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Electronic Supporting Information

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

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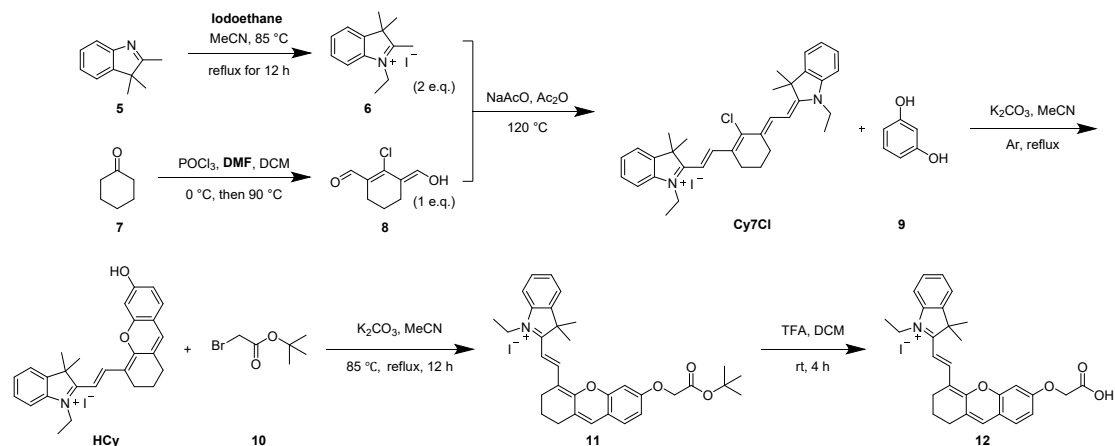
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1. Synthetic procedures of D1-D4.

Synthesis of HCy derivatives.



Synthesis of 6. 2,3,3-trimethylindolenine (9.55g, 60mmol) was dissolved in acetonitrile. Then, iodoethane (9.36g, 60mmol) 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 **6** (15.31g, yield: 81%) was used directly in the next reaction without further purification.

^1H 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 8. A solution of DMF (15mL) and DCM (15mL) in a round-bottom single-neck flask was cooled over ice bath in argon atmosphere. Then, phosphorus oxychloride (19mL, 0.2mol) was added drop wise with stirring for 30 min, followed by cyclohexanone (5.01g, 0.051mol). 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 (100mL \times 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 **8** 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 **6** (3.65g, 11.6mmol) and sodium acetate (0.95g, 36mmol) were added to a round-bottom double-neck flask containing the synthesized intermediate compound **8** (1.00g, 5.79mmol) in 15 mL of acetic anhydride. The solution was stirred at room temperature for 4 h. The mixture was extracted with water and dichloromethane (60mL \times 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%).

^1H 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 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 (1.10g, 8mmol) was added to a stirred solution of resorcinol (0.88g, 8mmol) in acetonitrile (15mL), and stirred for 20 min at room temperature. Then, a solution of **Cy7Cl** (2.56g, 4mmol) in acetonitrile (10mL) was added to the above mixture, and heated at 50°C for 4 h. The mixture was extracted with water and dichloromethane (30mL \times 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 (1.62g, yield: 77%).

^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.48 (d, J = 14.5 Hz, 1H), 7.72 (d, J = 6.4 Hz, 1H), 7.57 (d, J = 5.4 Hz, 2H), 7.55 – 7.44 (m, 2H), 7.38 (t, J = 7.9 Hz, 1H), 6.87 – 6.79 (m, 2H), 6.40 (d, J = 14.6 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 2.76 – 2.65 (m, 4H), 1.84 (t, J = 6.0 Hz, 2H), 1.74 (s, 6H), 1.36 (t, J = 7.1 Hz, 3H).

^{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.

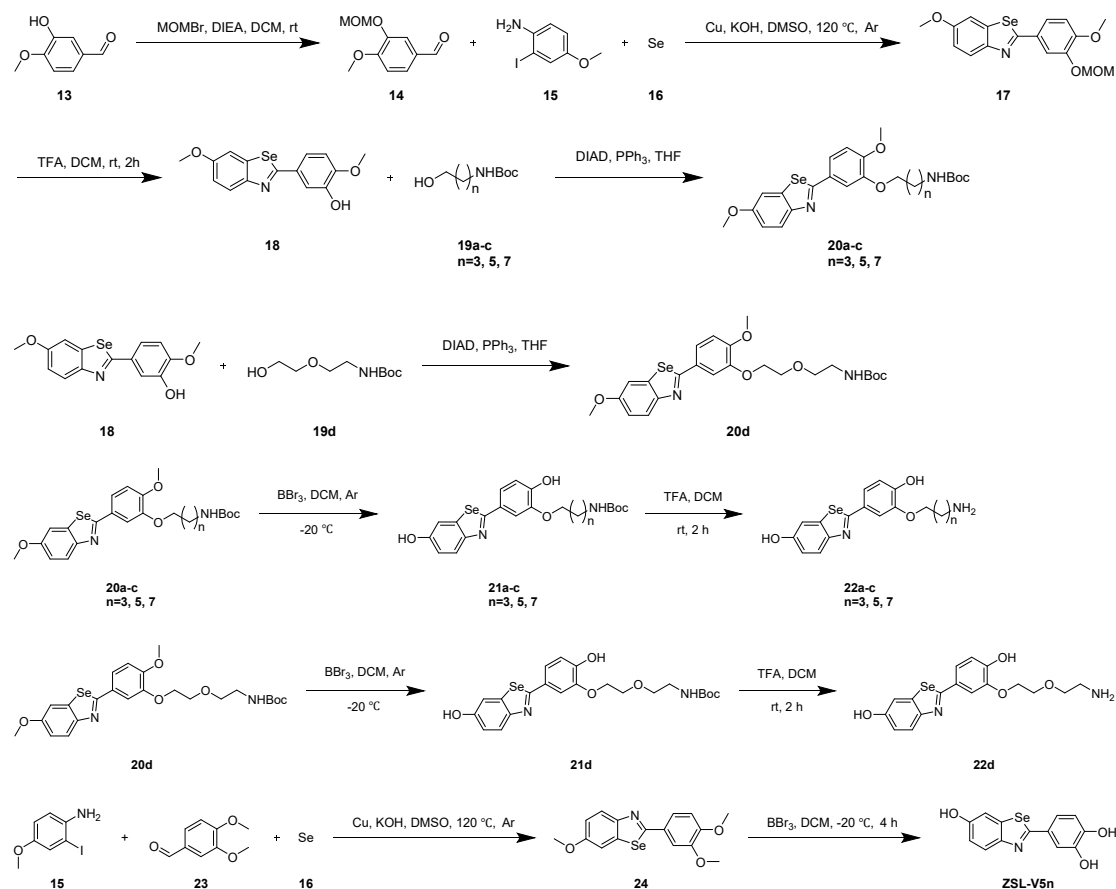
Synthesis of 11. KI (0.03g, 0.19mmol) was added to a solution of *tert*-butyl 2-bromoacetate (0.56g, 2.9mmol) in acetonitrile (15mL), and stirred at room temperature for 30 min. Then, **HCy** (1.00g, 1.9mmol) and K₂CO₃ (0.39g, 2.9mmol) were added, and heated to reflux at 85°C for 12 h. The solution was cooled to room temperature and extracted with water and dichloromethane (30mL × 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 (1.03g, yield: 83%).

¹H 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).

¹³C NMR (151 MHz, CDCl₃) 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** (0.20g, 0.3mmol) was dissolved in dichloromethane (1mL), and trifluoroacetic acid (1mL) was added slowly over ice 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 (4.56g, 30mmol) was dissolved in dichloromethane (30mL). Then, a solution of bromomethyl methyl ether (4.87g, 39mmol) in dichloromethane (10mL) was added slowly over ice bath, followed by *N,N*-diisopropylethylamine (7.39mL, 45mmol). 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 (5.41g, yield: 92%).

Synthesis of 17. 2-Iodo-4-methoxyaniline (1.00g, 4 mmol), **14** (0.95g, 4.8 mmol), selenium powder (0.95g, 12mmol), copper powder (25mg, 0.4mmol), potassium hydroxide (0.45g, 8mmol) were dissolved in dimethylsulfoxide (20mL) and heated at 120°C for 12 h in argon atmosphere. Then, it was cooled to room temperature, filtered and washed with a small amount of ethyl acetate. The filtrate was extracted with water and ethyl acetate (30mL \times 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 (497mg, yield: 33%). ¹H 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** (0.50g, 1.3mmol) was dissolved in dichloromethane (2mL), and trifluoroacetic acid (2mL) 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 (0.43g, yield: 97%).

¹H 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).

¹³C NMR (151 MHz, CDCl₃) 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 (0.24g, 1.2mmol), triphenylphosphine (0.31g, 1.2mmol) were dissolved into a 5 mL sample vial with tetrahydrofuran (2mL). The solution was ultrasonicated for 5 min at room temperature to produce a milky solid. Then, **18** (0.10g, 0.3mmol) and linker **19a-d** (0.6mmol) 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 yellow liquid (yield: 25%-100%).

Synthesis of 21a-d. In argon atmosphere, **20a-d** (0.15g, 1.0eq) was dissolved in dichloromethane (5mL) at -20°C. The BBr₃ (4.0eq) was added slowly into the solution. The solution was stirred at -20°C for 4 h. Then, the reaction was quenched by drop wise addition of anhydrous methanol at -20°C. The solution was extracted with water and ethyl acetate (15mL \times 3), and the organic phase was evaporated under reduced pressure to get compounds **21a-d** as yellow solid. The products **21a-d** were used directly in the next reaction without further purification.

Synthesis of 22a-d. **21a-d** (mentioned above) were dissolved in dichloromethane (1mL), and trifluoroacetic acid (1mL) 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 to get compounds **22a-d** as yellow solid. The products **22a-d** were used directly in the next reaction without further purification.

