Electronic Supporting Information

An estrogen receptor β-targeted near-infrared probe for theranostic imaging of prostate cancer

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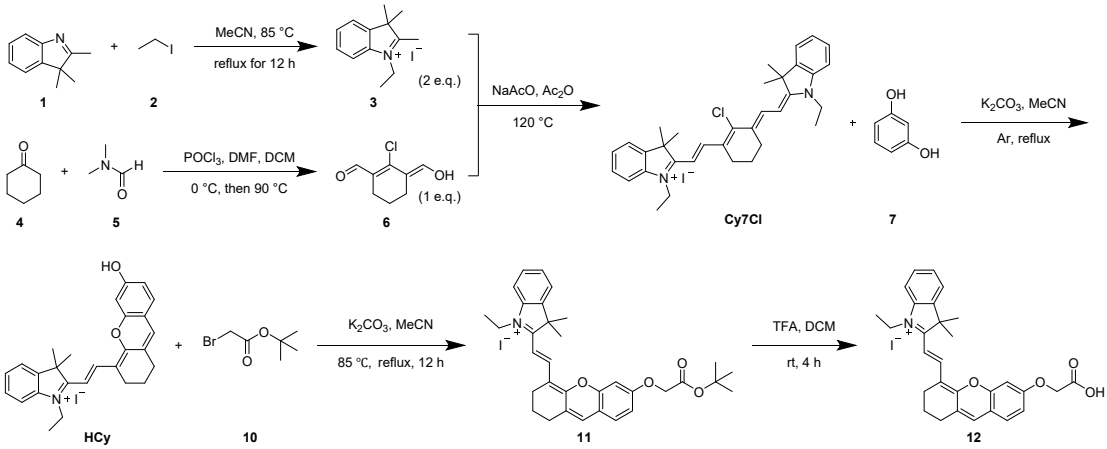
1. Synthetic procedures of D1-D4.

Synthesis of HCy derivatives.



*Synthesis of **3***. 2,3,3-trimethylindolenine (9.55 g, 60 mmol) was dissolved in acetonitrile, then, iodoethane (9.36 g, 60 mmol) was added slowly at room temperature. The mixture was heated at 85 °C for 12 h. After filtration and washes with the minimum amount of cold petroleum ether, a pink solid was generated. The product **3** (15.31 g, yield: 81%) was used directly in the next reaction without further purification.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.82 – 7.76 (m, 1H), 7.63 (dd, *J* = 5.5, 3.6 Hz, 1H), 7.62 – 7.58 (m, 1H), 4.73 (q, *J* = 7.5 Hz, 2H), 3.15 (s, 3H), 1.66 (s, 6H), 1.64 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.70, 142.44, 140.52, 130.77, 129.56, 123.49, 116.69, 55.10, 44.73, 23.11, 17.02, 13.08.

*Synthesis of **6***. A solution of DMF (15 mL) and DCM (15 mL) in a round-bottom single-neck flask was cooled over ice bath in argon atmosphere. Then, phosphorus oxychloride (19 mL, 0.2 mol) was added dropwise with stirring for 30 min, followed by cyclohexanone (5.01 g, 0.051 mol). The solution was refluxed at 90 °C for 6 h. After the solution was cooled to room temperature, it was stirred over ice bath and quenched with drops of ice water. The mixture was extracted with water and dichloromethane (100 mL × 3). Eventually, the organic phase was evaporated under reduced pressure, and the crude product was purified by flash column chromatography (DCM/MeOH = 50:1) on silica gel, affording the desired compound **6** as a yellow solid (4.22 g, yield:

48%).

Synthesis of ***Cy7Cl****.* In argon atmosphere, 1-ethyl-2,3,3-trimethyl-3*H*-indol-1-ium iodide (**3**; 3.65 g, 11.6 mmol) and sodium acetate (0.95 g, 36 mmol) were added to a round-bottom double-neck flask containing the synthesized intermediate compound **6**; 1.00 g, 5.79 mmol) in 15 mL of acetic anhydride. The solution was stirred at room temperature for 4 h. The mixture was extracted with water and dichloromethane (60 mL × 3), and the organic phase was evaporated under reduced pressure. Eventually, the crude product was purified by flash column chromatography (DCM/MeOH = 15:1) on silica gel, affording compound **Cy7Cl** as a dark-green solid with metallic luster (5.32 g, yield: 72%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 14.0 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.27 (t, *J* = 7.9 Hz, 0H), 7.23 (d, *J* = 7.8 Hz, 1H), 6.20 (d, *J* = 14.1 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 2.75 (t, *J* = 6.2 Hz, 2H), 1.99 (p, *J* = 6.3 Hz, 1H), 1.73 (s, 5H), 1.47 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 171.92, 150.64, 144.50, 141.69, 141.11, 128.88, 127.24, 125.37, 122.33, 110.81, 100.87, 49.36, 40.09, 28.05, 26.71, 20.67, 12.48.

Synthesis of ***HCy****.* In argon atmosphere, K_2CO_3 (1.10 g, 8 mmol) was added to a stirred solution of resorcinol (0.88 g, 8 mmol) in acetonitrile (15 mL), and stirred for 20 min at room temperature. Then, a solution of **Cy7Cl** (2.56 g, 4 mmol) in acetonitrile (10 mL) was added to the above mixture, and heated at 50 °C for 4 h. The mixture was extracted with water and dichloromethane (30 mL × 3), and the organic phase was evaporated under reduced pressure. Eventually, the crude product was purified by flash column chromatography (DCM/CH_3OH = 10:1) on silica gel, affording compound **HCy** as a blue-green solid with metallic luster (1.62 g, yield: 77%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 14.0 Hz, 2H), 7.44 – 7.39 (m, 4H), 7.27 (t, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 6.20 (d, *J* = 14.1 Hz, 2H), 4.26 (q, *J* = 7.2 Hz, 4H), 2.75 (t, *J* = 6.2 Hz, 4H), 1.99 (p, *J* = 6.3 Hz, 2H), 1.73 (s, 12H), 1.47 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) *δ* 179.28, 167.24, 161.37, 159.21, 144.50, 140.61, 129.84, 128.42, 126.08, 123.97, 121.12, 117.74, 116.16, 115.91, 107.98, 104.44, 47.97,

29.13, 28.20, 24.59, 22.03, 12.44.

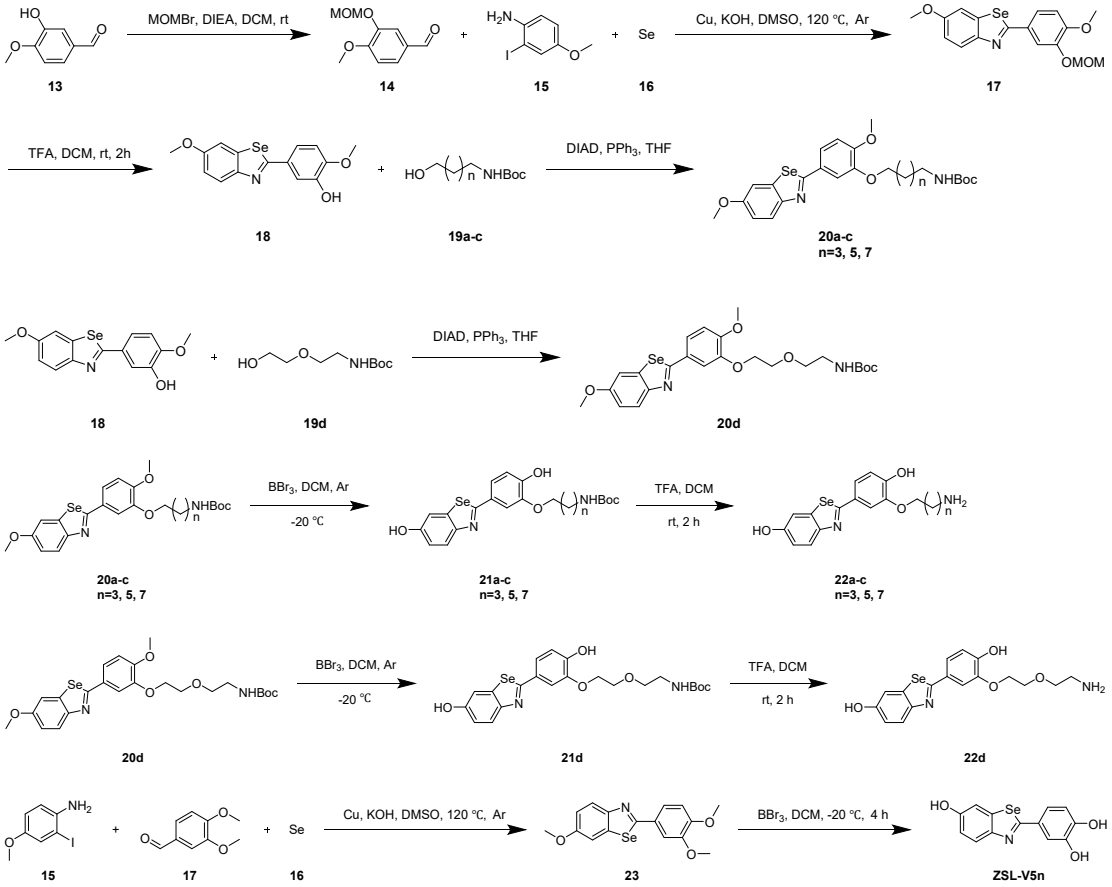
*Synthesis of **11***. KI (0.03 g, 0.19 mmol) was added to a solution of tert-butyl 2-bromoacetate (0.56 g, 2.9 mmol) in acetonitrile (15 mL), and stirred at room temperature for 30 min. Then, **HCy** (1.00 g, 1.9 mmol) and K_2CO_3 (0.39 g, 2.9 mmol) were added, and heated to reflux at 85 ℃ for 12 h. The solution was cooled to room temperature and extracted with water and dichloromethane (30 mL × 3). The organic phase was evaporated under reduced pressure. Eventually, the crude product was purified by flash column chromatography (DCM/MeOH = 10:1) on silica gel, affording compound **11** as a blue-green solid with metallic luster (1.03 g, yield: 83%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.68 (d, J = 14.9 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.50 (d, J = 7.9 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.41 (d, J = 8.5 Hz, 1H), 7.31 (s, 2H), 7.21 (s, 1H), 6.92 (d, J = 2.3 Hz, 1H), 6.88 (dd, J = 8.6, 2.4 Hz, 1H), 6.77 (d, J = 14.9 Hz, 1H), 4.70 (s, 2H), 2.88 (t, J = 6.1 Hz, 2H), 2.78 (d, J = 5.8 Hz, 2H), 2.32 – 2.22 (m, 1H), 1.99 (t, J = 6.1 Hz, 2H), 1.83 (s, 9H), 1.56 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 176.88, 167.13, 161.37, 160.93, 154.13, 145.95, 141.83, 141.05, 133.26, 129.37, 129.00, 127.97, 127.42, 122.49, 116.51, 115.26, 112.80, 112.56, 104.39, 102.24, 65.98, 50.64, 41.76, 29.25, 28.17, 28.08, 24.69, 20.28, 13.07.

*Synthesis of **12***. **11** (0.20 g, 0.3 mmol) was dissolved in dichloromethane (1 mL), and trifluoroacetic acid (1 mL) was added slowly over ice bath bath. Then, the solution was stirred at room temperature for 4 h. Eventually, the solution was evaporated under reduced pressure to get compounds **12** as a blue-green solid. The product was used directly in the next reaction without further purification.

Synthesis of ZLS-V5n derivatives.



*Synthesis of **14***. 3-Hydroxy-4-methoxybenzaldehyde (4.56 g, 30 mmol) was dissolved in dichloromethane (30 mL), then, a solution of bromomethyl methyl ether (4.87 g, 39 mmol) in dichloromethane (10 mL) was added slowly over ice bath bath, followed by *N*,*N*-diisopropylethylamine (7.39 mL, 45 mmol). The solution was stirred at room temperature for 12 h. Eventually, the solution was evaporated under reduced pressure, and the crude product was purified by flash column chromatography (PE/EA = 1:1) on silica gel, affording compound **14** as a white solid (5.41 g, yield: 92%).

