Supporting Information

Multiple Non-covalent Interactions Directed Supramolecular Double Helices: The Orthogonality of Hydrogen, Halogen and Chalcogen Bonding

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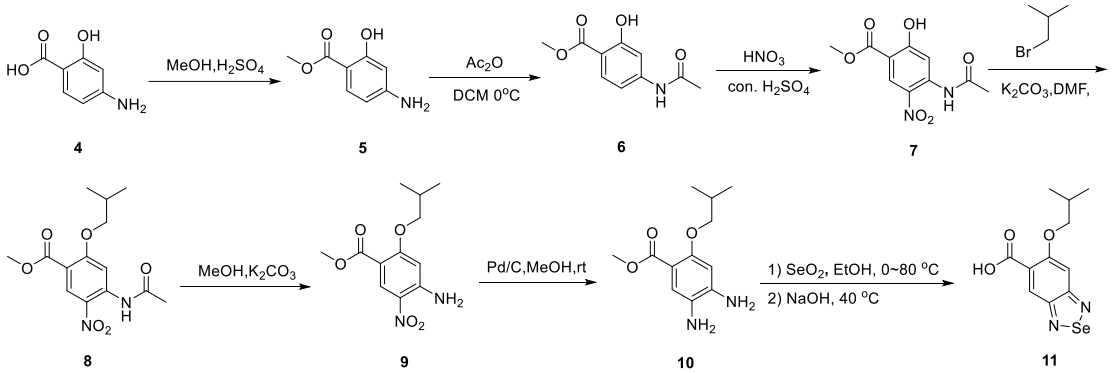
Contents

General methods. All reagents were obtained from commercial suppliers and used without further purification unless otherwise noted. ^{1}H and ^{13}C NMR spectra were recorded with a 400 MHz or 100 MHz spectrometer in the indicated solvents at 25 °C. Chemical shifts are expressed in parts per million (δ) using residual proton resonances of the deuterated solvents as the internal standards. Crystals were measured using Bruker D8 Venture-Metaljet diffractometer equipped with an PHOTON II area detector and HELIOS multilayer optics monochrommated Cu-K alpha radiation (lambda = 1.54184). Crystal structures were solved by direct method and refined by full-matrix least-squares methods based on F2 using SHELXL-2018 software. Co-crystals of **1** and **2** were grown by evaporating their solution of dichloromethane, n-hexane and dimethyl sulfoxide (*V*:*V* = 5:1:0.01). Crystals of solvate **3** was grown by evaporation of the same mixed solvent as co-crystal of **1** and **2**. CCDC (Nos. 2344590, 2344598) contains the related crystallographic data, which can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Compound 5. To a mixture of compound **4** (30 g, 1.96 mol) in anhydrous methanol (100 mL) was added concentrated H_2SO_4 (10 mL) by dropwise. The mixture was heated to reflux and stirred at this temperature for 12 hours. Then water (100 mL) was added to quench to reaction. The aqueous was treated with saturated $NaHCO_3$ solution by dropwise to adjust the pH to 7-8 (The addition of $NaHCO_3$ solution must be slowly to prevent excessive bubbles from overflowing in a short time). Then the solution was extracted with EtOAc (3*100 mL). The combined organic phase was washed with saturated sodium chloride solution (100 mL) and fresh water (100 mL) in sequence. Then the organic phase was dried and concentrated to get crude brown solid. The crude product was further purified by recrystallization to get the pure product (28 g, 86%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 8.36 (s, 8H), 7.42 (d, J = 8.4 Hz, 8H), 7.11 (d, J = 8.8 Hz, 8H), 2.08 (s, 24H). This compound was known.[1]

Compound 6. To a solution of compound **5** (5 g, 29.9 mmol) in anhydrous DCM (250 mL) at 0^{o}C was added Ac_2O (9.15 g, 89.7 mmol). The mixture was stirred for 5 hours at room temperature. Then the solvent was evaporated under reduced pressure, and the solid residue was slurry in water (20 mL). The isolated product was recrystrallized from methanol/water (2:1) to provide compound **6** (5.6 g, 90%) as a white solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 10.13 (s, 1H), 7.09 (s, 1H), 6.83-6.75 (m, 2H), 3.86 (s, 3H), 3.37 (s, 2H). This compound was known.[2]