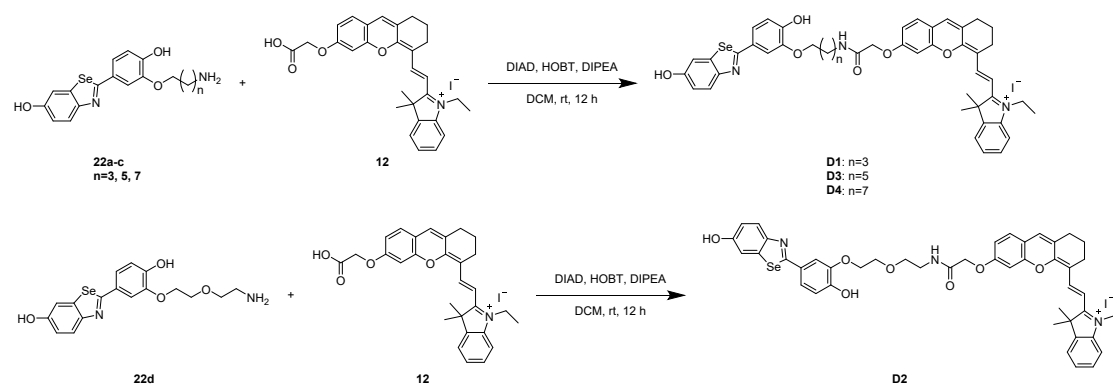
Synthesis of ZSL-V5n. The synthesis method of **ZSL-V5n** was similar to **17** mentioned above.

^1H 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 $\text{C}_{13}\text{H}_{10}\text{NO}_3\text{Se}$ $[\text{M} + \text{H}]^+$, 307.9826, found 307.9825.

Synthesis of NIR probes.



Synthesis of D1-D4. **12** (150mg, 0.26mmol, 1.05eq), 1-Hydroxybenzotriazole (HOBT, 50.88mg, 0.38mmol, 1.5eq), Diisopropyl azodicarboxylate (DIAD, 76.09 mg, 0.38 mmol, 1.5eq) were dissolved in the dichloromethane (2mL), and stirred at room temperature for 30min. Subsequently, the solution was added with **22a-d** (1.00eq) and *N,N*-diisopropylethylamine (DIPEA, 0.25mL, 1.5mmol, 6.0eq) and stirred at room temperature for 12 h. The solution was extracted with water and dichloromethane (15 mL \times 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 compounds **D1-D4** as a blue solid with metallic luster (yield: 4.06% – 10.42%).

(*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 **D1**, yield: 4.06%. ¹H 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). ¹³C 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 C₄₆H₄₇N₃O₆Se [M + H]⁺, 944.1675; found 944.1679.

(*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 **D2**, yield 7.73%. ¹H 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). ¹³C 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 C₄₆H₄₇N₃O₇Se [M + H]⁺, 960.1624, found 960.1631.

(*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 **D3**, yield 10.42%. ¹H 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 $\text{C}_{48}\text{H}_{51}\text{N}_3\text{O}_6\text{Se}$ $[\text{M} + \text{H}]^+$, 972.1988, found 972.1996.

(*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 **D4**, yield 4.81%. ^1H 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 $\text{C}_{50}\text{H}_{55}\text{N}_3\text{O}_6\text{Se}$ $[\text{M} + \text{H}]^+$, 1000.2301, found 1000.2308.

2. Optical properties of D1, D2 and D4.

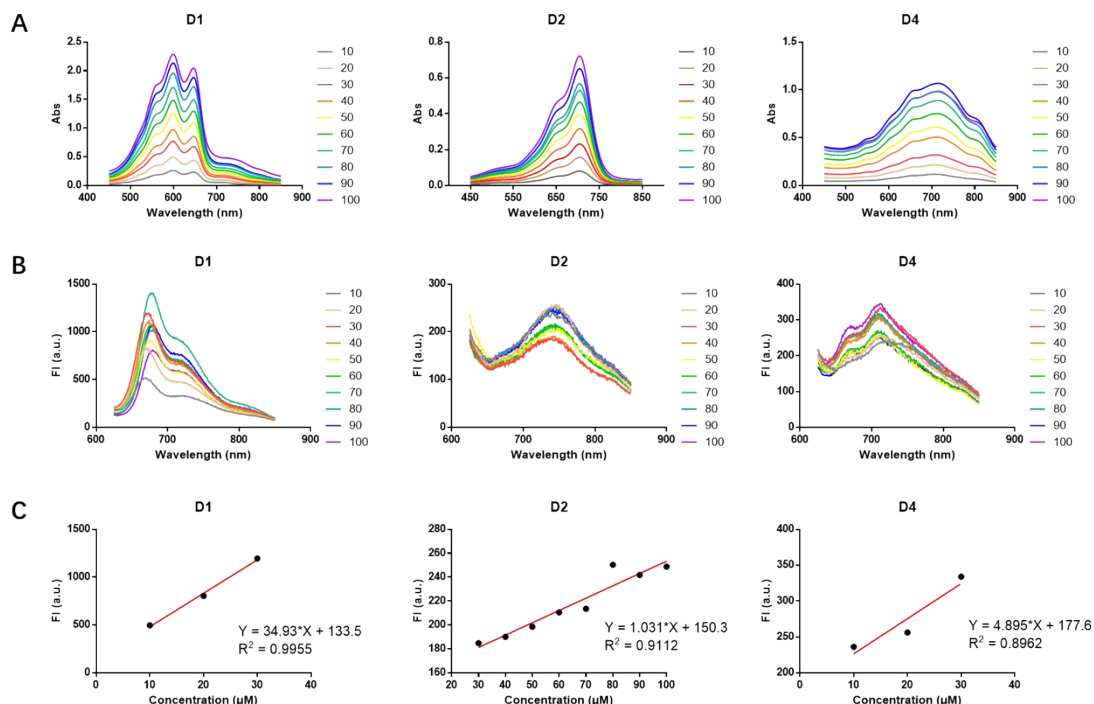


Figure S1. Optical properties of **D1**, **D2** and **D4**. Relationship curve of (A) UV absorption and (B) fluorescence intensity at different concentrations. (C) Linear relationship derived from (B) (R^2 : **D1** = 0.9955, **D2** = 0.9112, **D4** = 0.8962). All the experiments were conducted in a pH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

3. NMR spectra of probes.

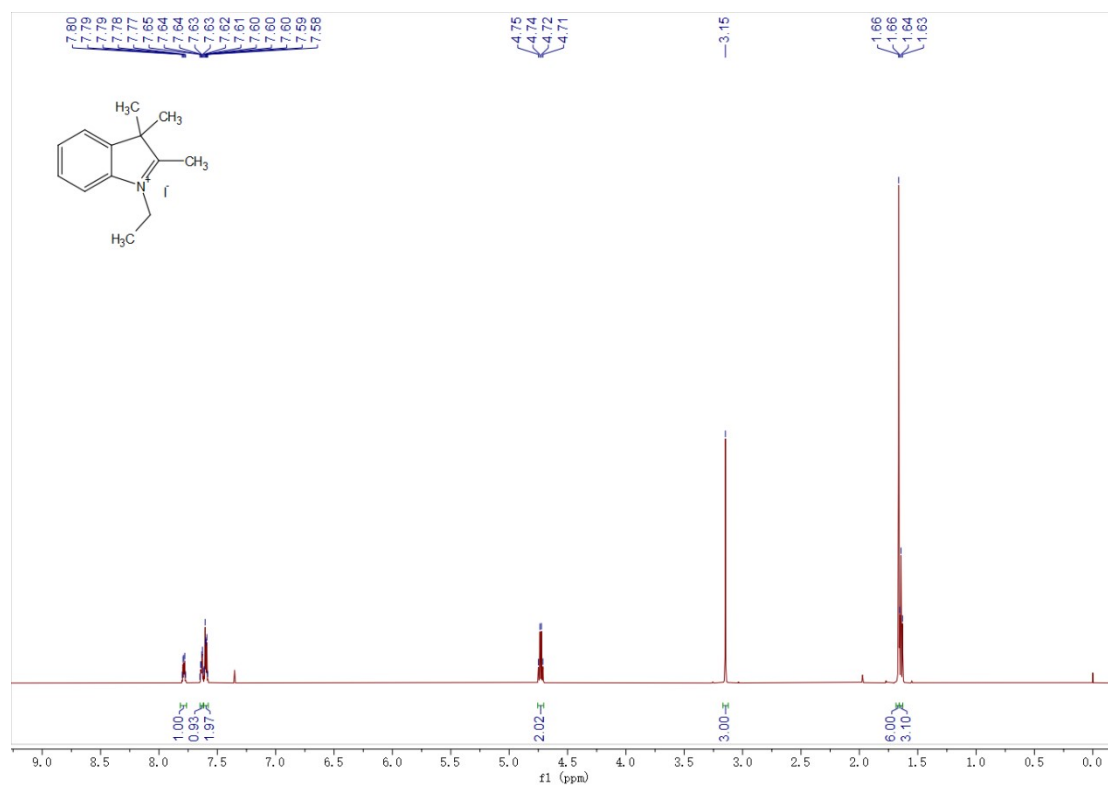


Figure S2. ¹H NMR of **3**.

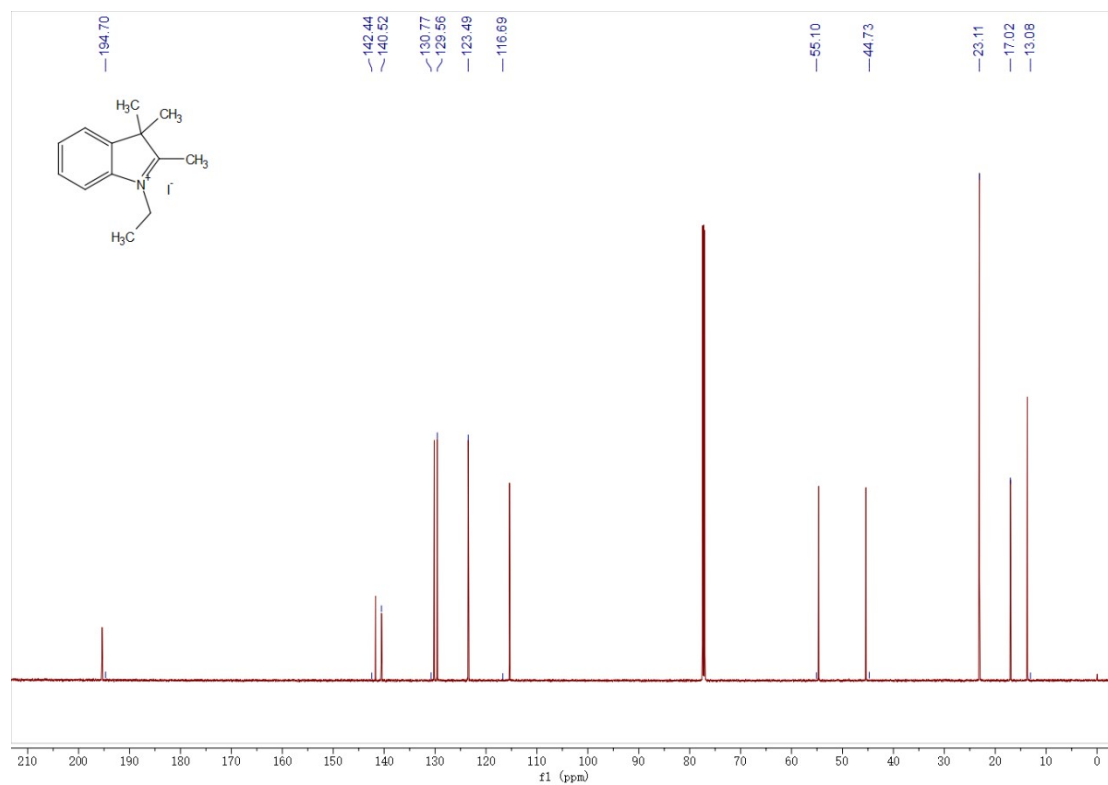


Figure S3. ¹³C NMR of **3**.