*Synthesis of **17***. 2-Iodo-4-methoxyaniline (1.00 g, 4 mmol), **14** (0.95 g, 4.8 mmol), selenium powder (0.95 g, 12 mmol), copper powder (25 mg, 0.4 mmol), potassium hydroxide (0.45 g, 8 mmol) were dissolved in dimethylsulfoxide (20 mL) and heated at 120 °C for 12 h in argon atmosphere. Then, it was cooled to room temperature, filtered through diatomaceous earth and washed with a small amount of ethyl acetate. The filtrate was extracted with water and ethyl acetate (30 mL × 3), and

the organic phase was evaporated under reduced pressure. Eventually, the crude product was purified by flash column chromatography (DCM/PE = 10:1) on silica gel, affording compound **17** as an orange solid (497 mg, yield: 33%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.9 Hz, 1H), 7.84 (d, J = 2.1 Hz, 1H), 7.56 (dd, J = 8.4, 2.2 Hz, 1H), 7.40 (d, J = 2.6 Hz, 1H), 7.09 – 7.03 (m, 1H), 6.97 (d, J = 8.5 Hz, 1H), 5.32 (s, 2H), 3.97 (s, 3H), 3.90 (s, 3H), 3.59 (s, 3H).

*Synthesis of **18***. **17** (0.50 g, 1.3 mmol) was dissolved in dichloromethane (2 mL), and trifluoroacetic acid (2 mL) was added slowly over ice bath. Then, the solution was stirred at room temperature for 2 h. Eventually, the solution was evaporated under reduced pressure, the crude product was purified by flash column chromatography (PE/EA = 3:1) on silica gel, affording compound **18** as an orange solid (0.43 g, yield: 97%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.83 (s, 1H), 7.50 – 7.35 (m, 3H), 7.06 – 6.87 (m, 2H), 3.98 – 3.85 (m, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 191.30, 169.47, 157.54, 152.10, 146.97, 139.49, 130.78, 129.94, 124.79, 120.29, 114.27, 109.94, 108.10, 56.34, 55.94.

*Synthesis of **20a-d***. Diisopropyl azodicarboxylate (0.24 g, 1.2 mmol), triphenylphosphine (0.31 g, 1.2 mmol) were dissolved into a 5 mL sample vial with tetrahydrofuran (2 mL). The solution was ultrasonicated for 5 min at room temperature to produce a milky solid. Then, **18** (0.10 g, 0.3 mmol) and Linkers **19a-d** (0.6 mmol) were added into the sample vial, and the solution was ultrasonicated at room temperature for 30 min. Eventually, the solution was evaporated under reduced pressure, the crude product was purified by flash column chromatography (PE/EA = 3:1) on silica gel, affording compounds **20a-d** as a yellow liquid (yield: 25%-100%).

*Synthesis of **21a-d***. In argon atmosphere, **20a-d** (0.15 g, 1.0 eq) was dissolved in dichloromethane (5 mL) at -20 °C. The BBr_3 (4.0 eq) was added slowly into the solution. The solution was stirred at -20 °C for 4 h, then, the reaction was quenched by dropwise addition of anhydrous methanol at -20 °C. The solution was extracted with water and ethyl acetate (15 mL × 3), and the organic phase was evaporated under reduced pressure to get compound **21a-d** as yellow solid, The product **21a-d** were

used directly in the next reaction without further purification.

*Synthesis of **22a-d***. **21a-d** (mentioned above) were dissolved in dichloromethane (1 mL), and trifluoroacetic acid (1 mL) was added slowly over ice bath bath. Then, the solution was stirred at room temperature for 2 h. Eventually, the solution was evaporated under reduced pressure to get compounds **22a-d** as yellow solid. The product **22a-d** were used directly in the next reaction without further purification.

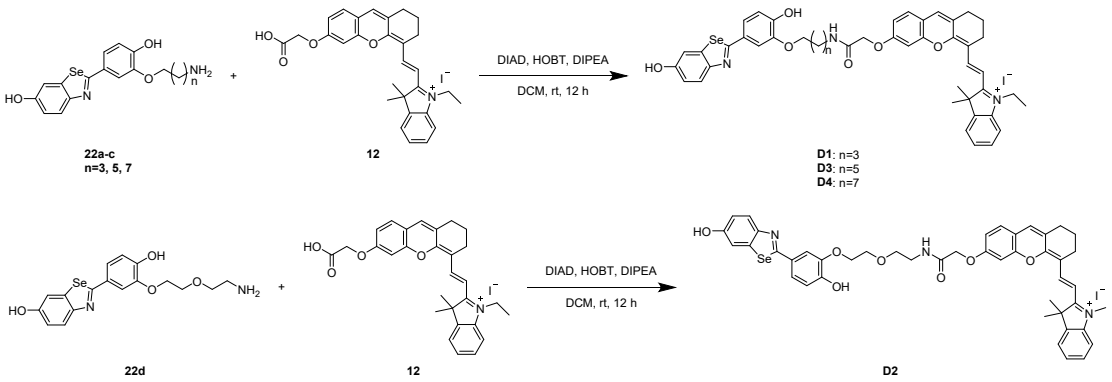
*Synthesis of **ZSL-V5n***. The synthesis method of **ZSL-V5n** was similar to **18** mentioned above.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.79 (s, 1H), 9.64 (s, 1H), 9.43 (s, 1H), 7.77 (d, J = 8.7 Hz, 1H), 7.42 (d, J = 11.5 Hz, 2H), 7.24 (d, J = 10.6 Hz, 1H), 6.92 (d, J = 8.8 Hz, 1H), 6.85 (d, J = 8.2 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-d) δ 170.65, 155.44, 150.34, 147.95, 145.37, 139.16, 128.66, 123.57, 121.02, 115.54, 113.17, 109.83.

HR-MS (ESI) calcd. for $C_{13}H_{10}NO_3Se$ $[M + H]^+$, 307.9826, found 307.9825.

Synthesis of NIR probes.



*Synthesis of **D1-D4***. **12** (150 mg, 0.26 mmol, 1.05 eq), 1-Hydroxybenzotriazole (HOBT, 50.88 mg, 0.38 mmol, 1.5 eq), Diisopropyl azodicarboxylate (DIAD, 76.09 mg, 0.38 mmol, 1.5 eq) were dissolved in the dichloromethane (2 mL), and stirred at room temperature for 30 min. Subsequently, the solution was added with *N*,*N*-diisopropylethylamine (DIPEA, 0.25 mL, 1.5 mmol, 6.0 eq) and stirred at room temperature for 12 h. The solution was extracted with water and dichloromethane (15 mL × 3). The organic phase was evaporated under reduced pressure. Eventually, the

crude product was purified by flash column chromatography (DCM/MeOH = 15:1) on silica gel, affording compound **D1**-**D4** as a blue solid with metallic luster (yield: 4.06% – 10.42%).

D1 (*E*)-1-Ethyl-2-(2-(6-(2-((4-(2-hydroxy-5-(6-hydroxybenzo[*d*][1,3]selenazol-2-yl)phenoxy)butyl)amino)-2-oxoethoxy)-2,3-dihydro-1*H*-xanthen-4-yl)vinyl)-3,3-dimethyl-3*H*-indol-1-ium iodide, yield: 4.06%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.70 (d, J = 14.8 Hz, 1H), 8.62 (s, 1H), 7.54 (d, J = 7.4 Hz, 1H), 7.46 (t, J = 7.7 Hz, 2H), 7.38 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 7.3 Hz, 2H), 7.14 (s, 1H), 7.01 (s, 2H), 6.88 (d, J = 8.7 Hz, 2H), 6.66 (s, 1H), 6.34 (d, J = 14.9 Hz, 1H), 5.35 (s, 1H), 5.02 – 4.91 (m, 1H), 4.74 (s, 2H), 4.31 (q, J = 7.3 Hz, 2H), 2.70 (s, 2H), 2.66 (s, 2H), 1.81 (s, 6H), 1.69 (s, 6H), 1.51 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 180.85, 177.85, 161.61, 155.96, 147.02, 143.01, 141.02, 133.81, 130.79, 129.24, 128.92, 128.59, 128.32, 127.57, 123.29, 119.97, 116.97, 112.01, 102.19, 88.52, 70.33, 51.21, 39.96, 29.52, 28.11, 21.73, 19.74, 14.94, 12.84.

HR-MS (ESI) calcd. for $C_{46}H_{47}N_3O_6Se$ $[M + H]^+$, 944.1675; found 944.1679.

D2 (*E*)-1-ethyl-2-(2-(6-(2-((2-(2-(2-hydroxy-5-(6-hydroxybenzo[*d*][1,3]selenazol-2-yl)phenoxy)ethoxy)ethyl)amino)-2-oxoethoxy)-2,3-dihydro-1*H*-xanthen-4-yl)vinyl)-3,3-dimethyl-3*H*-indol-1-ium iodide, yield 7.73%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.55 (d, J = 13.9 Hz, 1H), 7.57 (d, J = 8.9 Hz, 1H), 7.41 (dd, J = 20.0, 7.6 Hz, 2H), 7.32 – 7.22 (m, 3H), 7.14 – 7.02 (m, 4H), 6.84 (d, J = 7.8 Hz, 1H), 5.95 (d, J = 14.0 Hz, 1H), 5.37 (s, 1H), 4.73 (s, 2H), 4.10 (s, 2H), 3.76 (s, 2H), 2.68 (s, 2H), 2.51 (s, 2H), 1.77 (d, J = 10.9 Hz, 6H), 1.57 (s, 3H), 1.52 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.26, 165.06, 163.95, 163.04, 154.06, 144.59, 141.91, 139.42, 128.83, 128.34, 127.43, 126.99, 125.25, 122.71, 122.60, 122.19, 121.55, 115.79, 115.37, 110.21, 109.66, 101.57, 98.28, 86.77, 64.42, 49.49, 47.46, 40.03, 29.76, 28.71, 27.03, 24.17, 20.75, 12.83, 10.84.

HR-MS (ESI) calcd. for $C_{46}H_{47}N_3O_7Se$ $[M + H]^+$, 960.1624, found 960.1631.

D3 (*E*)-1-ethyl-2-(2-(6-(2-((6-(2-hydroxy-5-(6-hydroxybenzo[*d*][1,3]selenazol-2-yl)phenoxy)hexyl)amino)-2-oxoethoxy)-2,3-dihydro-1*H*-xanthen-4-yl)vinyl)-3,3-dimethyl-3*H*-indol-1-ium iodide, yield 10.42%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.57 (s, 1H), 7.90 (d, J = 8.9 Hz, 1H), 7.61 (d, J = 9.0 Hz, 2H), 7.47 (s, 1H), 7.44 – 7.35 (m, 2H), 7.32 – 7.23 (m, 3H), 7.10 (t, J = 7.2 Hz, 2H), 7.05 (d, J = 5.5 Hz, 3H), 6.87 (dd, J = 22.4, 8.1 Hz, 2H), 5.41 (s, 1H), 4.66 (s, 2H), 3.88 (d, J = 14.9 Hz, 4H), 3.70 (s, 2H), 2.72 (d, J = 15.6 Hz, 2H), 2.61 (s, 2H), 2.52 (s, 2H), 1.86 (tt, J = 12.9, 6.4 Hz, 2H), 1.78 (d, J = 5.2 Hz, 6H), 1.56 (s, 3H), 1.51 (s, 3H), 1.47 (d, J = 7.3 Hz, 3H), 1.36 (d, J = 6.7 Hz, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.27, 165.67, 163.93, 163.45, 162.44, 157.46, 153.98, 149.26, 144.48, 138.56, 128.81, 128.33, 127.55, 125.31, 124.68, 122.59, 122.28, 116.09, 115.82, 115.26, 114.89, 110.12, 109.25, 101.53, 98.00, 86.73, 69.07, 63.86, 55.90, 49.56, 48.00, 40.04, 29.67, 28.55, 27.04, 24.17, 20.73, 12.16, 11.41.

HR-MS (ESI) calcd. for $C_{48}H_{51}N_3O_6Se$ $[M + H]^+$, 972.1988, found 972.1996.

