826	MM	0.1435	5106.56396	593.15588	99.4056
总量 :				5137.09691	596.14437	



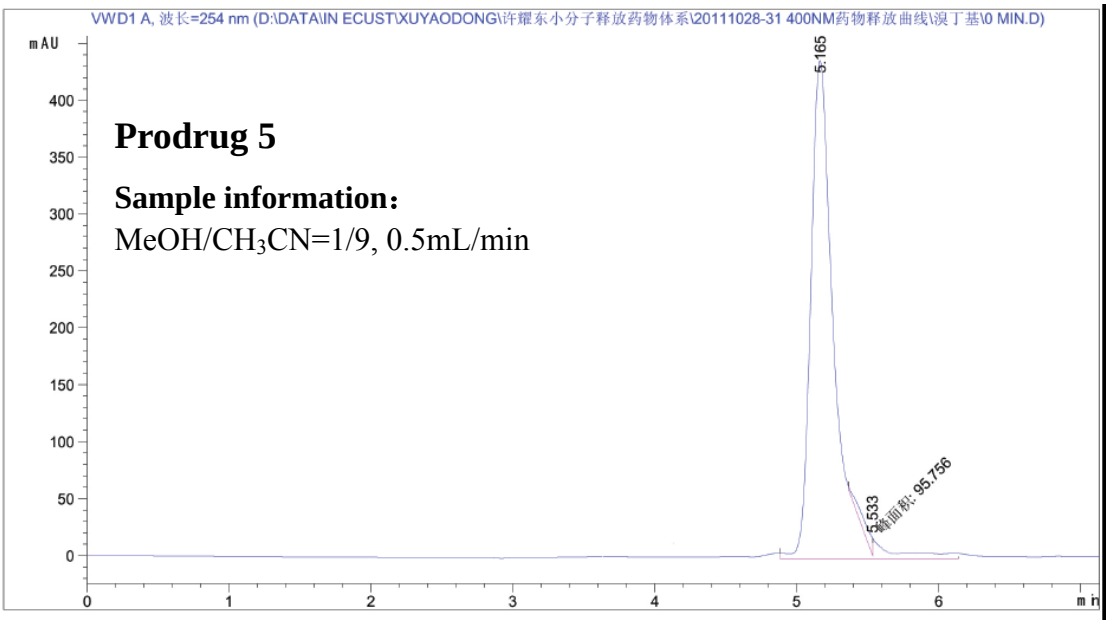
Prodrug 4

Sample information:

MeOH/CH_3CN=1/9, 0.5mL/min

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	3.491	MM	0.1796	44.14048	4.09524	0.7251
2	4.358	MM	0.1636	6043.25342	615.70886	99.2749
总量 :				6087.39390	619.80410	