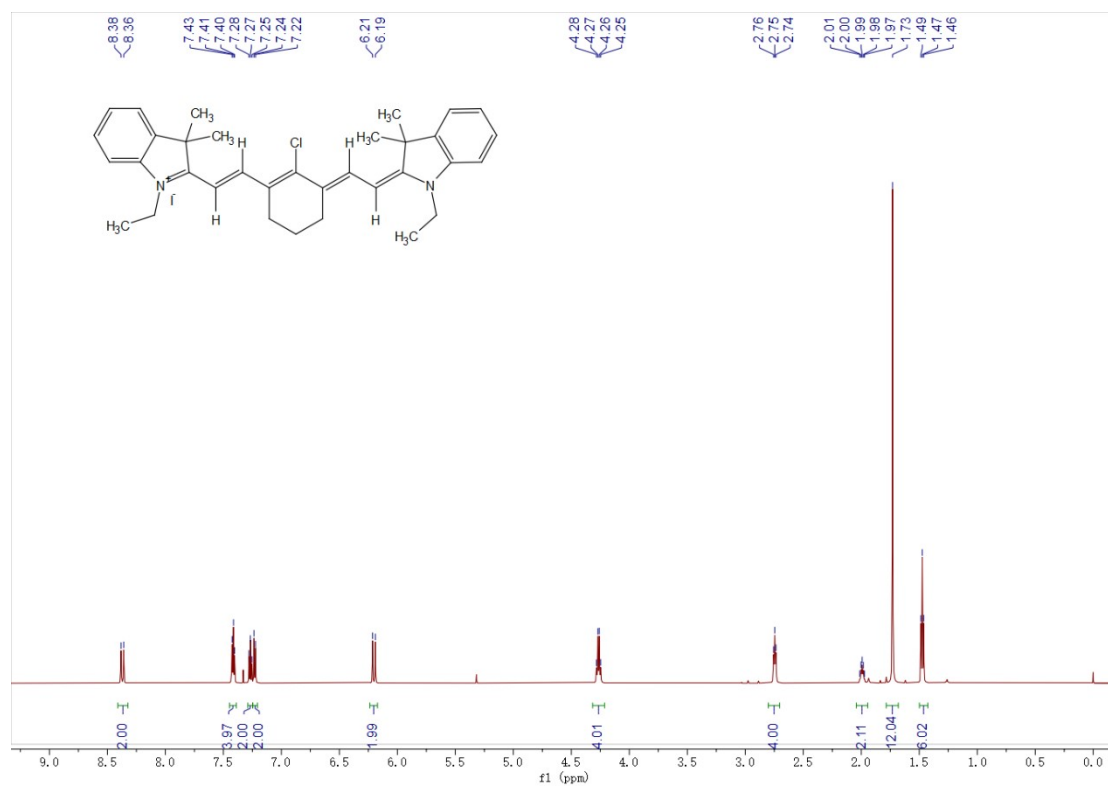


Figure S4. ¹H NMR of Cy7Cl.

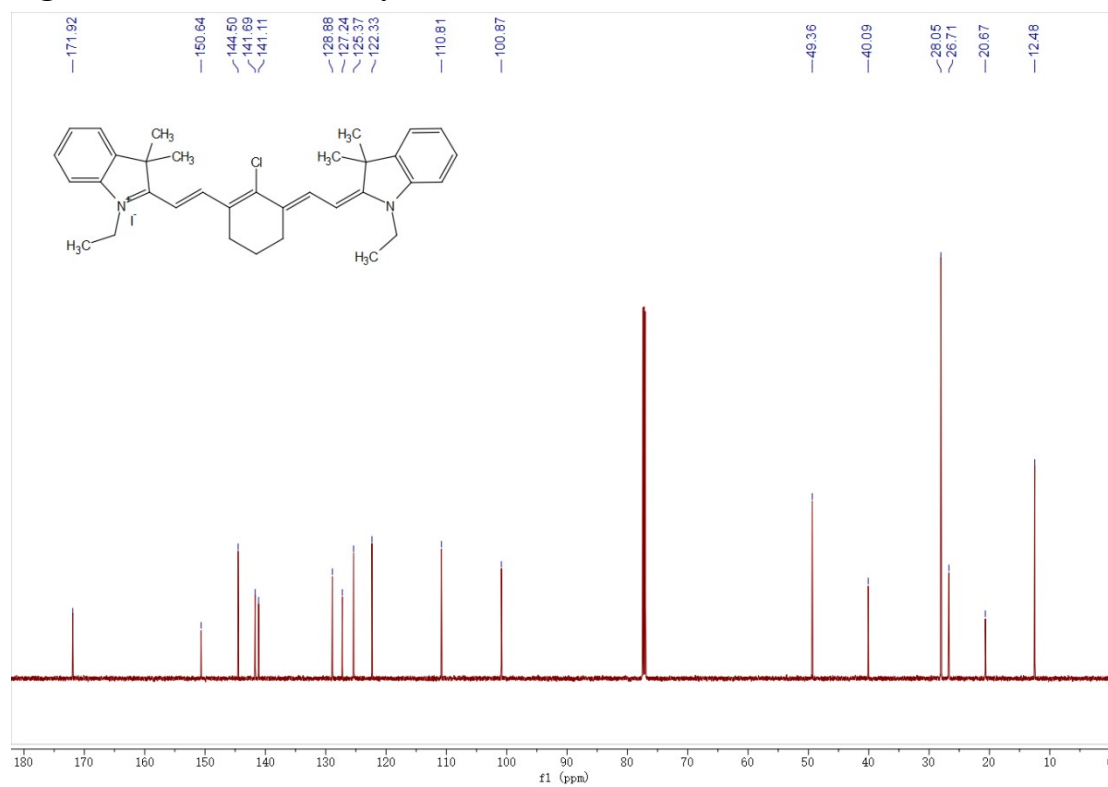


Figure S5. ¹³C NMR of Cy7Cl.

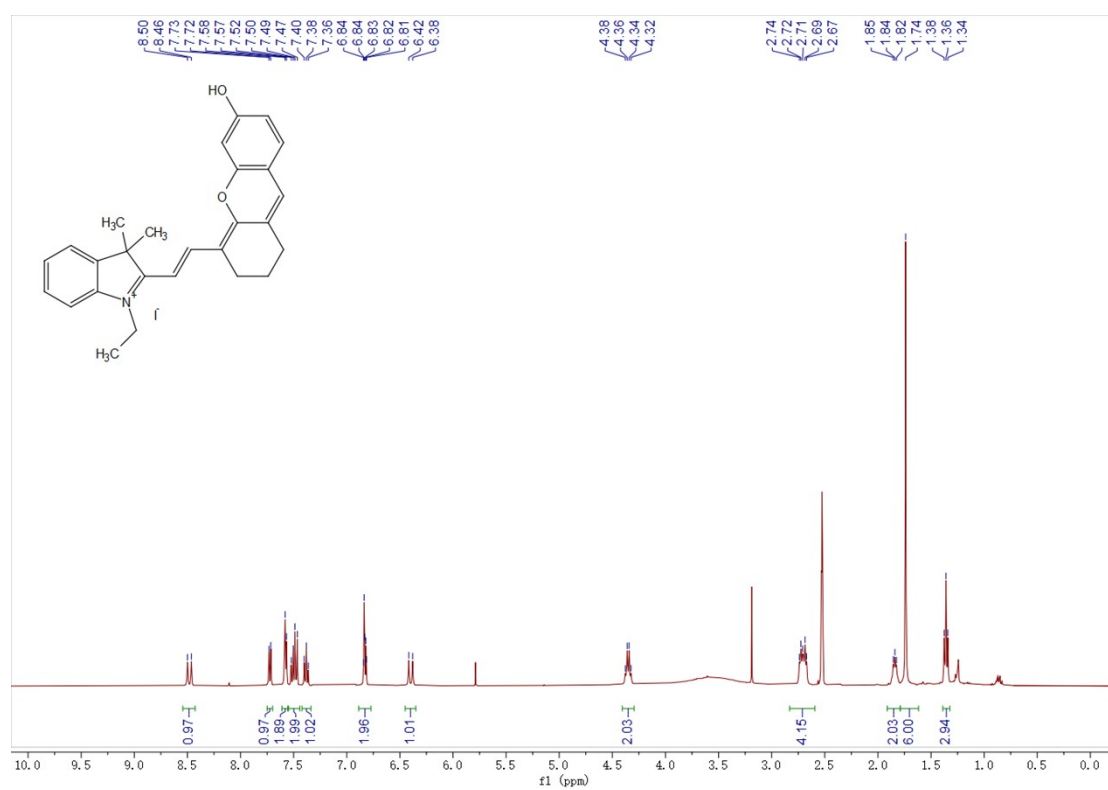


Figure S6. ^1H NMR of HCy.