D4 (*E*)-1-ethyl-2-(2-(6-(2-((8-(2-hydroxy-5-(6-hydroxybenzo[*d*][1,3]selenazol-2-yl)phenoxy)octyl)amino)-2-oxoethoxy)-2,3-dihydro-1*H*-xanthen-4-yl)vinyl)-3,3-dimethyl-3*H*-indol-1-ium iodide, yield 4.81%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.65 (dd, J = 36.5, 14.3 Hz, 2H), 7.64 (d, J = 8.8 Hz, 1H), 7.61 (d, J = 8.9 Hz, 1H), 7.54 (d, J = 7.4 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.42 – 7.36 (m, 2H), 7.15 (s, 2H), 7.08 – 7.00 (m, 2H), 6.95 (d, J = 11.5 Hz, 1H), 6.85 (dd, J = 13.5, 7.8 Hz, 2H),6.10 – 6.01 (m, 1H), 5.37 (d, J = 8.3 Hz, 1H), 4.35 (td, J = 18.2, 17.7, 7.6 Hz, 2H), 4.17 (t, J = 6.3 Hz, 2H), 1.87 (s, 3H), 1.80 (s, 3H), 1.60 – 1.52 (m, 8H), 1.51 (s, 3H), 1.49 – 1.45 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.28, 168.53, 167.82, 167.39, 162.69, 153.95, 153.49, 144.98, 141.04, 132.48, 131.00, 128.29, 127.82, 127.58, 124.03, 122.54, 122.13, 115.99, 115.52, 115.06, 111.58, 108.72, 86.53, 68.21, 64.60, 52.68, 47.50, 38.77, 31.75, 30.41, 29.74, 28.97, 23.79, 23.03, 22.17, 18.14, 17.42, 11.02.

HR-MS (ESI) calcd. for $C_{50}H_{55}N_3O_6Se$ $[M + H]^+$, 1000.2301, found 1000.2308.

2. Optical properties of D1, D2 and D4.

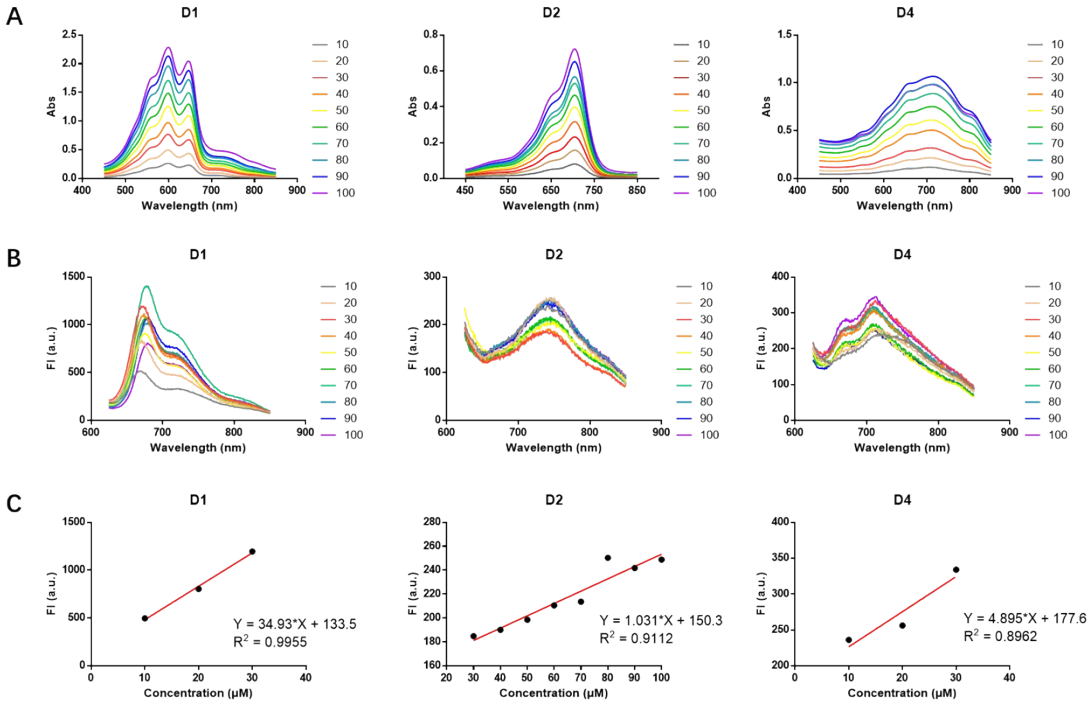


Figure S1. Optical properties of **D1**, **D2** and **D4**. Relationship curve of (A) UV absorption and (B) fluorescence intensity at different concentrations. (C) Linear relationship derived from (B) (R^2: **D1** = 0.9955, **D2** = 0.9112, **D4** = 0.8962). All the experiments were conducted in a pH 7.4 PBS solution containing 10 % DMSO at 37 ℃, with excitation at 600 nm. slit = 10/10 nm.

3. NMR spectra of probes.

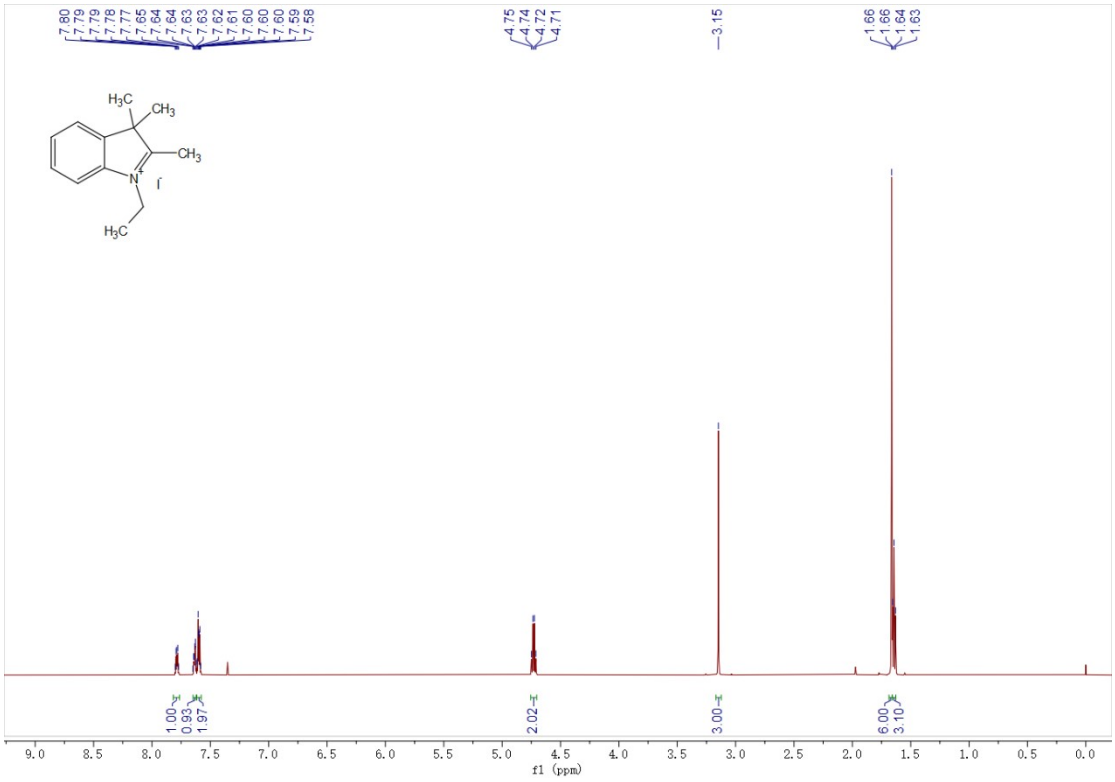


Figure S2. ^{1}H NMR of **3**.

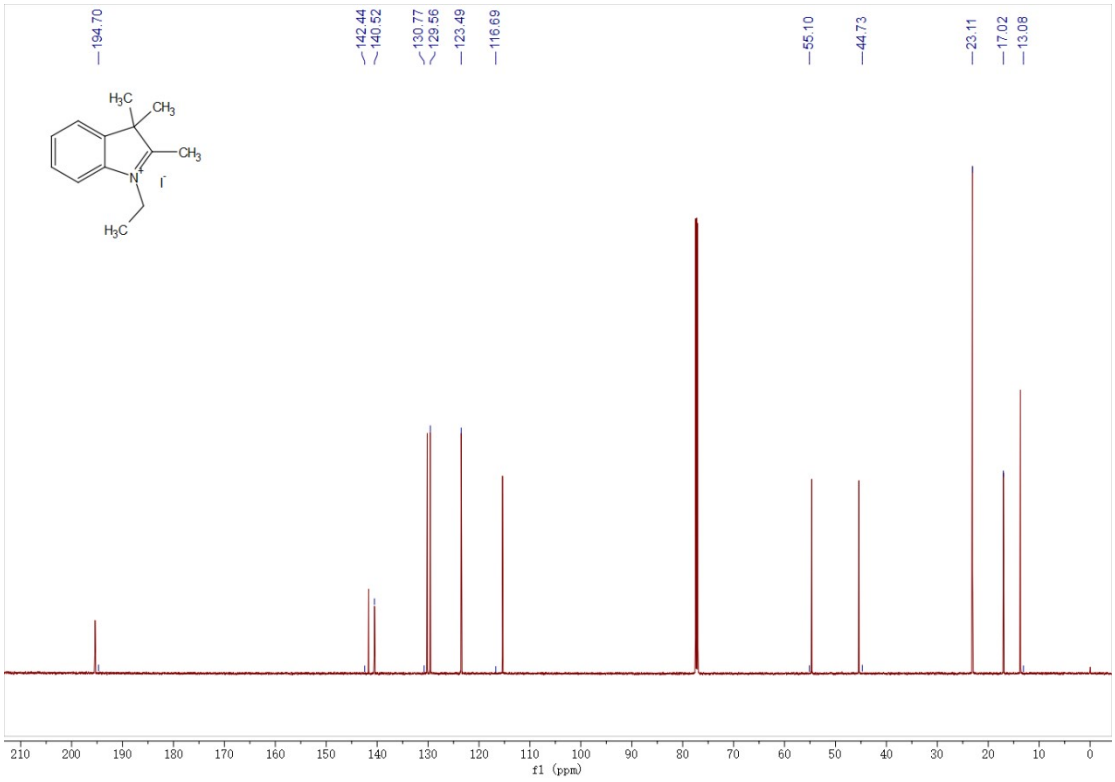


Figure S3. ^{13}C NMR of **3**.

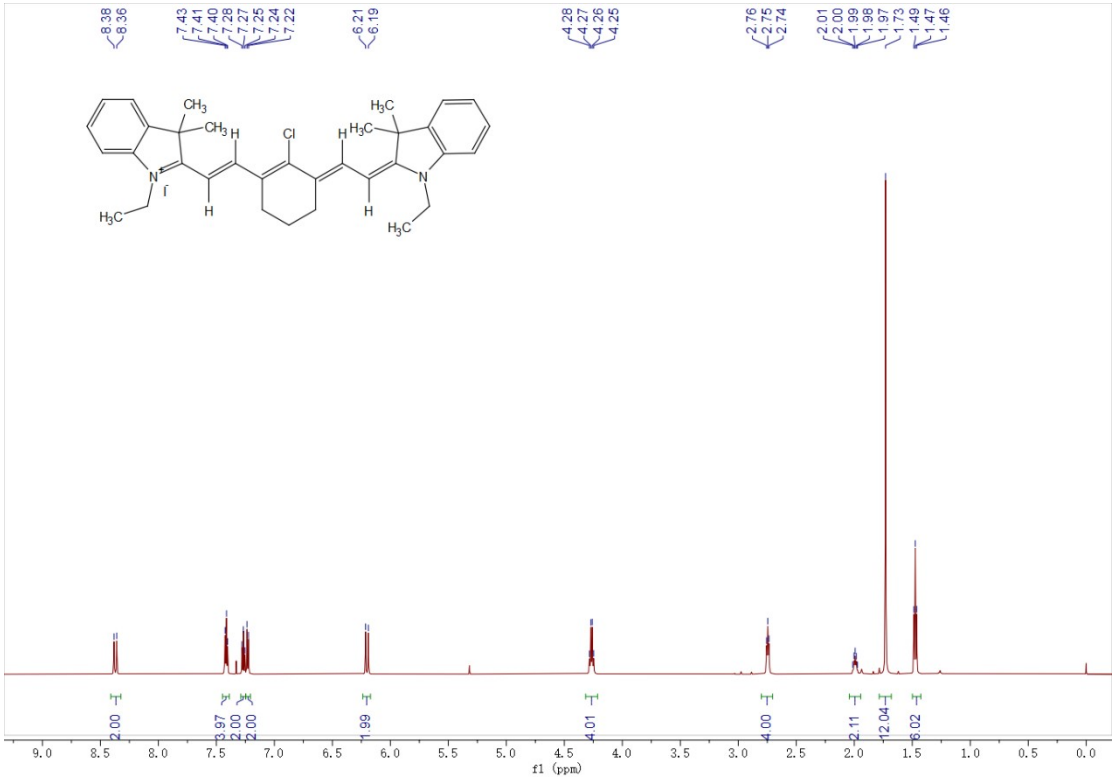


Figure S4. ^{1}H NMR of **Cy7Cl**.