Compound 7. To a solution of compound **6** (5.6 g, 26.8 mmol) in Ac_2O (50 mL) was

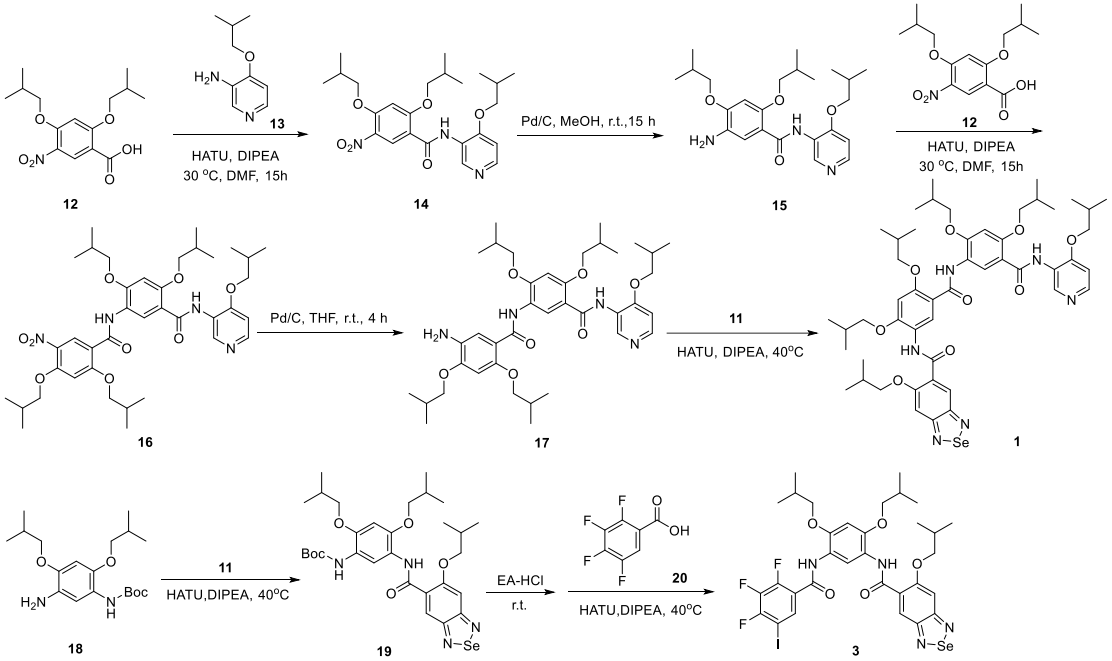
added con. HNO_3 (10 mL) by dropwise at 0°C. Then the solution was warmed to room temperature and stirred for 1 hour. Then the mixture was poured into ice-water (50 mL), and extracted with EtOAc (3*60 mL). The combined organic phase was washed with saturated $NaHCO_3$ (3*100 mL) and water (100 mL) in sequence. Then the organic phase was dried and concentrated. The residue was purified by column chromatography (petroleum ether and ethyl acetate, 5:1 to 2:1), the product was obtained as a yellow solid (4.9 g, 59%). ^{1}HNMR (400 MHz, DMSO-d_6): δ 11.17 (s, 1H), 10.27 (s, 1H), 8.47 (d, J = 2.8 Hz, 1H), 8.28 (d, J = 2.8 Hz, 1H), 3.94 (s, 3H), 2.05 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.14, 167.94, 149.19, 138.07, 131.20, 126.09, 120.82, 117.39, 53.61, 24.26. HR-MS (ESI): Calcd for $C_{10}H_{10}N_2NaO_6$ $[M+Na]^+$: 277.0437. Found: 277.0436.

Compound 8. To a solution of compound **7** (4.9 g, 19.3 mmol) in DMF (100 mL) was added 1-bromo-2-methylpropane (5.3 g, 38.6 mmol) and K_2CO_3 (5.3 g, 38.6 mmol). The mixture was heated to 80°C and stirred at this temperature for 15 hours. Then water (100 mL) was added to quench the reaction. The aqueous was extracted with EtOAc (3*100 mL) and the combined organic phase was washed (with fresh water for several times to remove residual DMF), dried and concentrated. The residue was purified by column chromatography (petroleum ether and ethyl acetate, 3:1 to 1:1), the pure product was obtained as a white solid (4.4 g, 73%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 10.88 (s, 1H), 8.83 (s, 1H), 8.55 (s, 1H), 3.93 (d, J = 6.4 Hz, 2H), 3.91 (s, 3H), 2.33 (s, 3H), 2.23-2.16 (m, 1H), 1.08 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.65, 164.56, 164.06, 139.94, 131.18, 128.03, 114.58, 103.59, 75.93, 52.23, 28.18, 25.94, 19.04. HR-MS (ESI): Calcd for $C_{14}H_{18}N_2NaO_6$ $[M+Na]^+$: 333.1063. Found: 333.1058.