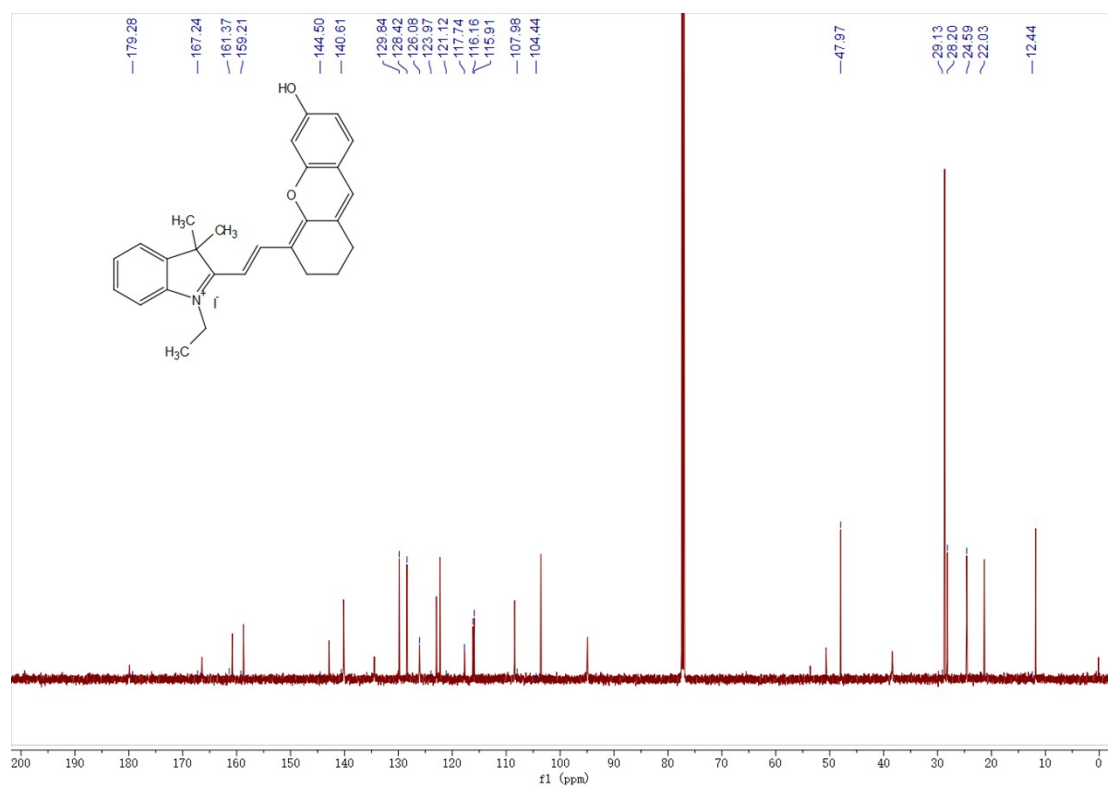


Figure S7. ^{13}C NMR of HCy.

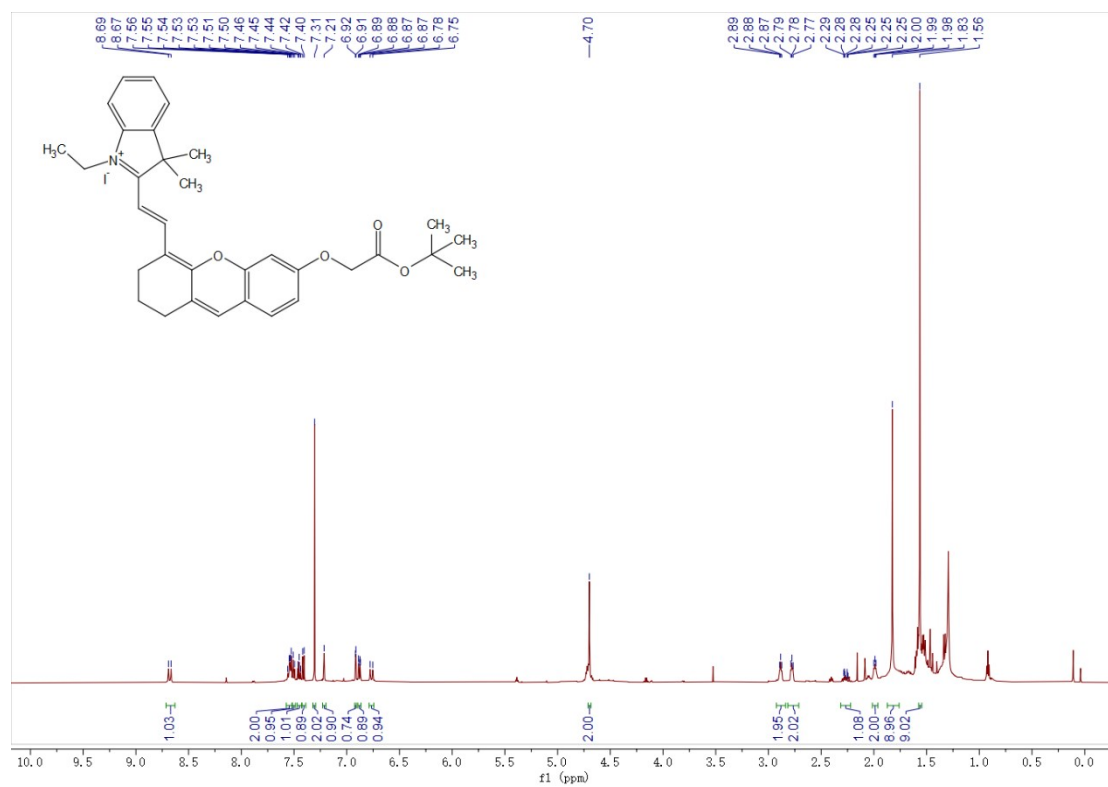


Figure S8. ¹H NMR of 11.

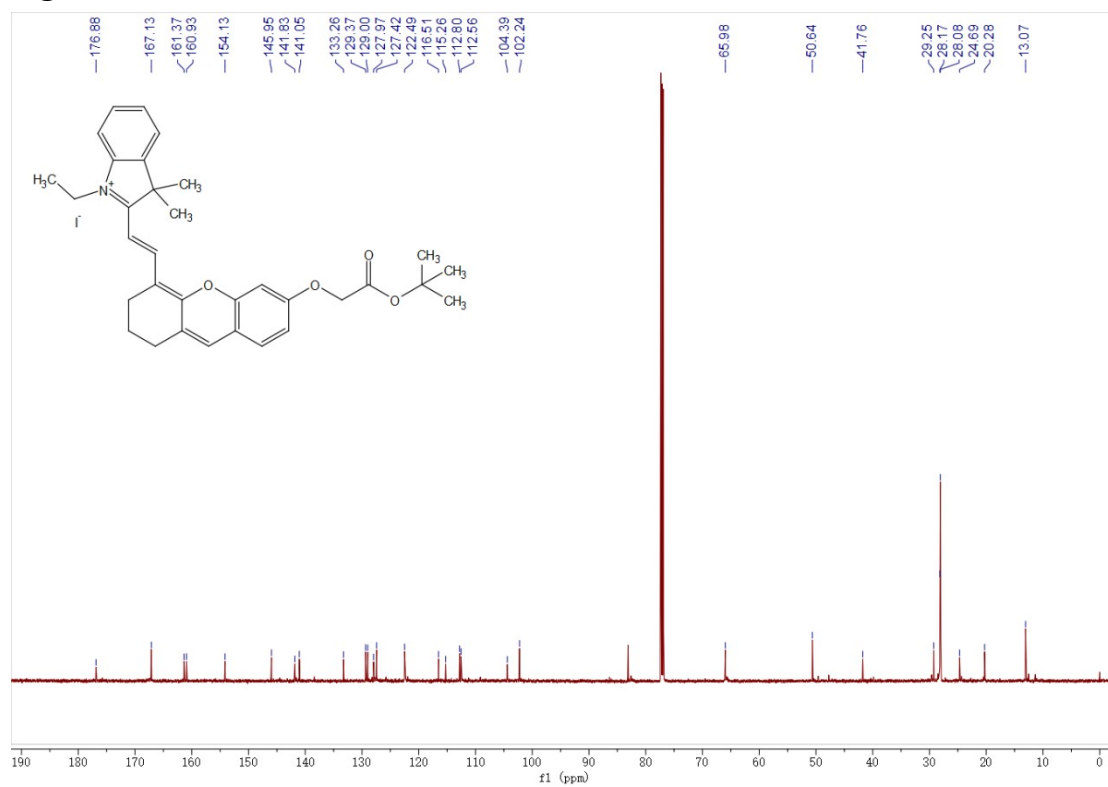


Figure S9. ¹³C NMR of 11.

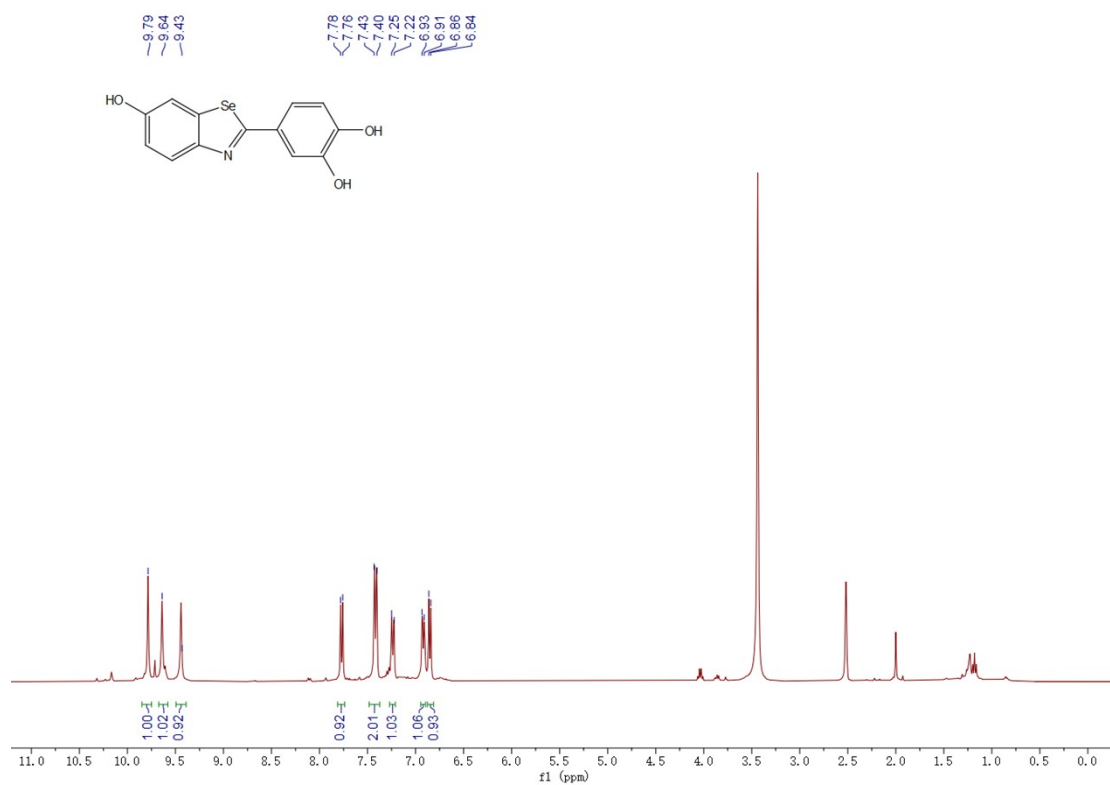


Figure S10. ¹H NMR of ZSL-V5n.