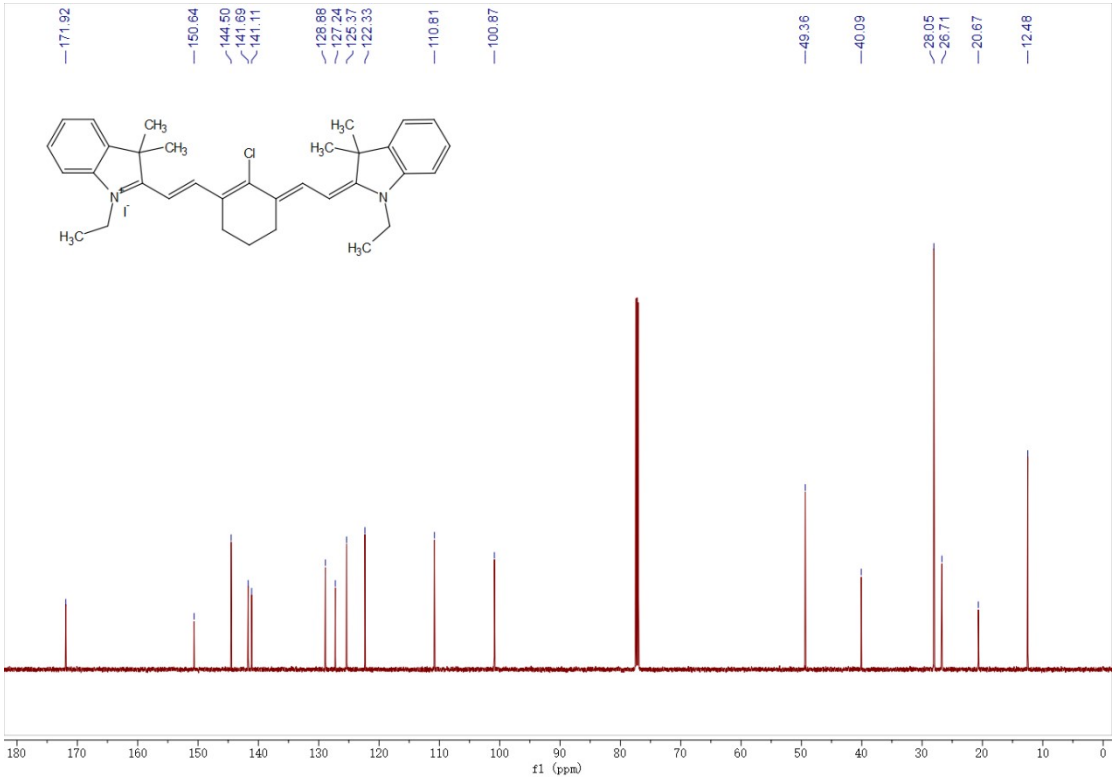


Figure S5. ^{13}C NMR of **Cy7Cl**.

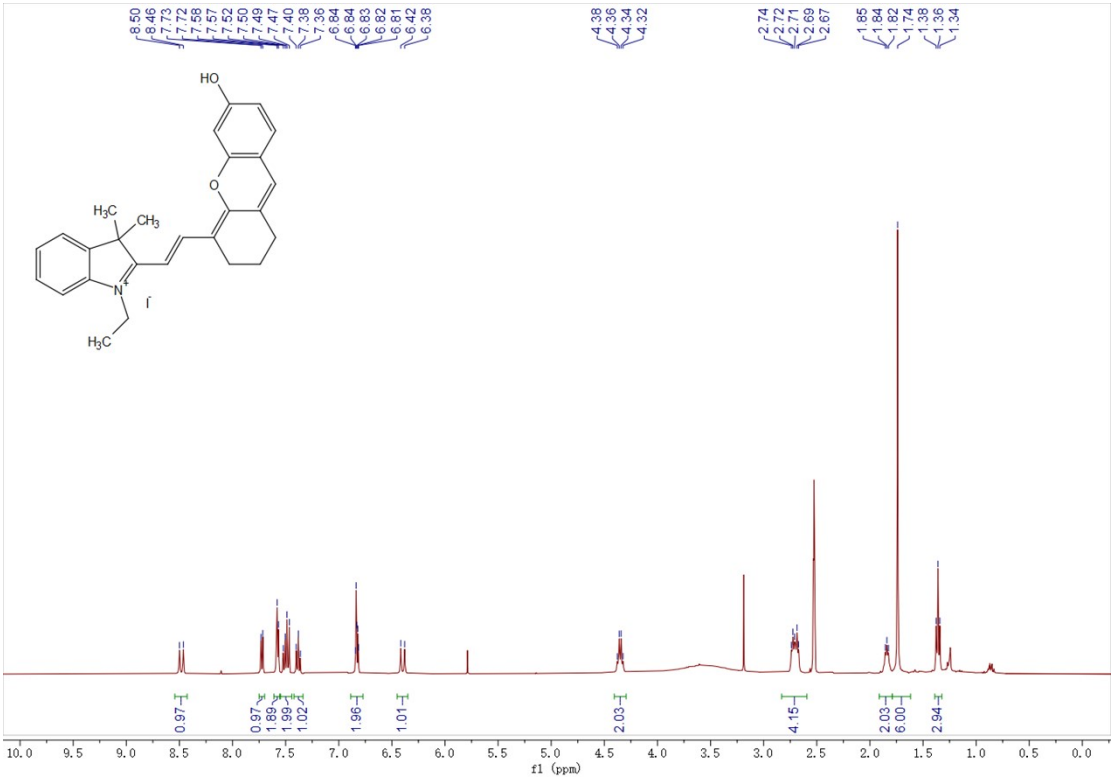


Figure S6. ^{1}H NMR of **HCy**.

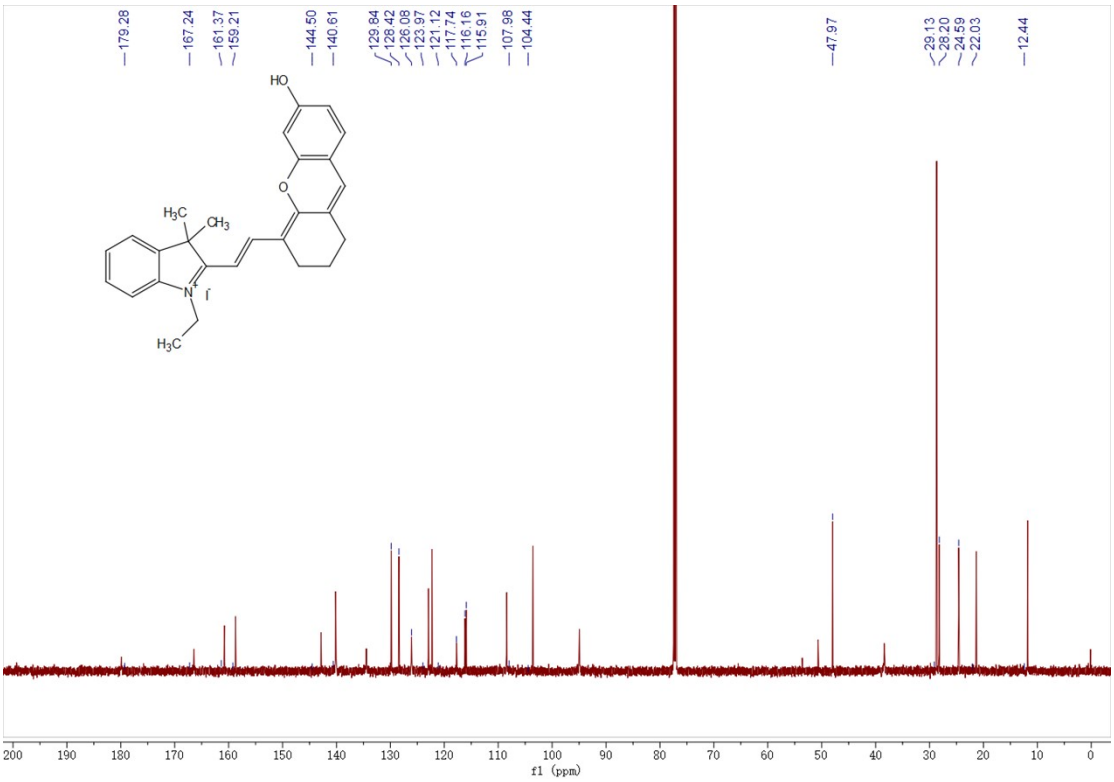


Figure S7. ^{13}C NMR of **HCy**.

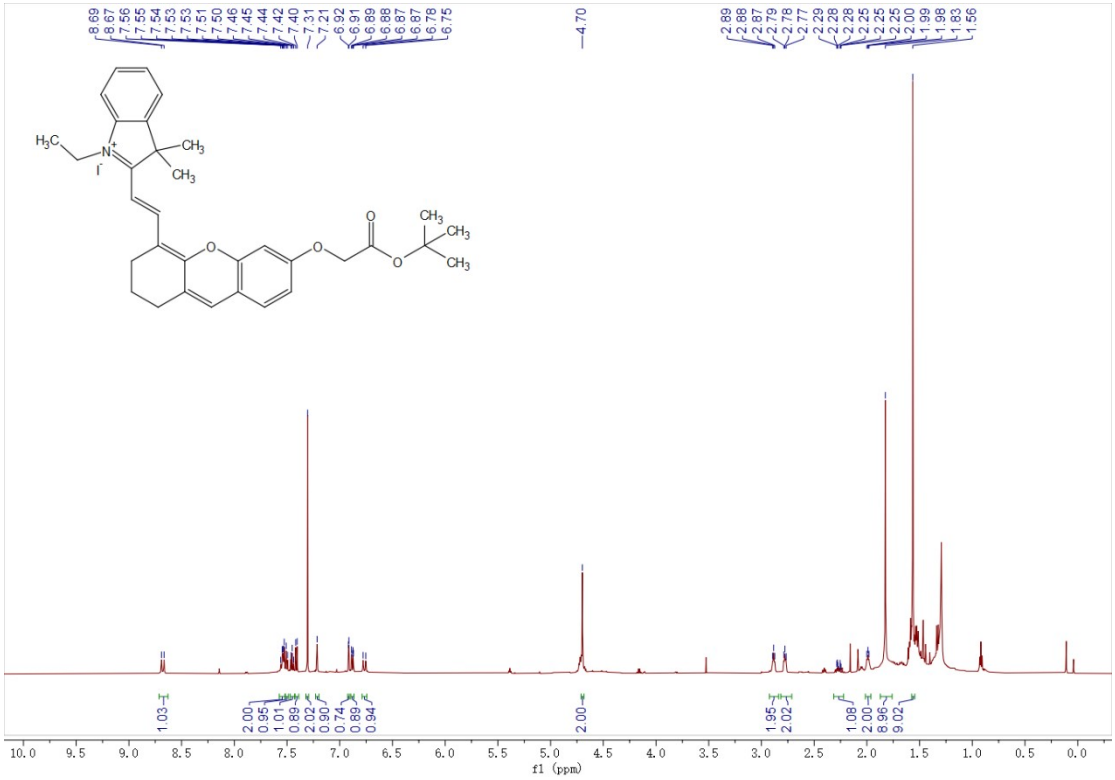


Figure S8. ^{1}H NMR of **11**.