Compound 9. To a solution of compound **8** (4.4 g, 14.2 mmol) in MeOH (50 mL) was added K_2CO_3 (3.9 g, 28.4 mmol). The solution was stirred at room temperature for 15 hours. After that, the solvent was removed under reduced pressure, the residue was dissolved in H_2O (50 mL) and EtOAc (50 mL). Then the EtOAc phase was separated and the aqueous phase was extracted with EtOAc (2*50 mL). The combined organic phase was dried with $NaSO_4$, and concentrated to get the yellow product (2.1 g, 55%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 8.78 (s, 1H), 6.50 (s, 2H), 6.16 (s, 1H), 3.86 (s, 3H), 3.78 (d, J = 6.4 Hz, 2H), 2.21-2.14 (m, 1H), 1.07 (d, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.50, 164.09, 148.94, 132.72, 125.64, 110.57, 98.90, 75.52, 51.88, 28.19, 19.08. HR-MS (ESI): Calcd for $C_{12}H_{16}N_2NaO_5$ $[M+Na]^+$: 291.0957. Found: 291.0954.

Compound 10. A mixture of compound **9** (2.1 g, 7.84 mmol) and Pd/C (210 mg) in MeOH (50 mL) under H_2 was stirred at room temperature for 4 hours. Then the mixture was filtered and the filtrated was concentrated to get crude product, and the crude product was purified by column chromatography (petroleum ether and ethyl acetate, 10:1 to 5:1) to get pure product as a brown solid (1.3 g, 70%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 7.32 (s, 1H), 6.27 (s, 1H), 3.83 (s, 3H), 3.69 (d, J = 6.4 Hz, 2H), 2.15-2.08 (m, 1H), 1.04 (d, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.77, 155.87, 142.77, 125.46, 121.93, 109.28, 100.97, 76.01, 51.43, 28.49, 19.27. HR-MS (ESI): Calcd for $C_{12}H_{18}N_2NaO_3$ $[M+Na]^+$: 261.1215. Found: 261.1220.

Compound 11. To a solution of compound **10** (2.0 g, 8.4 mmol) in EtOH (50 mL) at 0°C was added SeO_2 (0.93 g, 8.4 mmol). The solution was heated to 80°C and stirred at this temperature for 5 hours. Then the mixture was cooled to rt. NaOH (0.67 g, 16.8 mmol) in H_2O (10 mL) was added. The solution was reheated to 40°C and stirred at this temperature for 2 hours. Then the solvent was removed under reduced pressure, the residue was adjusted the pH to 3-4 with dilute hydrochloric acid (1 N). The precipitate was filtered and the yellow filter was product (2.2 g, 88%). ^{1}HNMR (400 MHz, DMSO-d_6): δ 13.33 (s, 1H), 7.93 (s, 1H), 7.20 (s, 1H), 3.91 (d, J = 6.4 Hz, 2H), 2.11-2.05 (m, 1H), 1.02 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.34, 160.85, 157.40, 155.90, 131.68, 122.83, 100.86, 74.99, 28.06, 19.40. HR-MS (ESI): Calcd for $C_{11}H_{12}N_2NaO_3Se$ $[M+Na]^+$: 322.9911. Found: 322.9908.