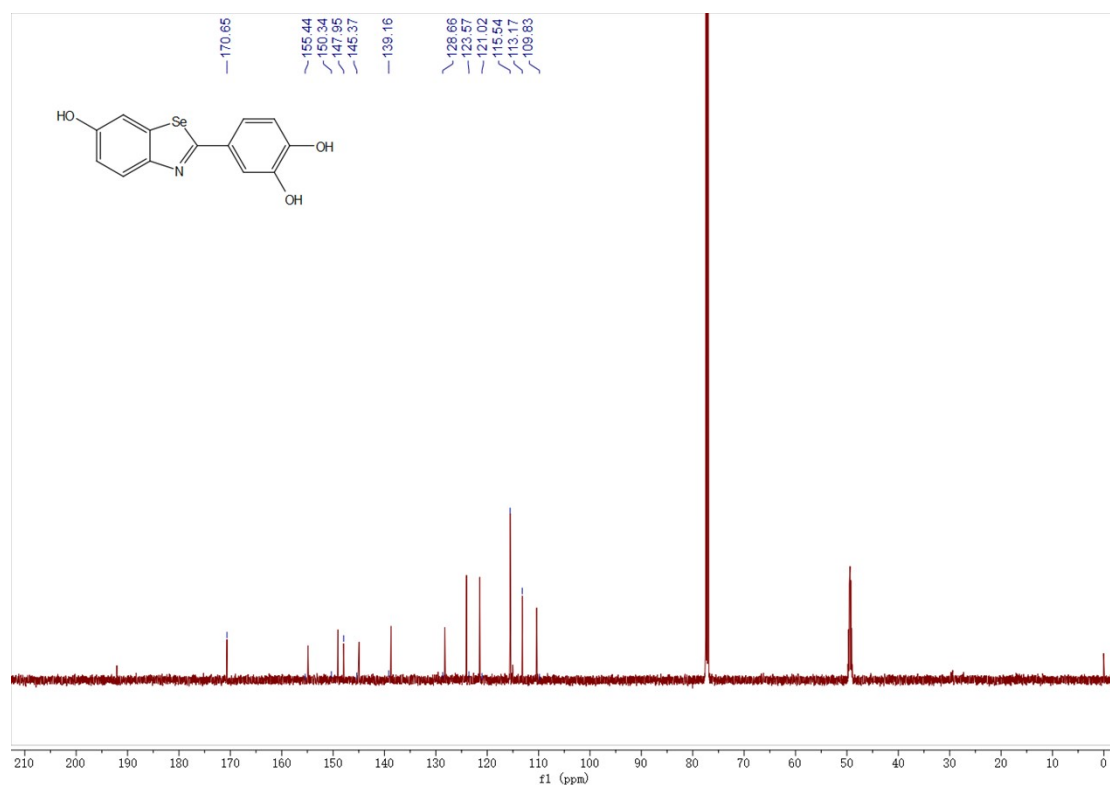


Figure S11. ¹³C NMR of ZSL-V5n.

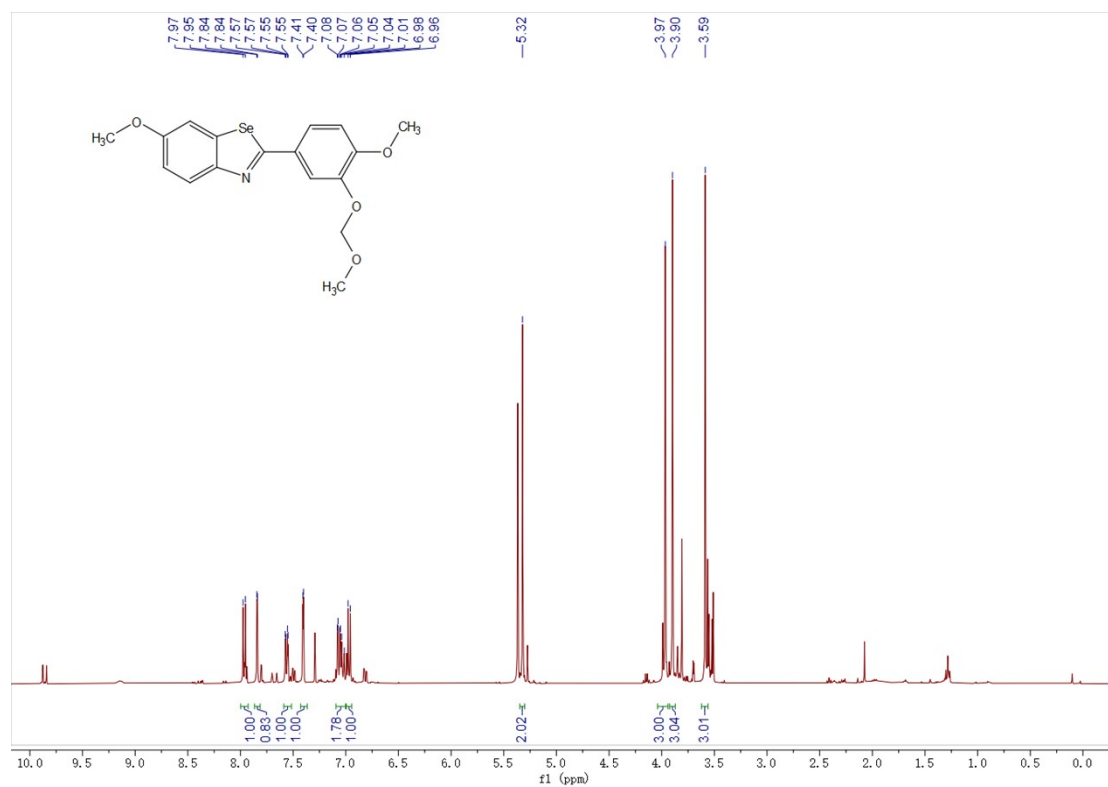


Figure S12. ¹H NMR of 17.

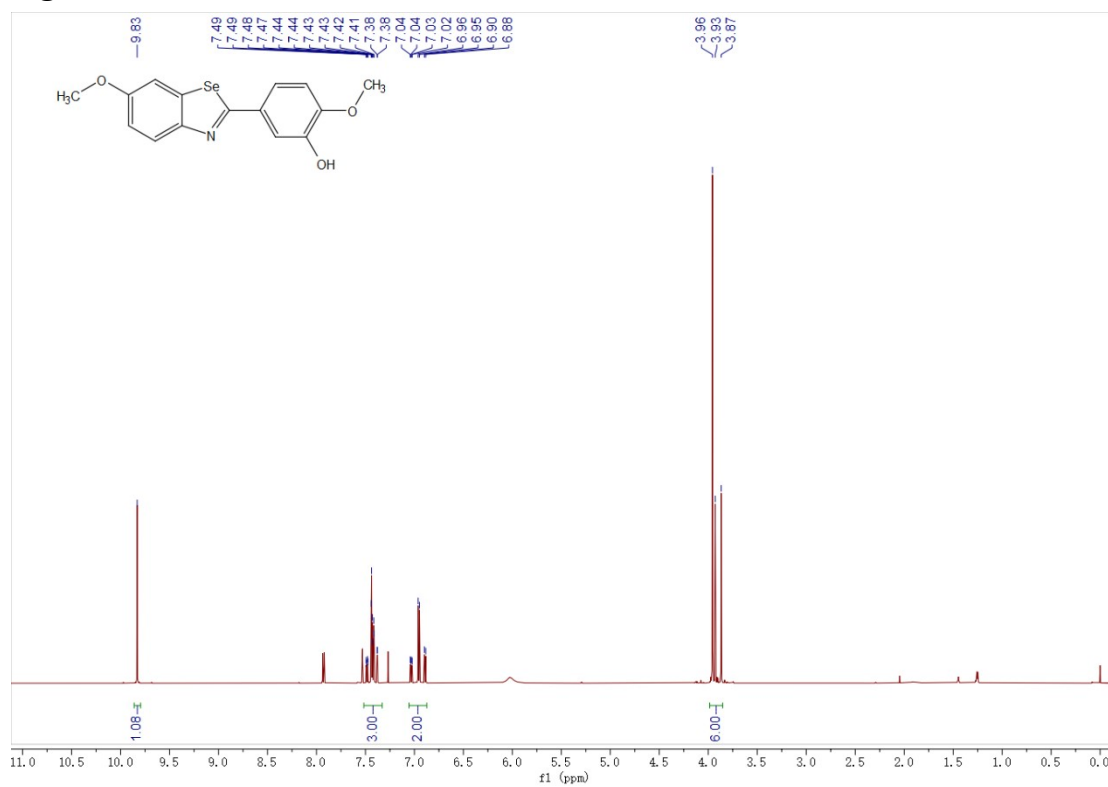


Figure S13. ¹H NMR of 18.