Figure S9. ^{13}C NMR of **11**.

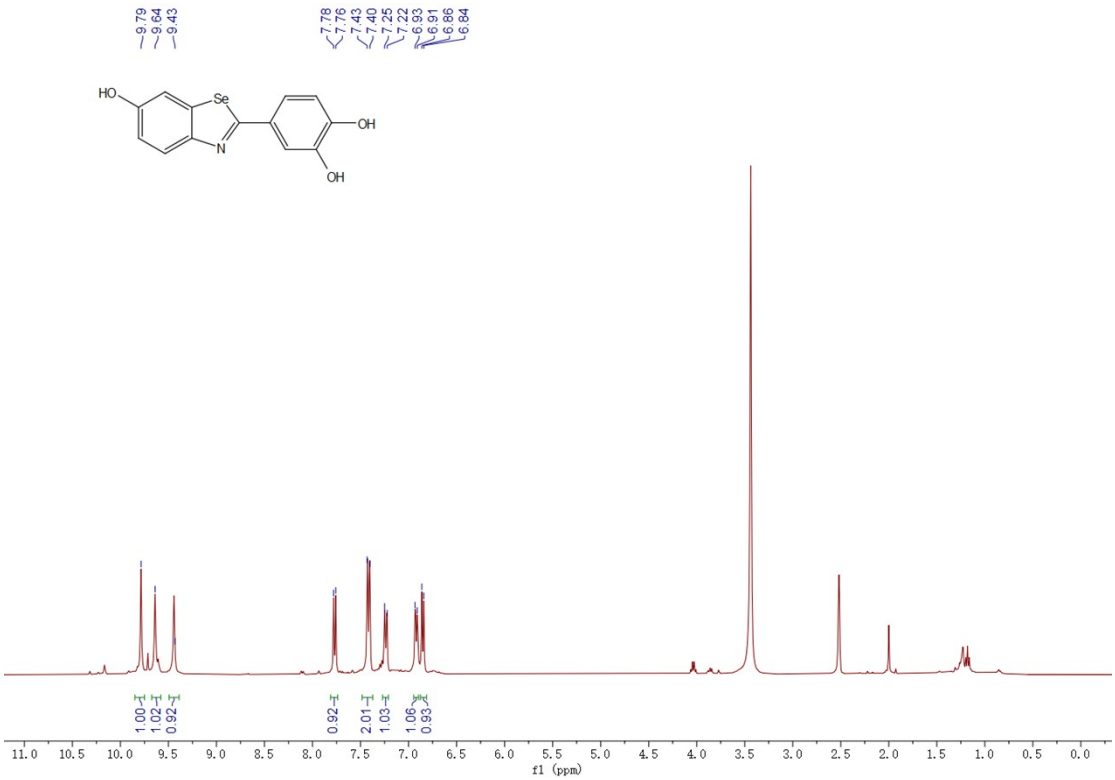


Figure S10. ^{1}H NMR of **ZSL-V5n**.

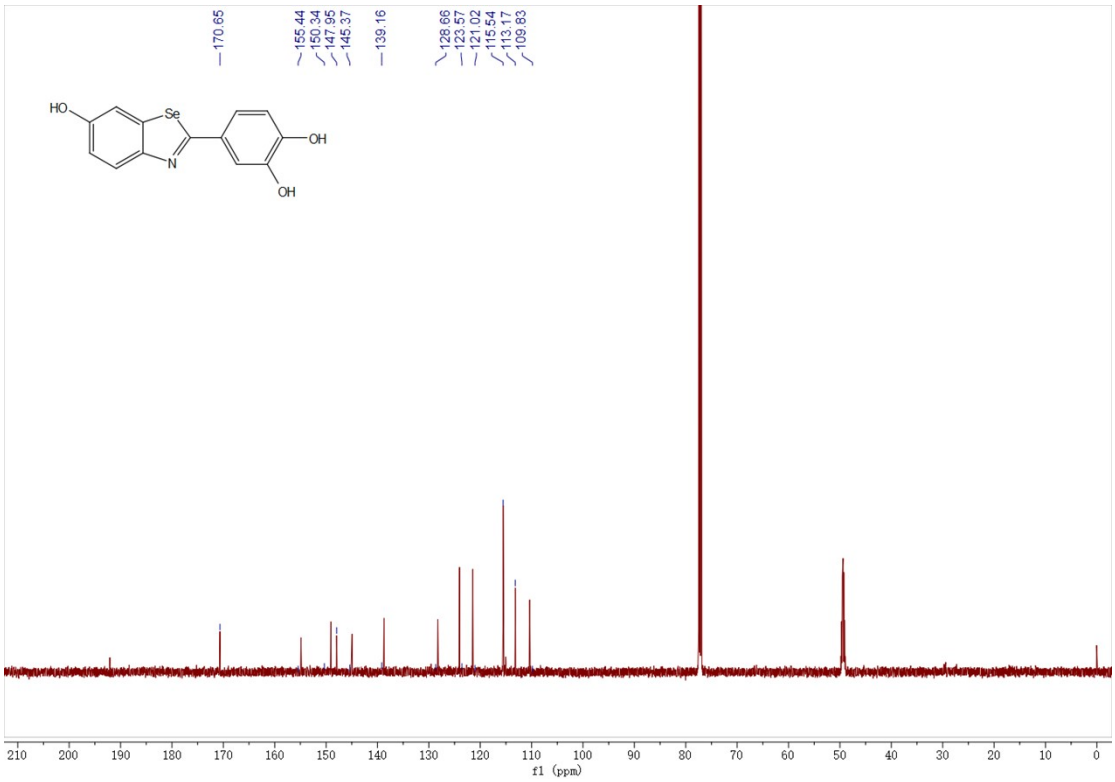


Figure S11. ^{13}C NMR of **ZSL-V5n**.

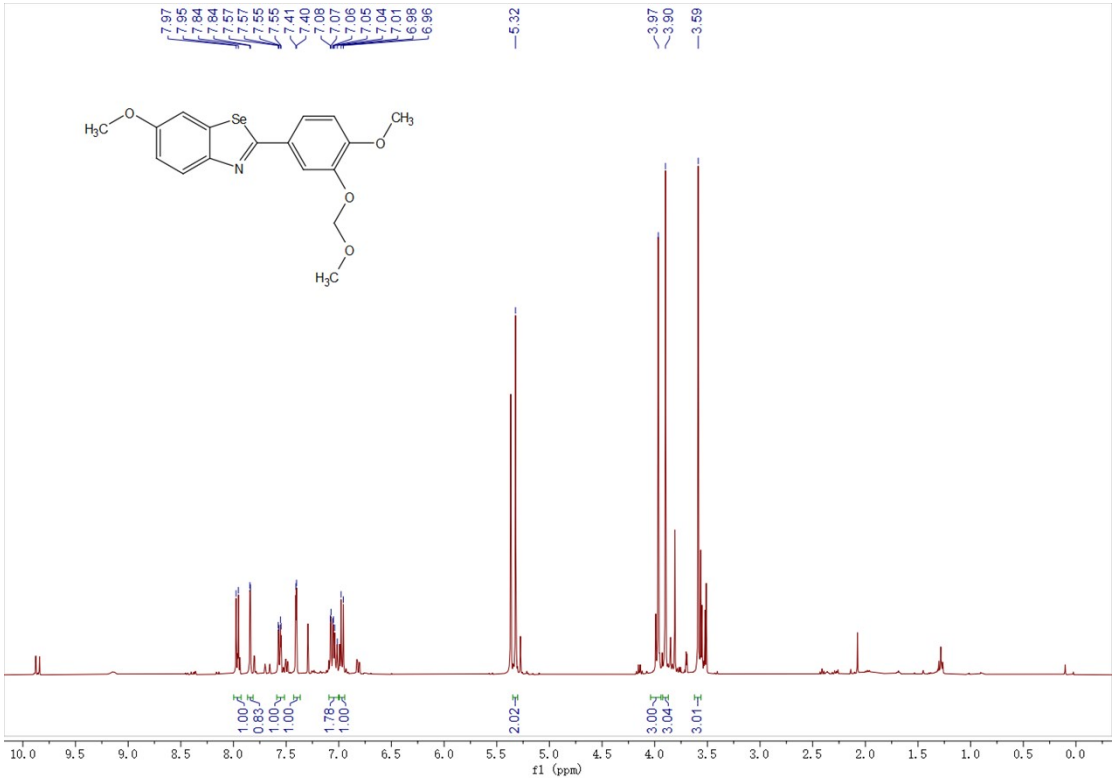


Figure S12. ^{1}H NMR of **17**.

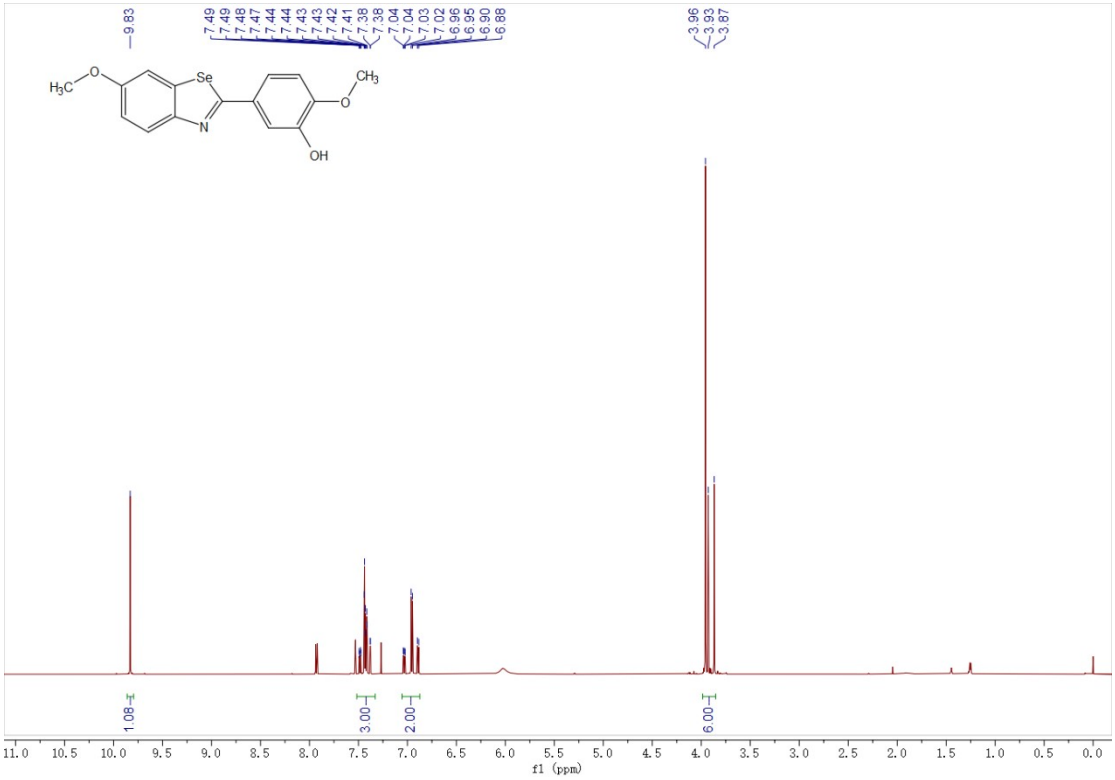


Figure S13. ^{1}H NMR of **18**.