Compound 14. A mixture of compound **13** (2.8 g, 16.8 mmol), compound **12** (4.3 g, 14.0 mmol), HATU (8.0 g, 21.0 mmol), and DIPEA (5.4 g, 42.0 mmol) in DMF (20 mL) was stirred at 30 °C for 15 h. Then water (60 mL) was added to quench to reaction. The aqueous was extracted with DCM (3*50 mL). The combined organic phase was washed with saturated sodium chloride solution (100 mL) and water (100 mL) in sequence. Then the organic phase was dried and concentrated to get crude product. The curde product was removed and the residue was purified by column chromatography (DCM/MeOH =20/1) to afford compound **14** (4.1 g, 64%) as a brown solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.52 (s, 2H), 8.89 (s, 1H), 8.29 (d, J =7.2 Hz, 1H), 6.84 (d, J =7.2 Hz, 1H), 6.55 (s, 1H), 4.06 (d, J =8.8 Hz, 2H), 3.92-3.90 (m, 4H), 2.32-2.10 (m, 3H), 1.11-1.02 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.26, 160.82, 156.85, 154.27, 146.47, 143.56, 133.57, 131.40, 124.88, 114.43, 106.67, 98.05, 76.15, 75.01, 28.30, 28.06, 27.85, 19.23, 19.11, 19.07. HR-MS (ESI): Calcd for $C_{24}H_{34}N_3O_6$ $[M+H]^+$: 460.2448. Found: 460.2447.

Compound 15. A mixture of compound **14** (4.0 g, 8.7 mmol) and Pd/C (400 mg) in MeOH (50 mL) under H_2 atmosphere was stirred at rt for 15 h. Then the mixture was filtered with celite, the filtrated was concentrated, the residue was purified by cloumn

chromatography (DCM/MeOH =20/1) to afford compound **15** (3.2 g, 86%) as a brown solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.96 (s, 1H), 9.60 (s, 1H), 8.25 (d, J =7.6 Hz, 1H), 7.59 (s, 1H), 6.82 (d, J =7.6 Hz, 1H), 6.46 (s, 1H), 3.91-3.87 (m, 4H), 3.81 (d, J =8.4 Hz, 2H), 3.68 (s, 2H), 2.22-2.10 (m, 3H), 1.09-0.99 (m, 18H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.67, 154.17, 150.80, 150.55, 145.73, 143.28, 130.75, 125.63, 117.31, 114.67, 106.51, 98.83, 77.72, 74.89, 74.85, 28.35, 28.19, 27.90, 19.33, 19.32, 19.14. HR-MS (ESI): Calcd for $C_{24}H_{36}N_3O_4$ $[M+H]^+$: 430.2706. Found: 430.2723.

Compound 16. A mixture of compound **15** (1.7 g, 3.96 mmol), compound **12** (1.23 g, 3.96 mmol), HATU (2.25 g, 5.94 mmol), and DIPEA (1.5 g, 11.88 mmol) in DMF (15 mL) was stirred at 30 ^{o}C for 15 h. Then water (50 mL) was added to quench to reaction. The aqueous was extracted with DCM (3*50 mL). The combined organic phase was washed with saturated sodium chloride solution (100 mL) and water (100 mL) in sequence. Then the organic phase was dried and concentrated to get crude product. The curde product was purified by column chromatography (DCM/MeOH =20/1) to afford compound **16** (1.6 g, 57%) as an off-white solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.68 (s, 1H), 9.62 (s, 1H), 9.28 (s, 1H), 8.86 (s, 1H), 8.81 (s, 1H), 8.24 (d, J =7.2 Hz, 1H), 6.81 (d, J =7.6 Hz, 1H), 6.54 (s, 2H), 4.04 (d, J =8.8 Hz, 2H), 3.95 (d, J =9.2 Hz, 2H), 3.90-3.85 (m, 6H), 2.27-2.07 (m, 5H), 1.08-1.01 (m, 30H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.01, 161.31, 160.95, 156.59, 155.01, 154.02, 153.96, 145.73, 143.19, 133.43, 131.31, 127.59, 125.59, 121.11, 114.94, 114.80, 106.50, 97.99, 97.91, 76.07, 75.41, 74.91, 28.29, 28.21, 28.14, 28.13, 27.88, 19.30, 19.28, 19.21, 19.15, 19.07. HR-MS (ESI): Calcd for $C_{39}H_{55}N_4O_9$ $[M+H]^+$: 723.3969. Found: 723.3979.