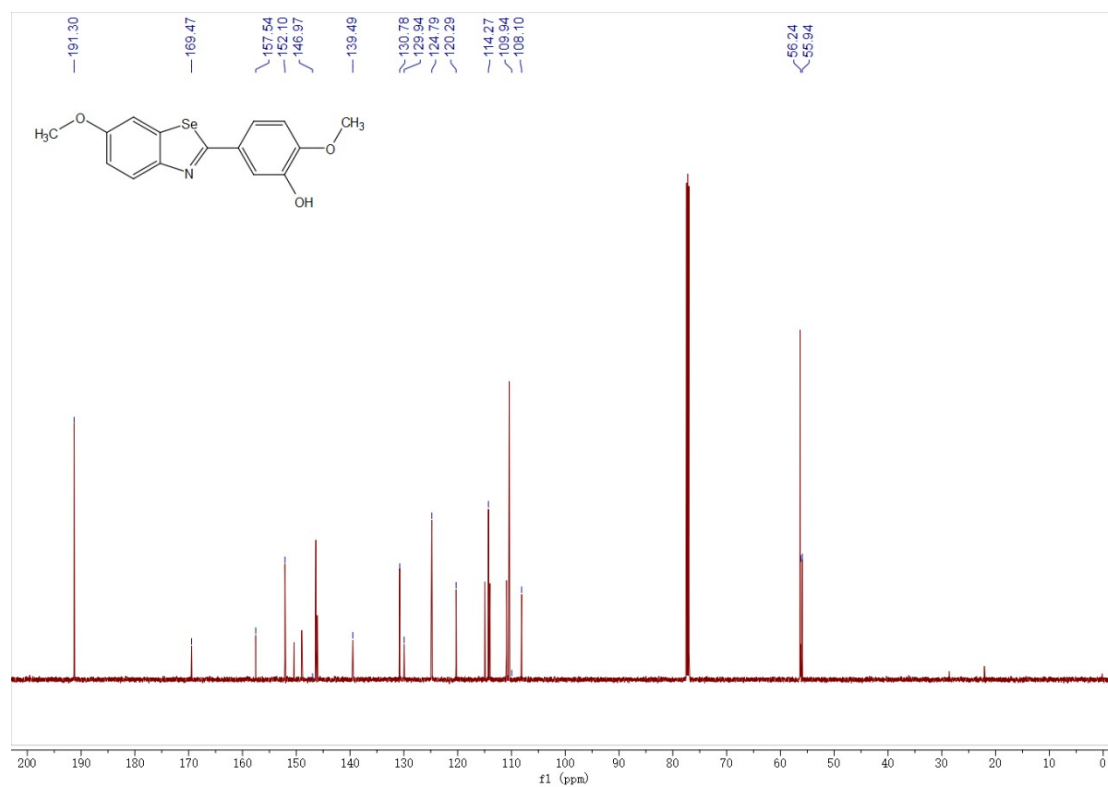


Figure S14. ¹³C NMR of 18.

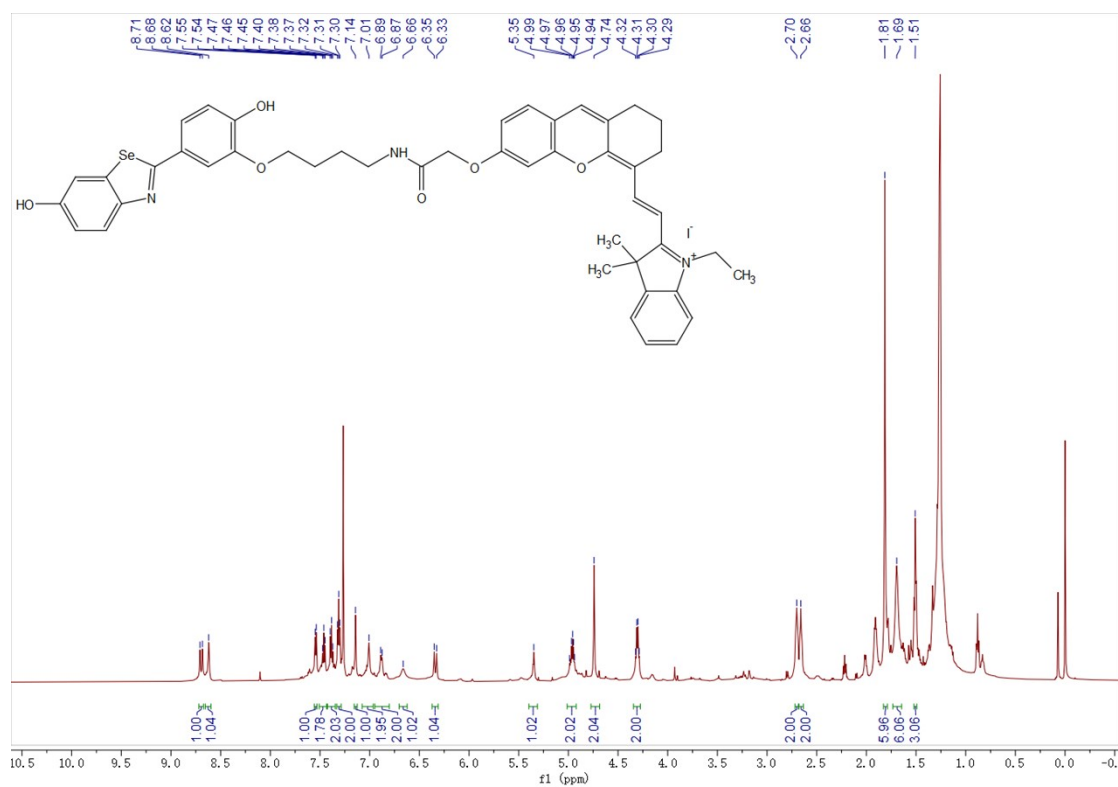
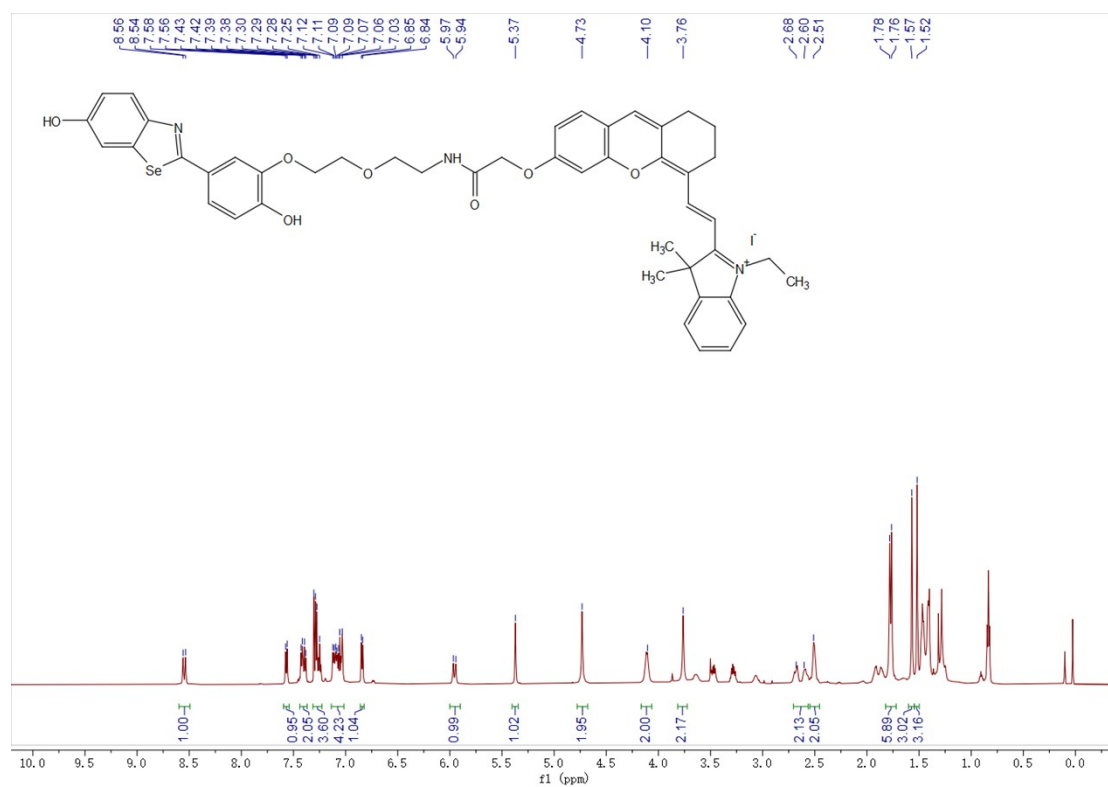
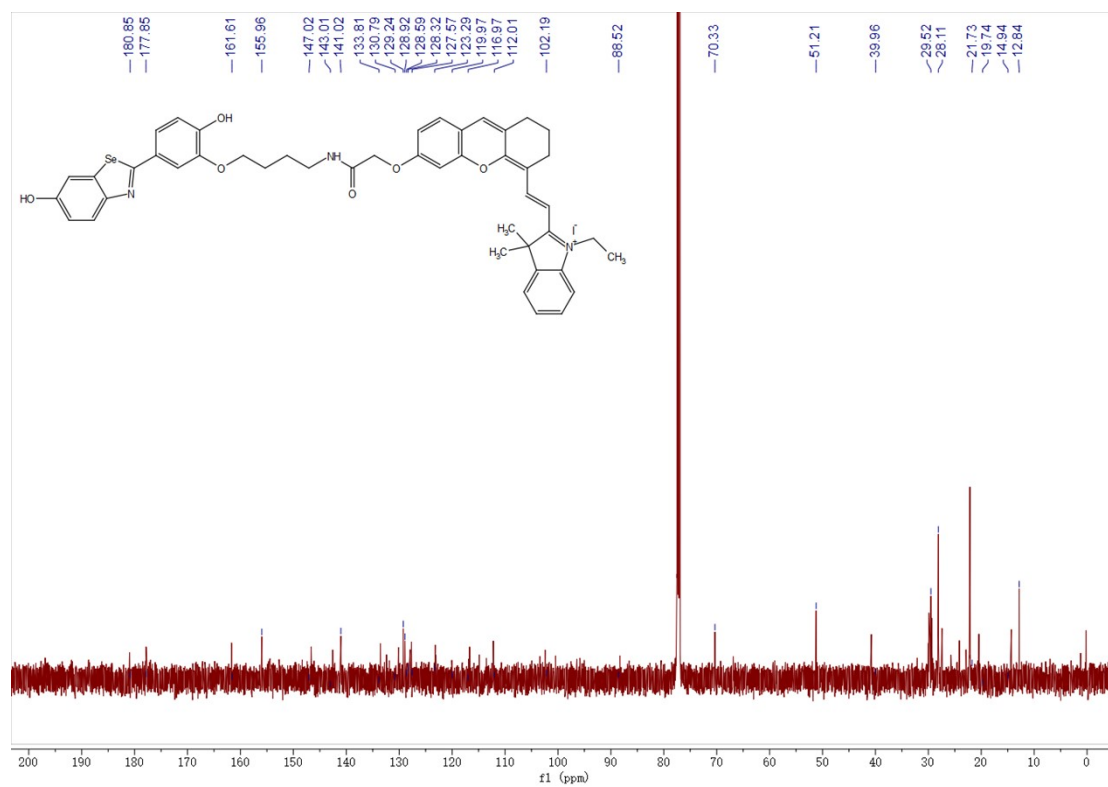


Figure S15. ¹H NMR of D1.