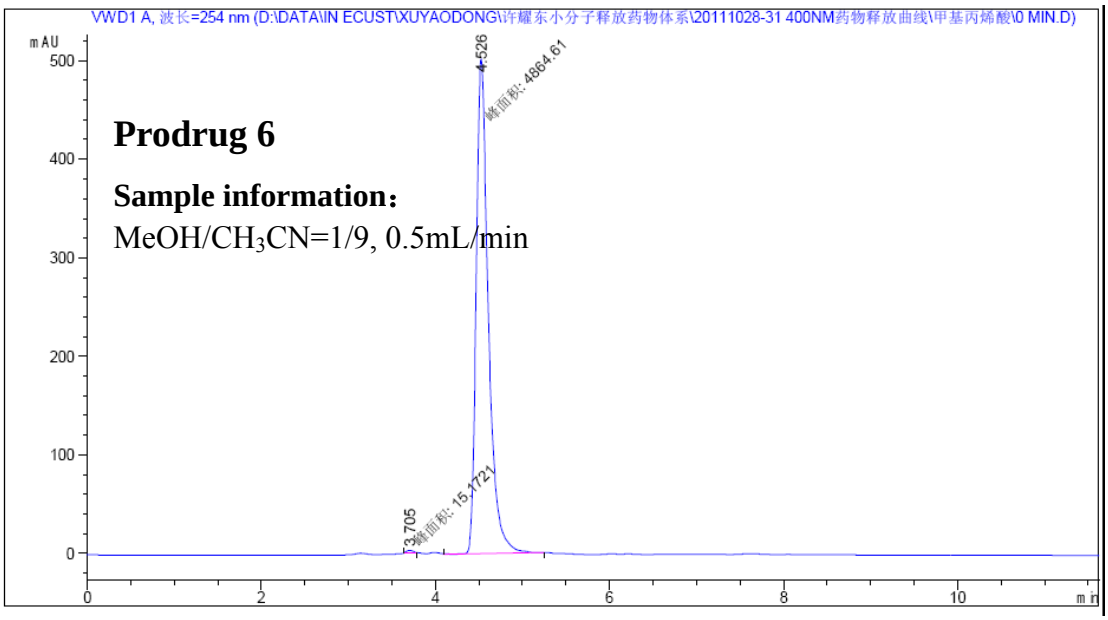
Prodrug 5

Sample information:

MeOH/CH_3CN=1/9, 0.5mL/min

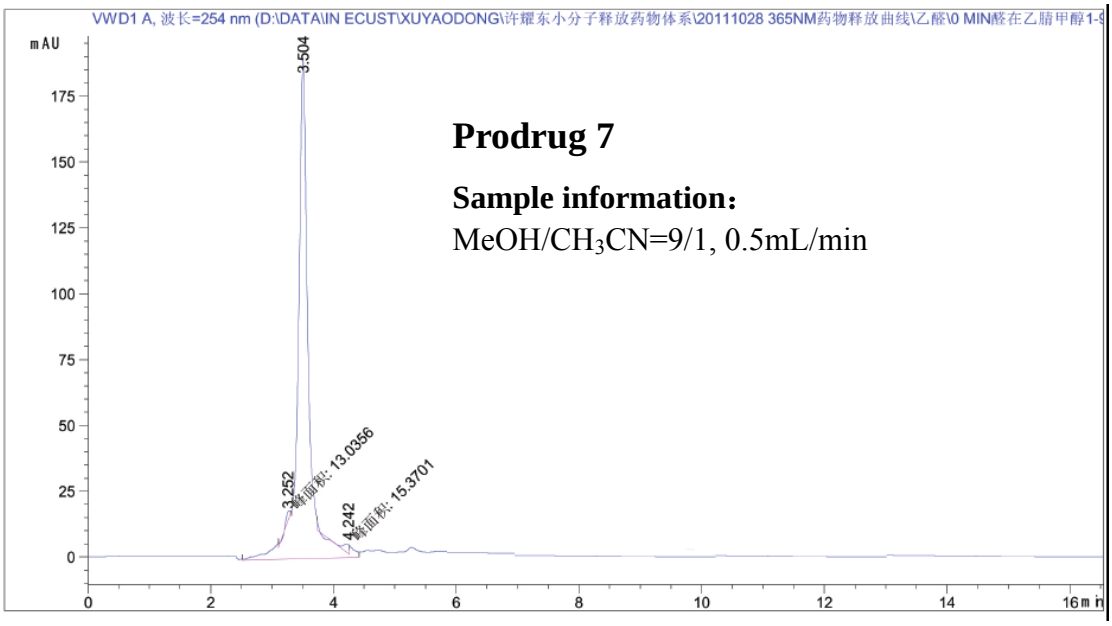
信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	5.165	MM R	0.2058	5409.70508	438.18723	98.2607
2	5.533	MM T	0.1068	95.75599	14.93771	1.7393
总量 :				5505.46107	453.12493	



信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	3.705	MM	0.0912	15.17206	2.77161	0.3109
2	4.526	MM	0.1615	4864.61035	501.91617	99.6891
总量 :				4879.78241	504.68778	



信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	3.252	MM T	0.0964	13.03555	3.35552	0.5469
2	3.504	MM R	0.2074	2354.99634	189.21007	98.8082
3	4.242	MM T	0.0755	15.37009	3.39299	0.6449