Compound 17. A mixture of compound **16** (1.3 g, 1.8 mmol) and Pd/C (130 mg) in THF (50 mL) under H_2 atmosphere was stirred at rt for 4 h, the mixture was filtered with celite, and the filtrated was concentrated, the residue was purified by column chromatography (DCM/MeOH =20/1) and Prep-TLC to afford compound **17** (902 mg, 72%) as an off-white solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.73 (s, 1H), 9.68 (s, 1H), 9.63 (s, 1H), 8.91 (s, 1H), 8.24 (d, J =7.2 Hz, 1H), 7.61 (s, 1H), 6.81 (d, J =7.6 Hz, 1H), 6.53 (s, 1H), 6.45 (s, 1H), 3.94 (d, J =8.8 Hz, 2H), 3.89-3.79 (m, 8H), 3.66 (s, 2H), 2.24-2.08 (m, 5H), 1.08-0.99 (m, 30H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.60, 163.23, 154.43, 153.99, 153.77, 150.79, 150.19, 145.63, 143.25, 130.62, 127.15, 125.69, 122.14, 117.60, 115.15, 115.04, 106.45, 98.91, 98.01, 77.72, 75.38, 74.87, 74.83, 28.37, 28.33, 28.25, 28.15, 27.90, 19.39, 19.33, 19.32, 19.25, 19.15. HR-MS (ESI): Calcd for $C_{39}H_{57}N_4O_7$ $[M+H]^+$: 693.4227. Found: 693.4228.

Compound 1. To a solution of compounds **11** (173 mg, 0.58 mmol) in DMF (20 mL) were added HATU (878 mg, 2.3 mmol) and DIPEA (0.4 mL). The mixture was stirred at room temperature for 20 mins. Then compound **17** (200 mg, 0.29 mmol) was added. The mixture was warmed to 40 ^{o}C and stirred for 12 hours. Then water (50 mL) was added to quench to reaction. The aqueous was extracted with DCM (3*50 mL). The combined organic phase was washed with saturated sodium chloride solution (100 mL) and water (100 mL) in sequence. Then the organic phase was dried and concentrated to get crude product. The crude product was purified by column chromatography (DCM/MeOH =20/1 to 25/1) to afford compound **1** (220 mg, 78%) as orange-yellow

solid. ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.75 (s, 1H), 9.69 (s, 1H), 9.46 (s, 1H), 9.19 (s, 1H), 8.88 (s, 2H), 8.62 (s, 1H), 8.23 (d, J =6.0 Hz, 1H), 7.19 (s, 1H), 6.92 (d, J =5.6 Hz, 1H), 6.57 (s, 2H), 4.03-3.95 (m, 8H), 3.88-3.86 (m, 4H), 2.31-2.10 (m, 6H), 1.08-1.02 (m, 36H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.22, 162.99, 162.23, 161.36, 157.56, 156.82, 155.32, 154.55, 154.38, 153.84, 144.86, 130.22, 127.51, 127.18, 127.12, 125.90, 121.91, 120.81, 115.39, 114.86, 106.62, 100.91, 97.95, 97.84, 76.13, 75.36, 75.33, 75.09, 28.27, 28.25, 28.13, 27.88, 27.85, 19.38, 19.33, 19.27, 19.23, 19.16. HR-MS (ESI): Calcd for $C_{50}H_{67}N_6O_9Se$ $[M+H]^+$: 975.4135. Found: 975.4126.

Compound 19. To a solution of compounds **11** (200 mg, 0.67 mmol) in DMF (10 mL) were added HATU (510 mg, 1.34 mmol) and DIPEA (259 mg, 2.01 mmol). The mixture was stirred at room temperature for 20 mins. Then compound **18** (259 mg, 0.74 mmol) was added. The mixture was warmed to 40 ^{o}C and stirred for 12 hours. Then water (100 mL) was added to quench to reaction. The aqueous was extracted with DCM (3*50 mL). The combined organic phase was washed with saturated sodium chloride solution (100 mL) and water (100 mL) in sequence. Then the organic phase was dried and concentrated to get crude product. The crude product was slurry in hexane (30 mL) and filtered to get compound **19** as orange-yellow solid (320 mg, 75%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.39 (s, 1H), 8.97 (s, 1H), 8.65 (s, 1H), 7.18 (s, 1H), 6.75 (s, 1H), 6.50 (s, 1H), 4.00 (d, J = 6.8 Hz, 2H), 3.76 (dd, J_1 = 6.8 Hz, J_2 = 1.6 Hz, 4H), 2.32-2.26 (m, 1H), 2.18-2.03 (m, 2H), 1.60 (s, 9H), 1.07-1.04 (m, 12H), 0.98 (d, J = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.73, 161.34, 157.57, 156.88, 152.94, 144.97, 130.51, 127.17, 121.43, 120.65, 114.22, 100.87, 98.32, 76.17, 76.16, 75.60, 28.41, 28.34, 28.33, 27.75, 19.36, 19.31, 19.24. HR-MS (ESI): Calcd for $C_{30}H_{42}N_4O_6NaSe$ $[M+Na]^+$: 657.2167. Found: 657.2169.