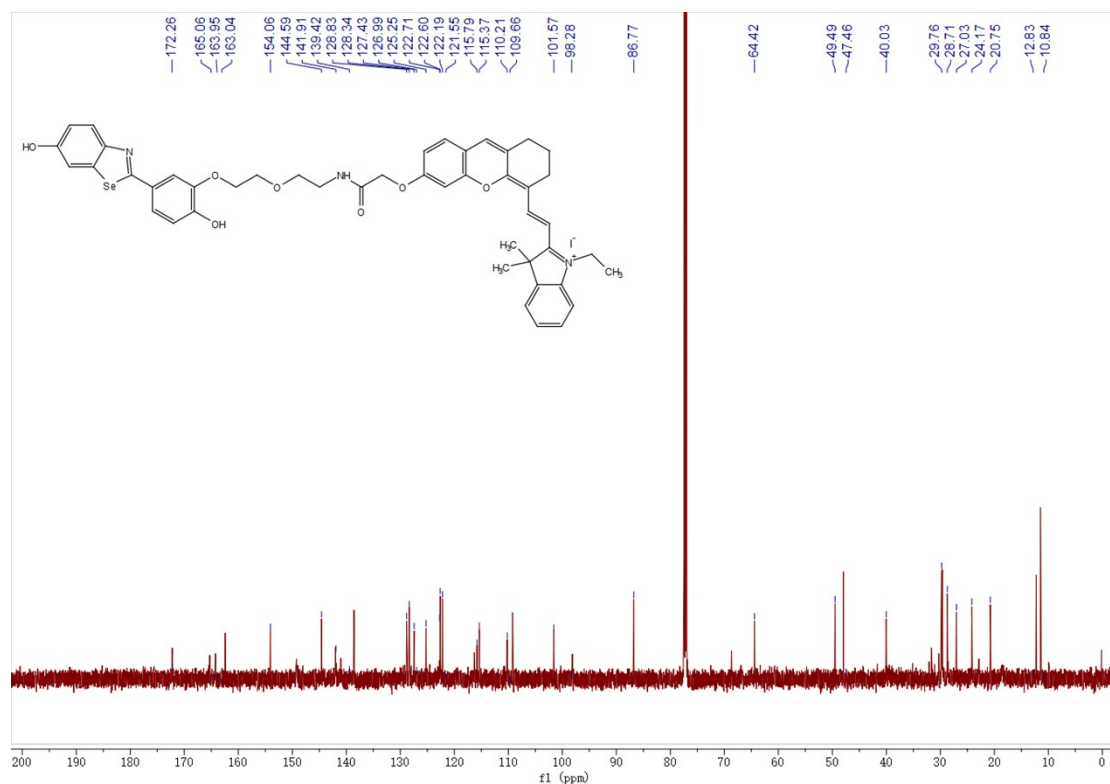


Figure S18. ^{13}C NMR of D2.

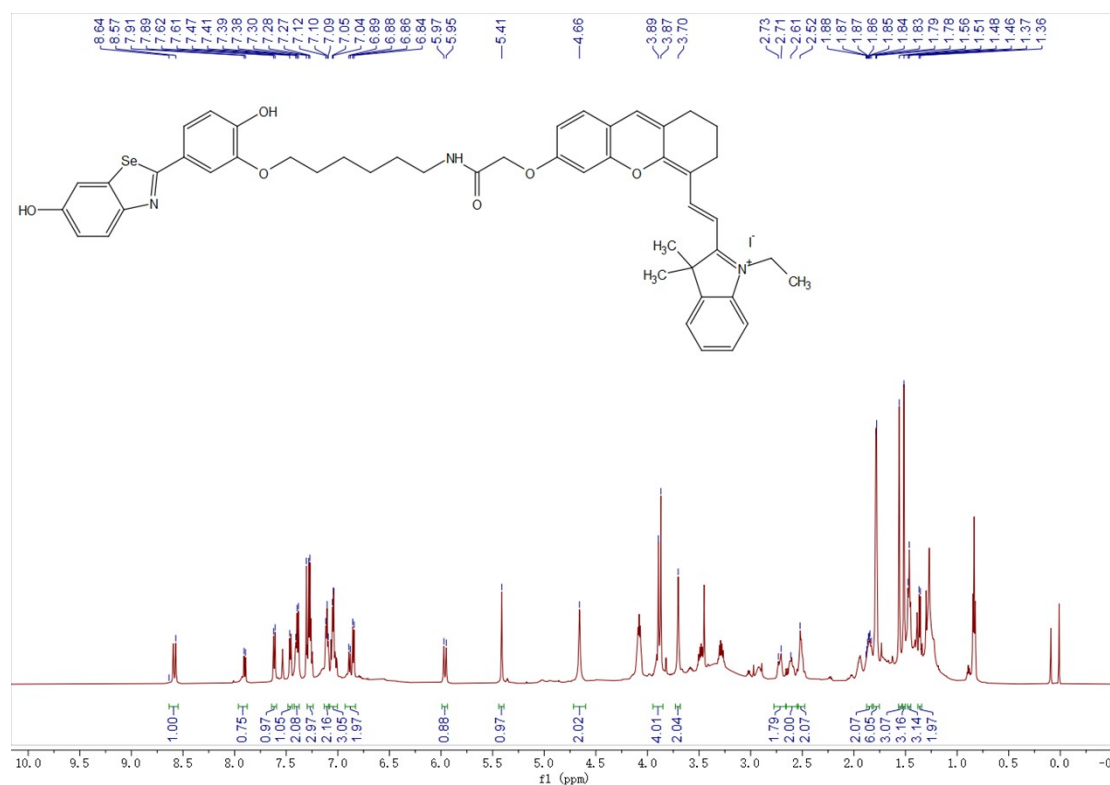


Figure S19. ^1H NMR of D3.

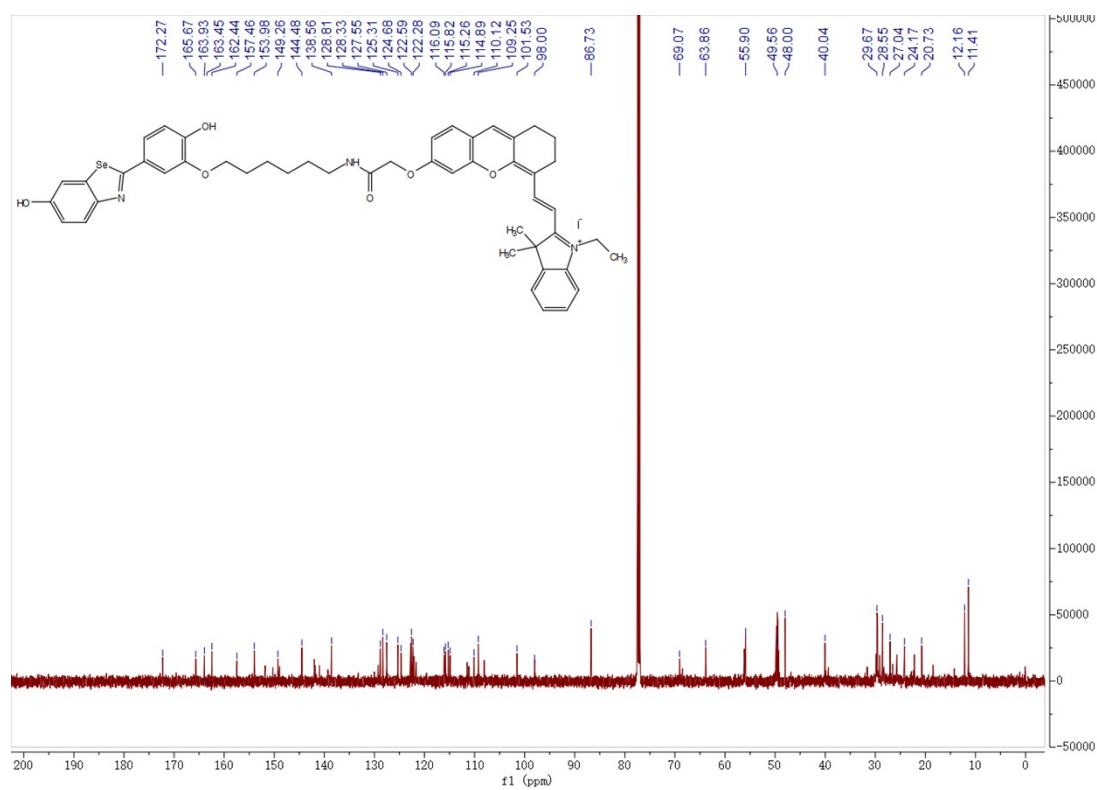


Figure S20. ¹³C NMR of D3.

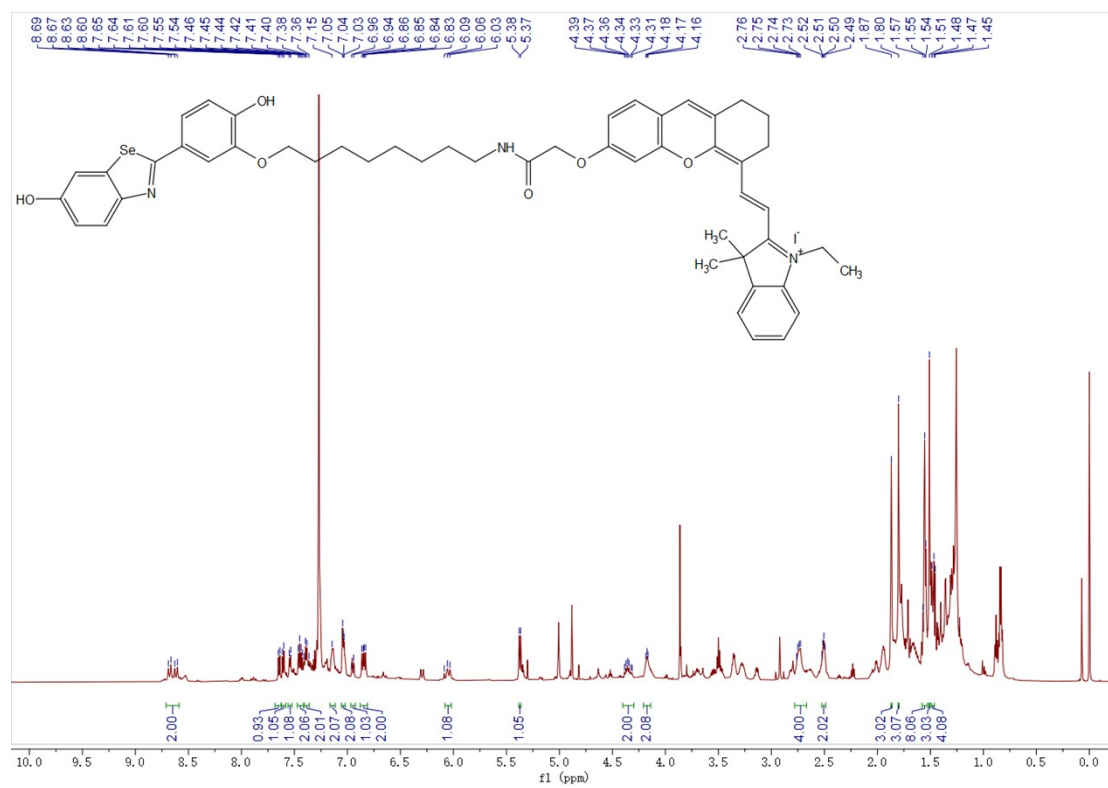


Figure S21. ¹H NMR of D4.