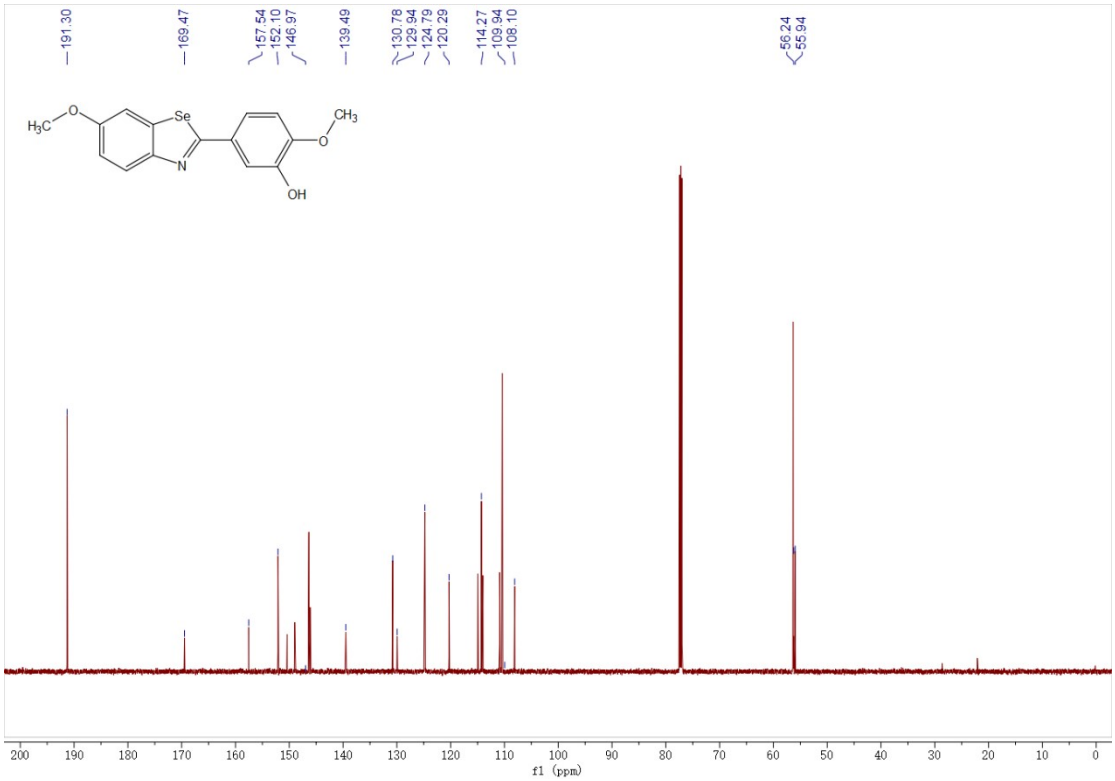


Figure S14. ^{13}C NMR of **18**.

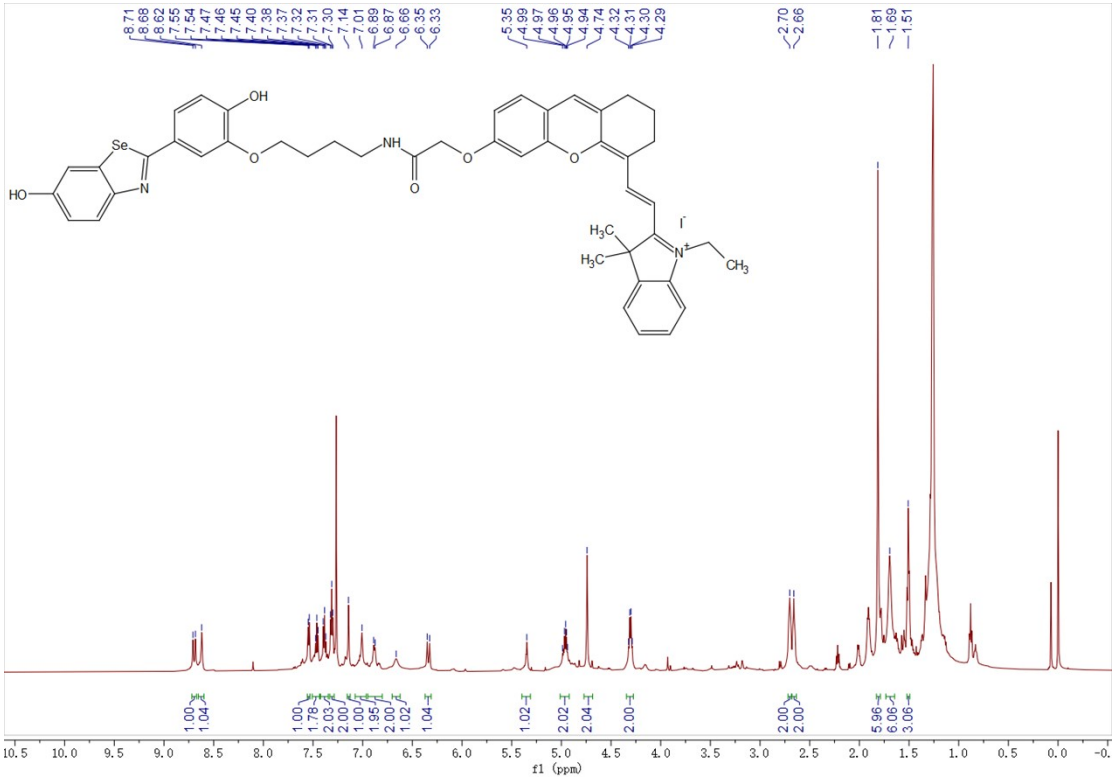


Figure S15. ^{1}H NMR of **D1**.

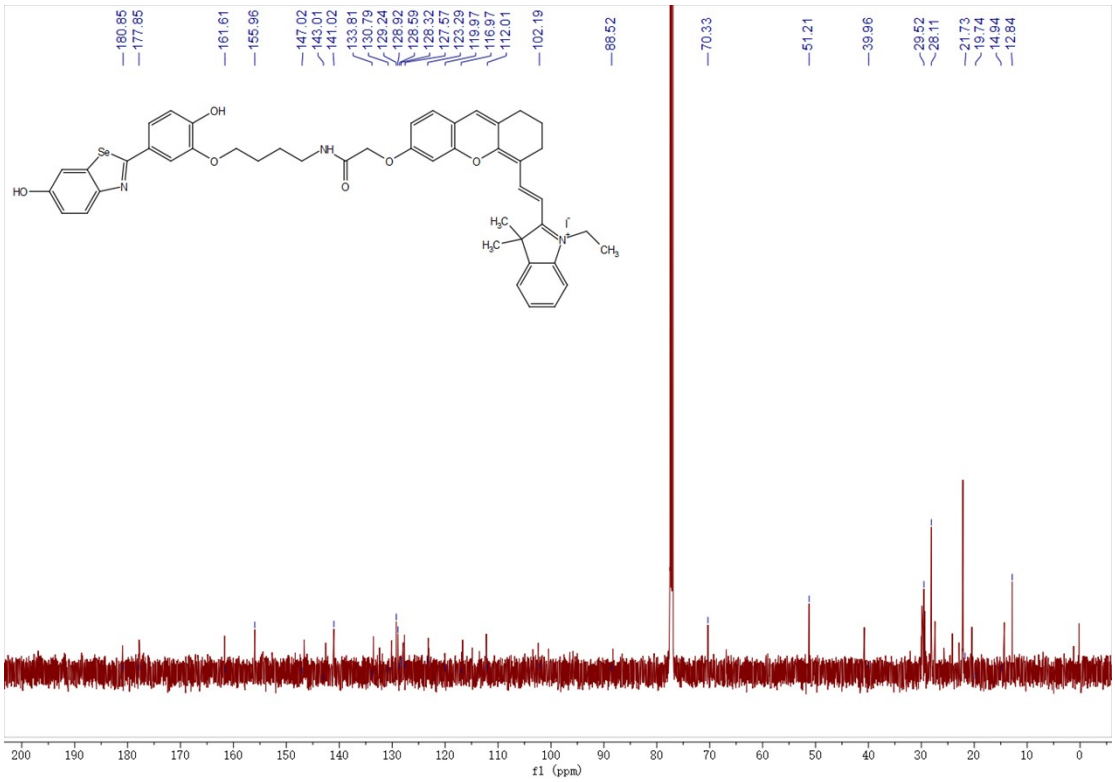


Figure S16. ^{13}C NMR of **D1**.

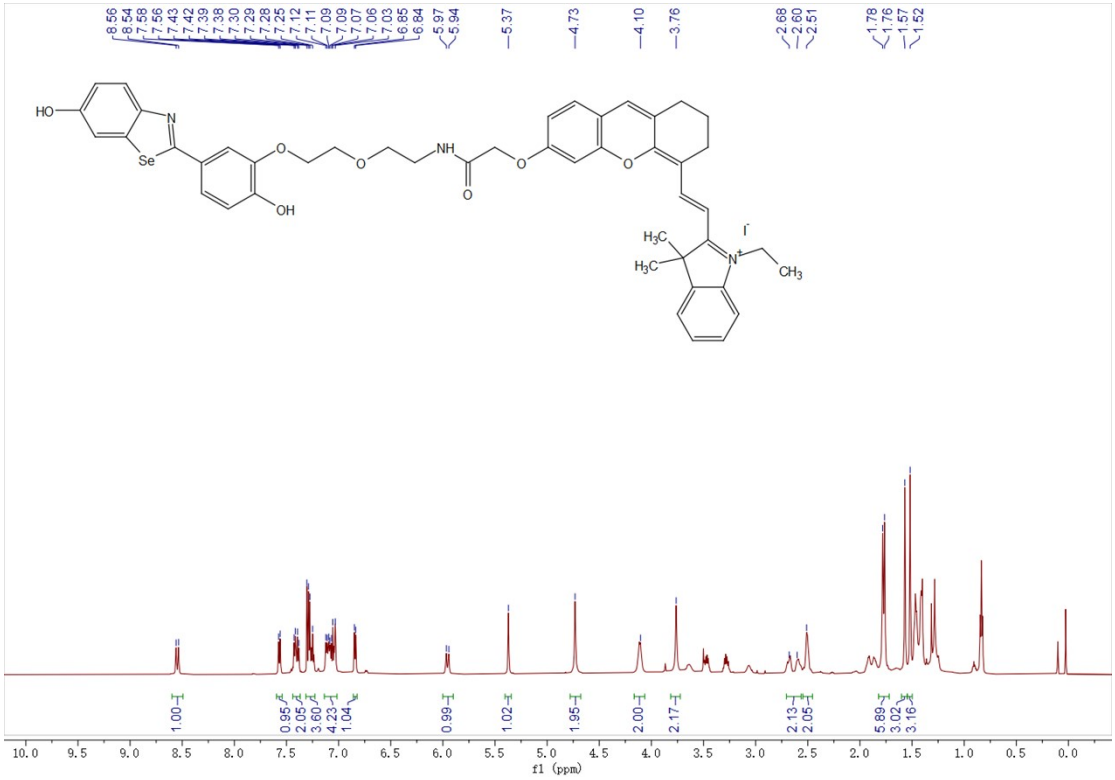


Figure S17. ^{1}H NMR of **D2**.