Compound 3. Compound **19** (279 mg, 0.44 mmol) was added to hydrochloride gas in ethyl acetate (30 mL) and the suspension was stirred for 1 hour and then concentrated to afford a residue. To a solution of compounds **20** (145 mg, 0.48 mmol) in DMF (10 mL) were added HATU (502 mg, 1.32 mmol) and DIPEA (0.7 mL). The mixture was stirred at room temperature for 20 mins. Then the previously obtained residue was added. The mixture was warmed to 40 ^{o}C and stirred for 12 hours. Then water (100 mL) was added to quench to reaction. The precipitated phase was filtered and recrystallized with EA (2 mL) and PE (20 mL) to get pure compound **3** as orange-yellow solid (285 mg, 79%). ^{1}HNMR (400 MHz, $CDCl_3$): δ 9.47-9.45 (m, 2H), 8.44 (d, J = 13.6 Hz, 1H), 8.69 (s, 1H), 8.51-8.46 (m, 1H), 7.20 (s, 1H), 6.56 (s, 1H), 4.03 (d, J = 6.4 Hz, 2H), 3.84-3.81 (m, 4H), 2.35-2.07 (m, 3H), 1.11-1.00 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.84, 161.39, 157.53, 157.27, 154.22, 151.70, 150.92, 148.52, 146.58, 145.65, 140.64, 140.47, 137.90 (t, J = 180 Hz), 135.08, 130.28, 127.38, 120.31, 120.02, 115.79, 100.95, 97.33, 76.20, 75.95, 75.43, 28.44, 28.34, 27.75, 19.34, 19.27, 19.23. ^{19}F NMR (300 MHz, $CDCl_3$): δ -106.3~-106.4 (m, 1F), -134.86~-134.94 (m, 1F), -155.0 (t, J = 17.1 Hz, 1F). HR-MS (ESI): Calcd for $C_{32}H_{34}N_4O_5NaF_3ISe$ $[M+Na]^+$: 841.0589. Found: 841.0582.

Reference

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S. Sun, *ACS Catal.* **2014**, *4*, 1777–1782.
[2] C. Wei, R. Wang, C. Zhang, G. Xu, Y. Li, Q. Z. Zhang, L. Y. Li, L. Yi, Z. Xi, *Chem-Asian J* **2016**, *11*, 1376–1381.