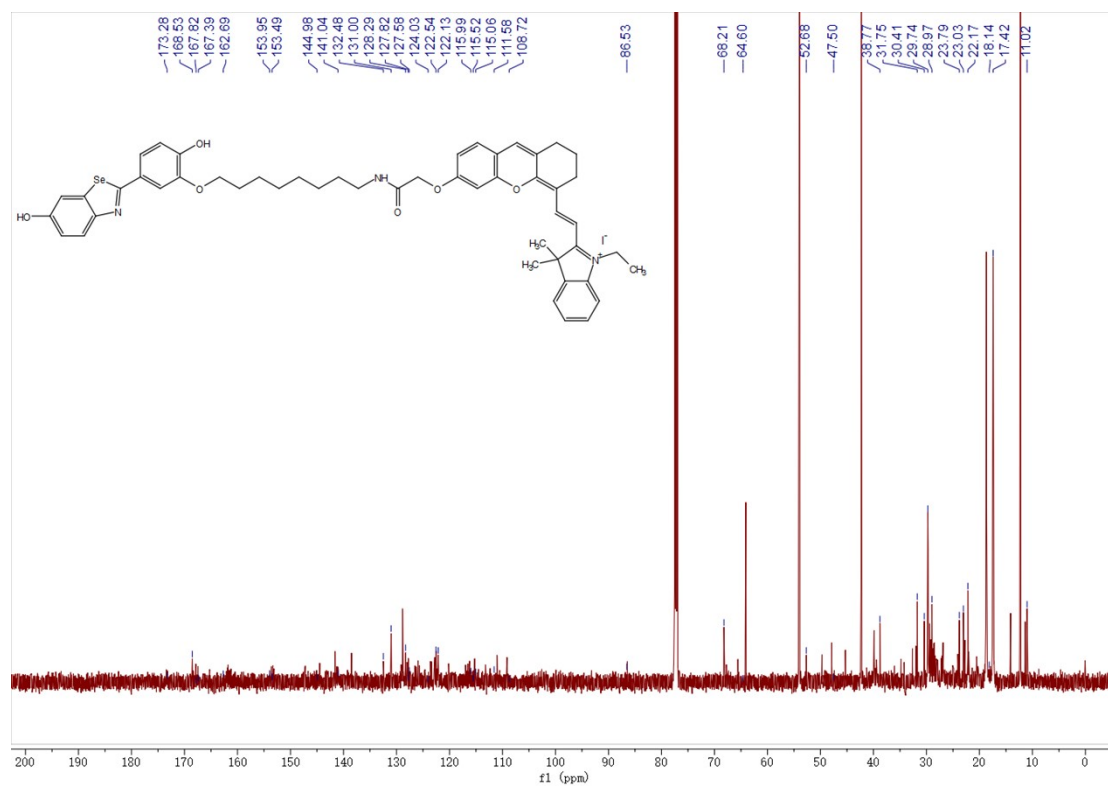
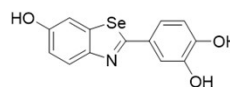


Figure S22. ¹³C NMR of D4.

4. High-resolution mass spectra of probes.

Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

217 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

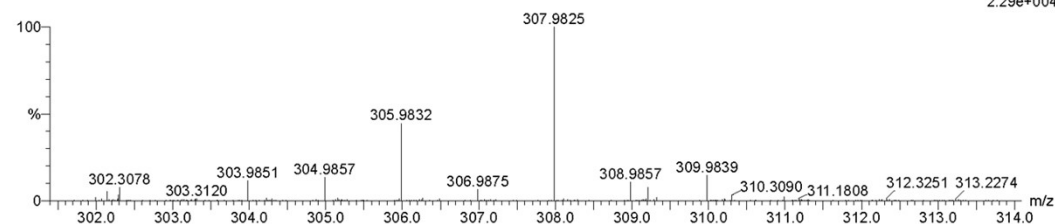
Elements Used:

C: 13-13 H: 10-10 N: 0-100 O: 0-100 Se: 1-1 Na: 0-1

27

240705-1-D-2 31 (0.219)

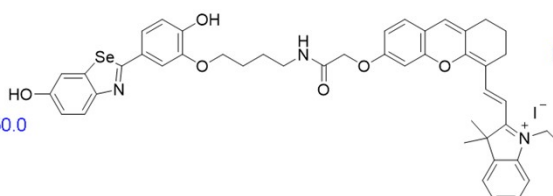
1: TOF MS ES+
2.29e+004



Minimum:				-1.5					
Maximum:	5.0	10.0		50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula	
307.9825	307.9826	-0.1	-0.3	10.5	403.2	n/a	n/a	C13 H10 N O3 Se	

Figure S23. HMRS spectra of ZSL-V5n.

Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2035 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

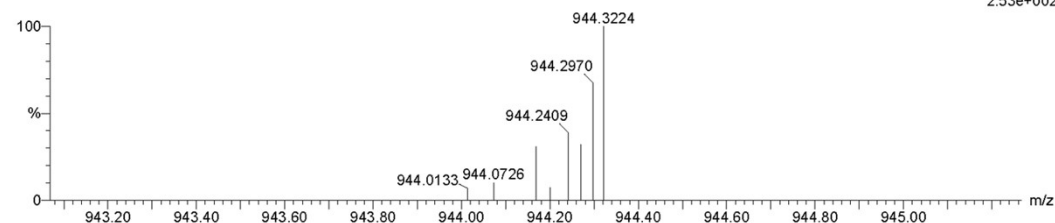
Elements Used:

C: 46-46 H: 47-47 N: 0-100 O: 0-100 Se: 1-1 I: 1-2

27

240705-1-D-3 21 (0.147)

1: TOF MS ES+
2.53e+002



Minimum:				-1.5					
Maximum:	5.0	10.0		50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula	
944.1679	944.1675	0.4	0.4	25.5	68.3	n/a	n/a	C46 H47 N3 O6 Se I	

Figure S24. HMRS spectra of D1.

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4117 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

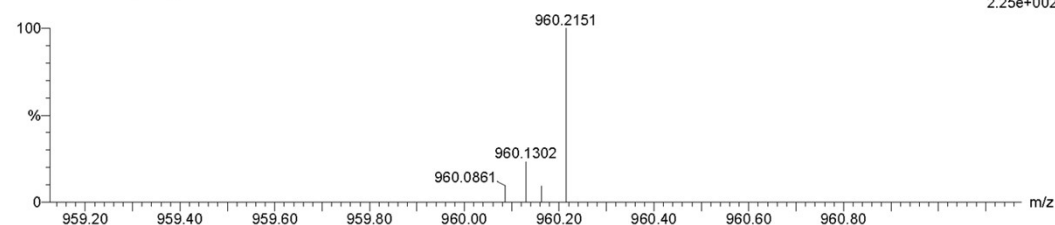
Elements Used:

C: 46-46 H: 47-47 N: 0-100 O: 0-100 Na: 0-1 Se: 1-1 I: 1-2

27

240705-1-D-4 42 (0.277)

1: TOF MS ES+
2.25e+002



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
960.1631	960.1624	0.7	0.7	25.5	31.3	n/a	n/a	C46 H47 N3 O7 Se I

Figure S25. HMRS spectra of D2.

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4288 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

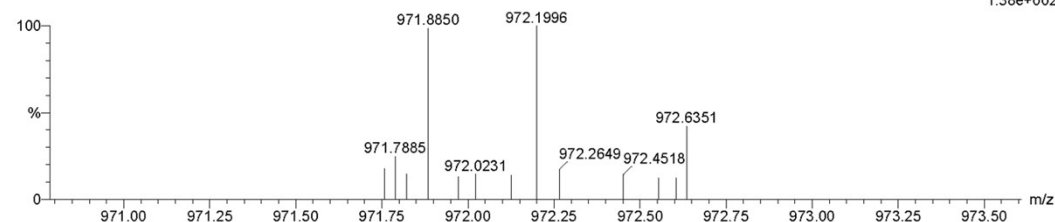
Elements Used:

C: 48-48 H: 51-51 N: 0-100 O: 0-100 Na: 0-1 Se: 1-1 I: 1-2

27

240705-1-D-5 57 (0.355)

1: TOF MS ES+
1.38e+002



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
972.1996	972.1988	0.8	0.8	25.5	56.3	n/a	n/a	C48 H51 N3 O6 Se I

Figure S26. HMRS spectra of D3.

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4635 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

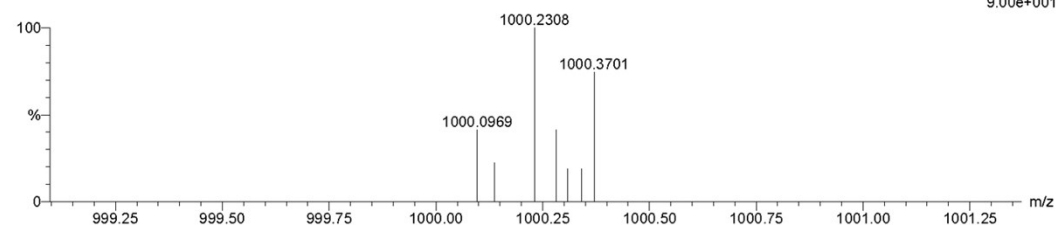
Elements Used:

C: 50-50 H: 55-55 N: 0-100 O: 0-100 Na: 0-1 Se: 1-1 I: 1-2

27

240705-1-D-6 31 (0.219)

1: TOF MS ES+
9.00e+001



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1000.2308	1000.2301	0.7	0.7	25.5	50.7	n/a	n/a	C50 H55 N3 O6 Se I

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