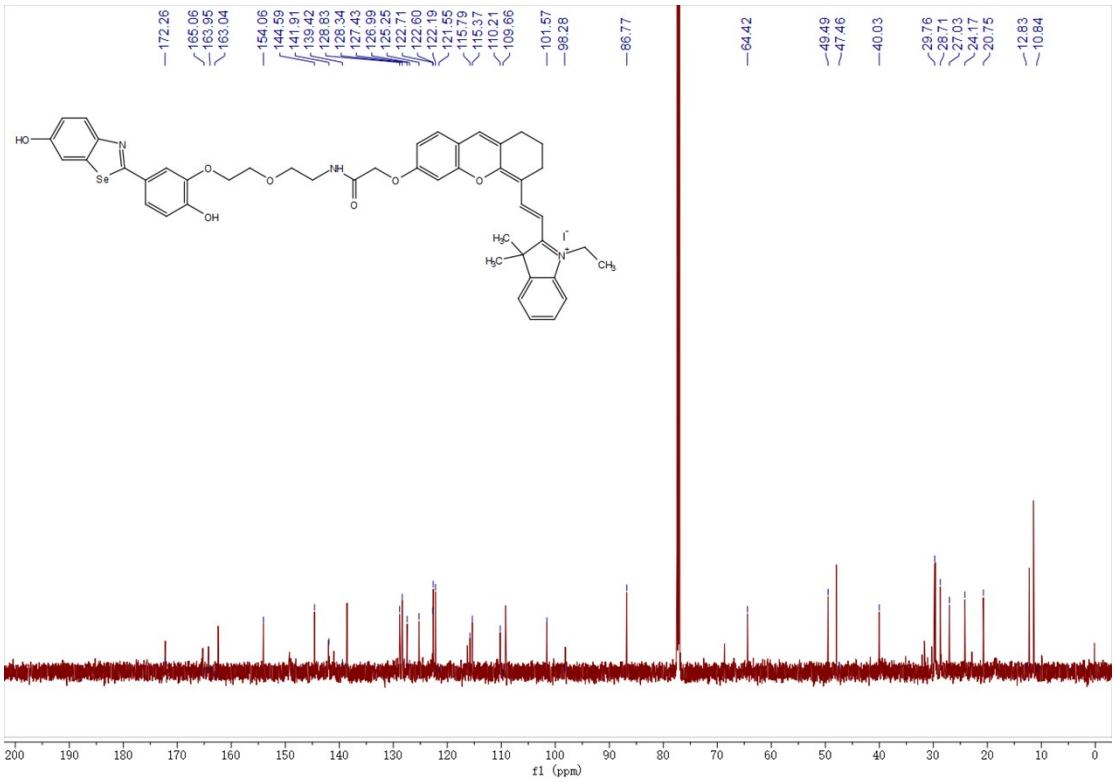


Figure S18. ^{13}C NMR of **D2**.

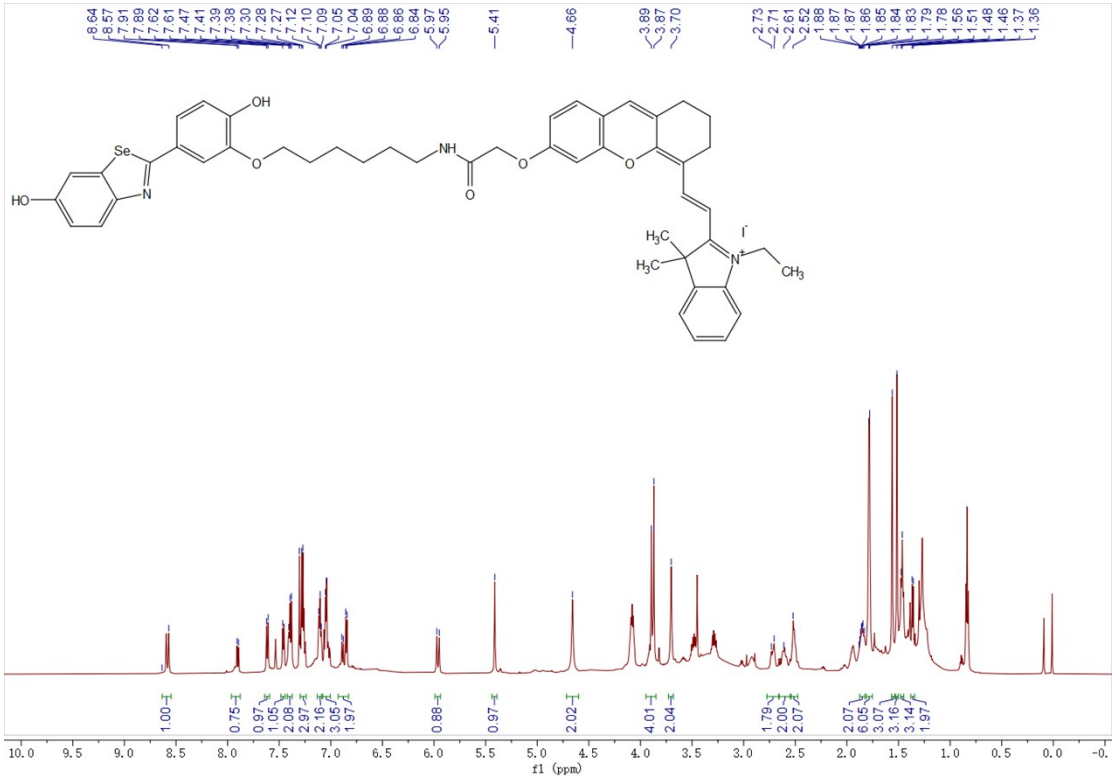


Figure S19. ^{1}H NMR of **D3**.

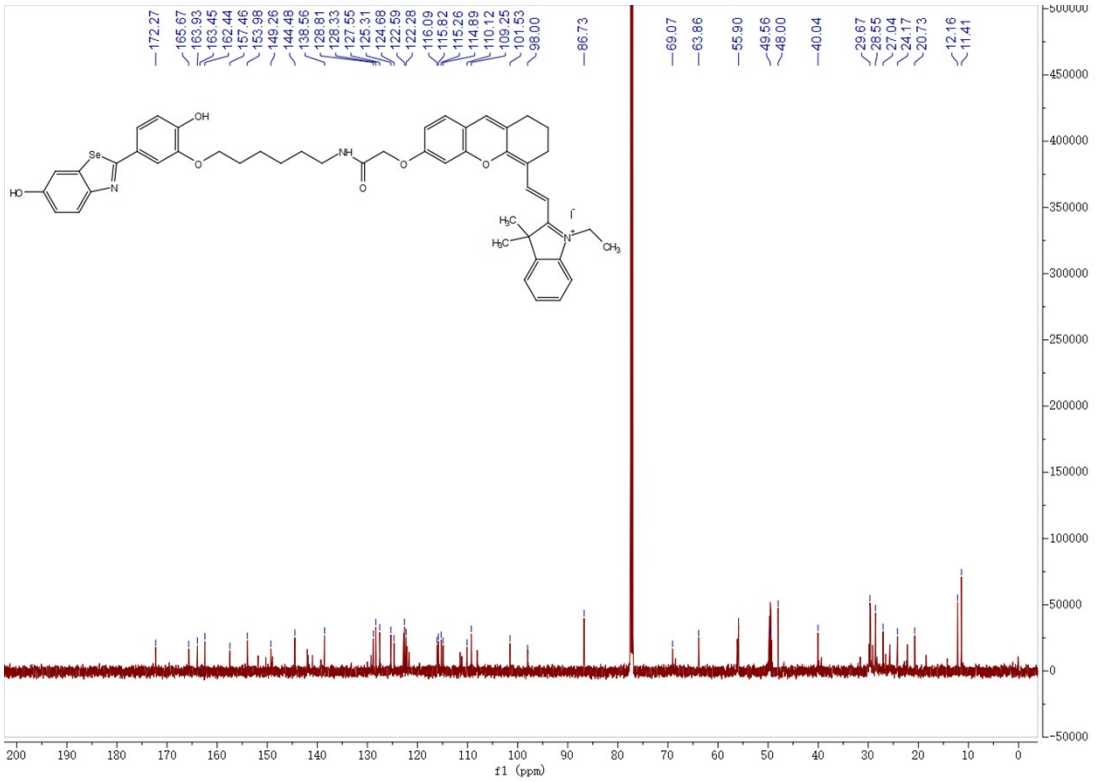


Figure S20. ^{13}C NMR of **D3**.

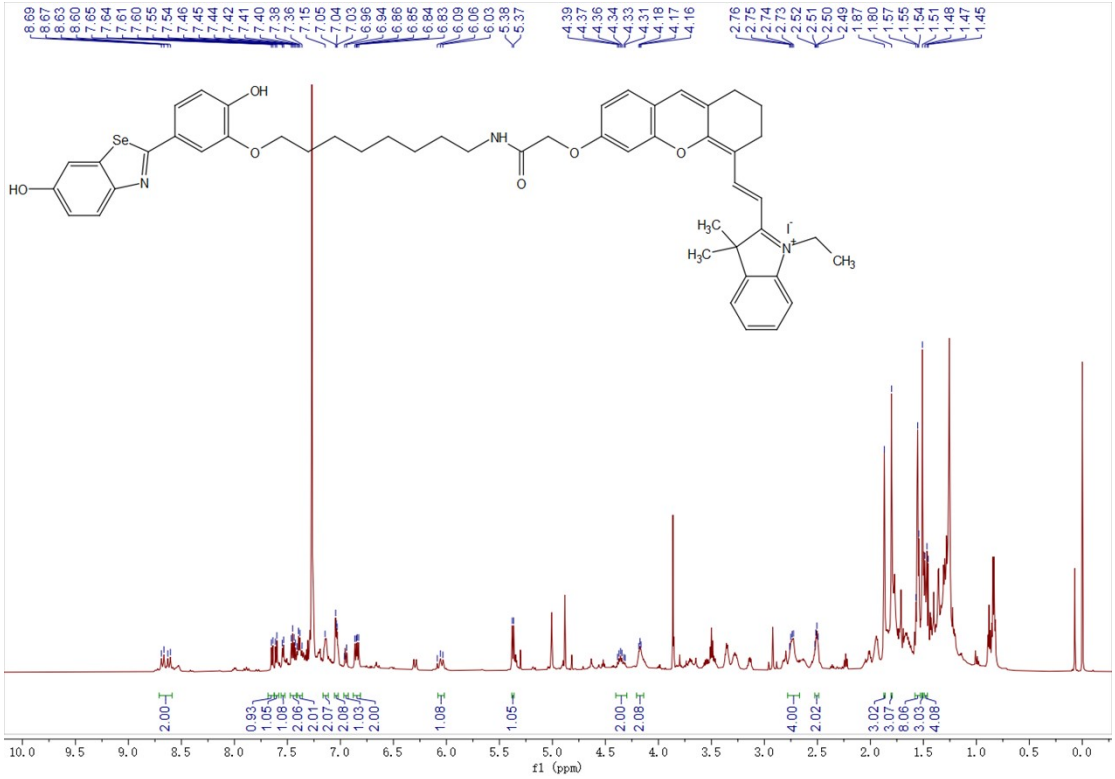


Figure S21. ^{1}H NMR of **D4**.

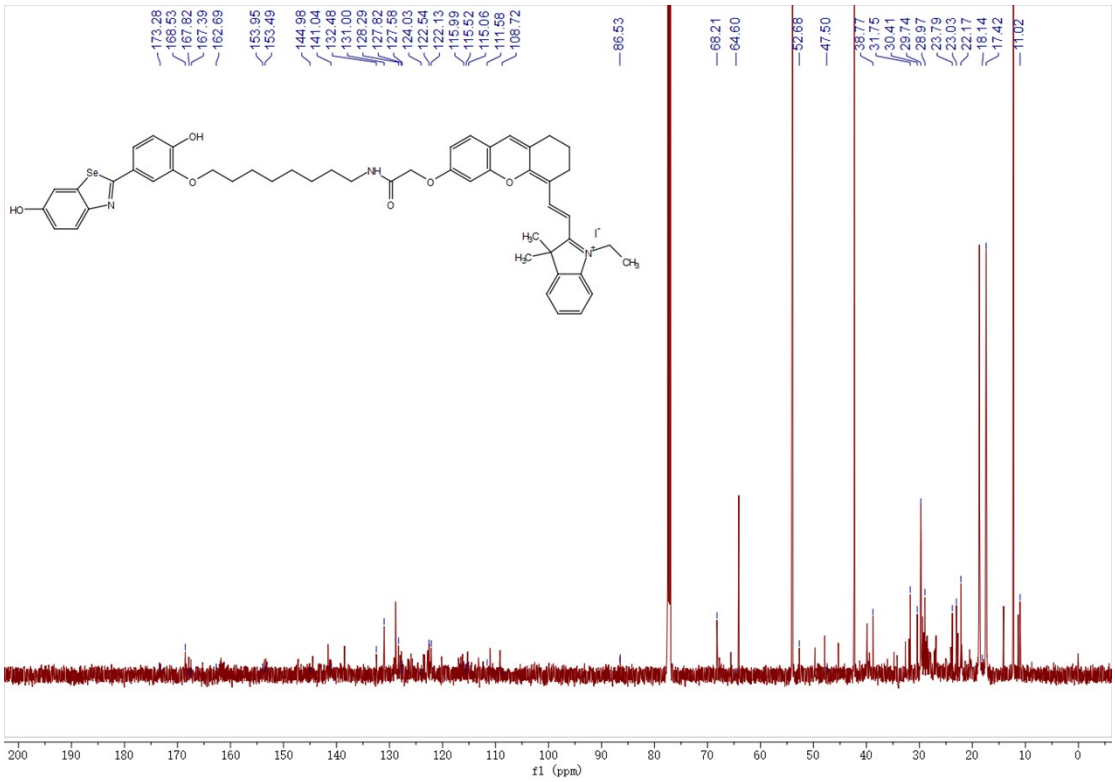


Figure S22. ^{13}C NMR of **D4**.

4. High-resolution mass spectra of probes.

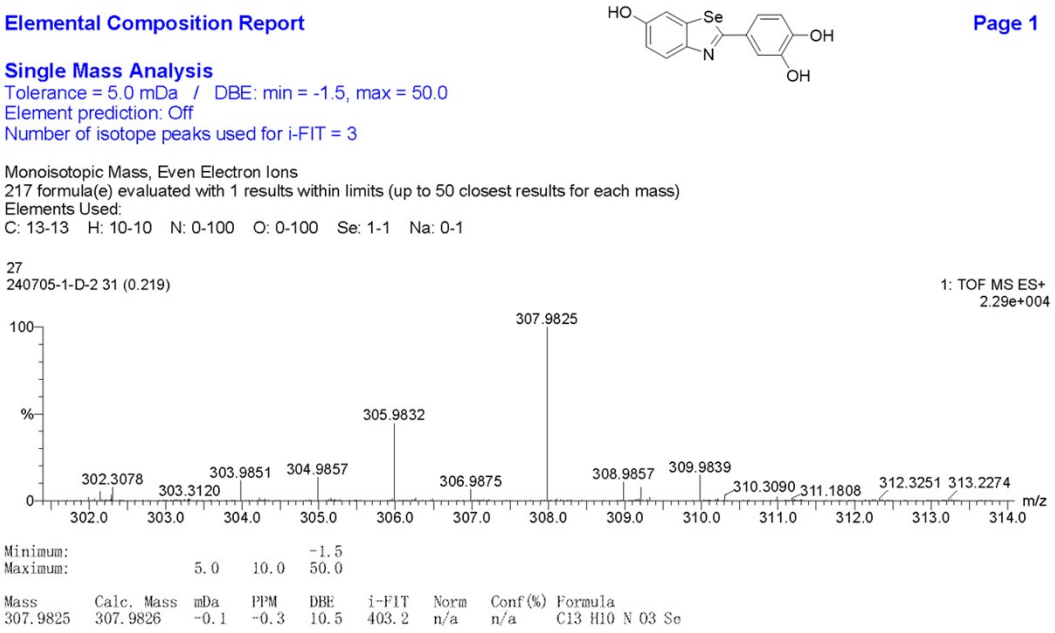


Figure S23. HMRS spectra of **ZSL-V5n**.

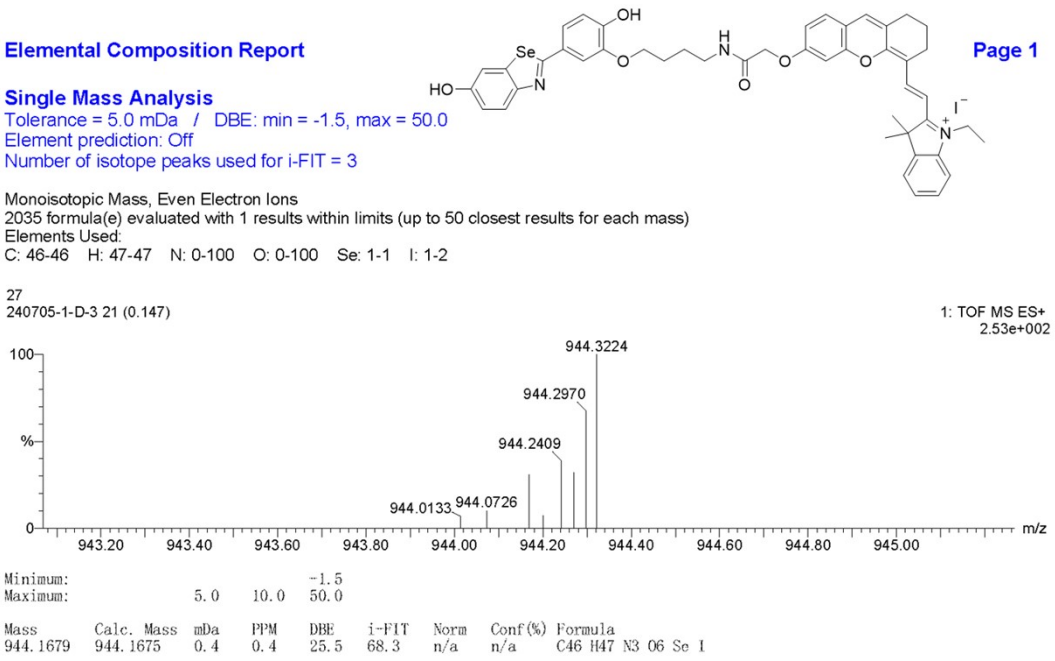


Figure S24. HMRS spectra of **D1**.

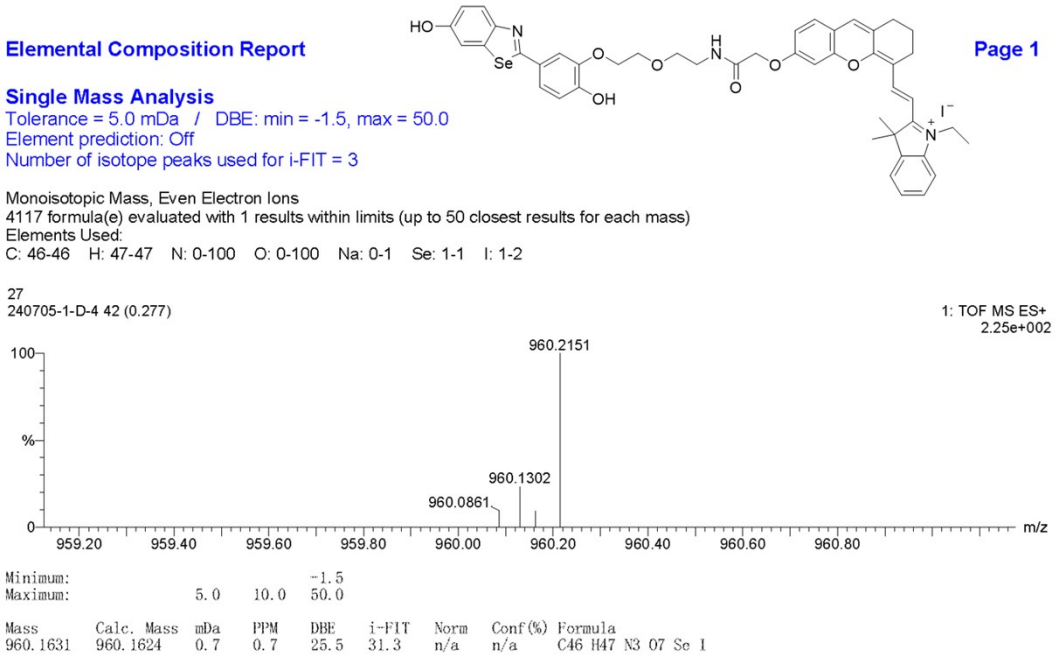


Figure S25. HMRS spectra of **D2**.

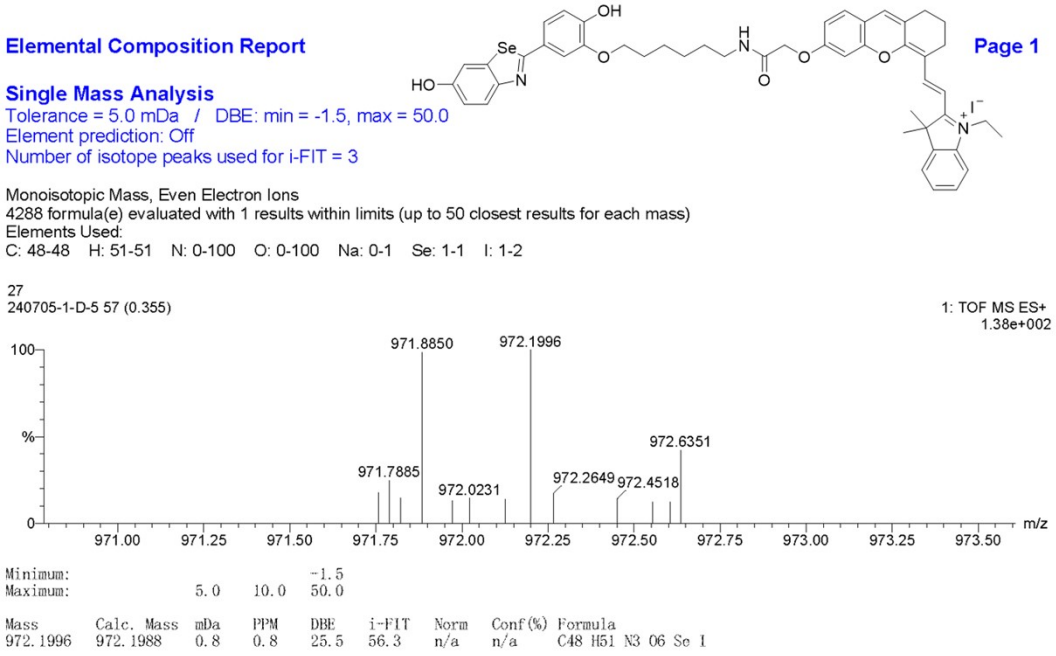


Figure S26. HMRS spectra of **D3**.

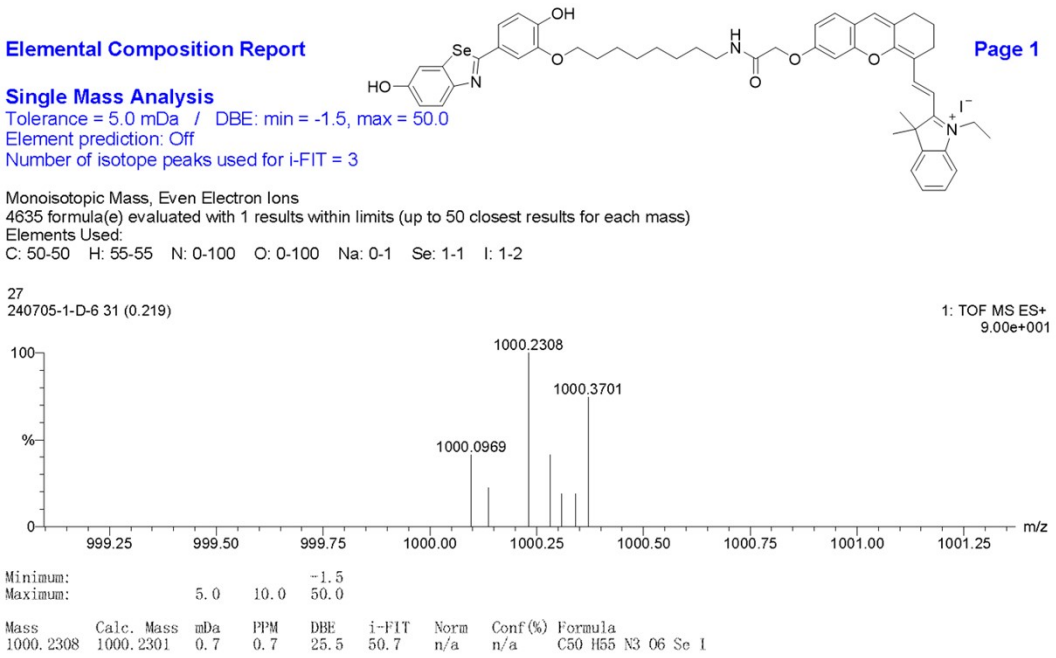


Figure S27. HMRS spectra of **D4**.