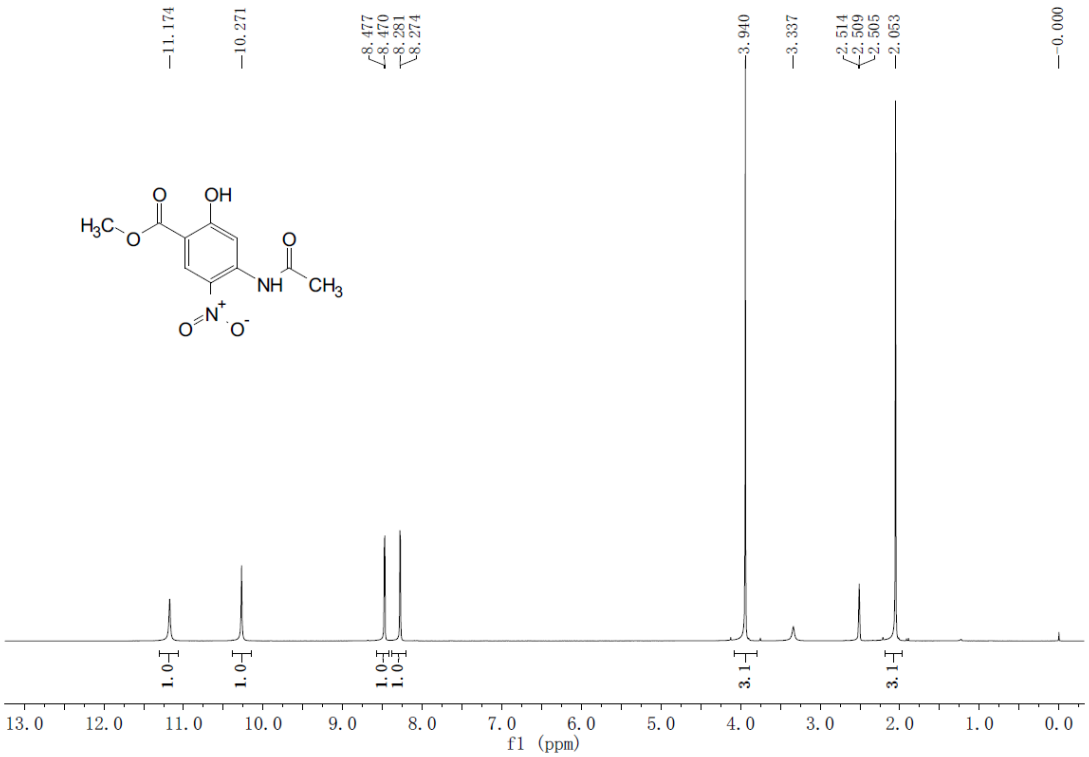


Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **7** at 25 °C.

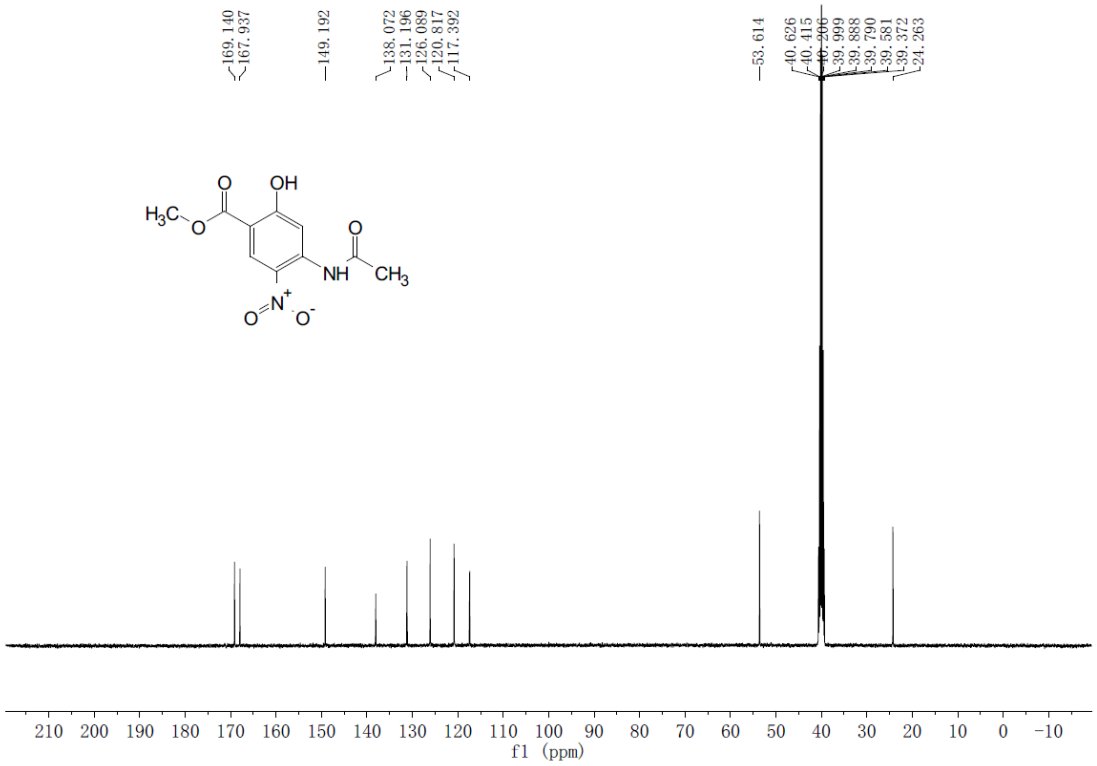


Figure S2. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **7** at 25 °C.

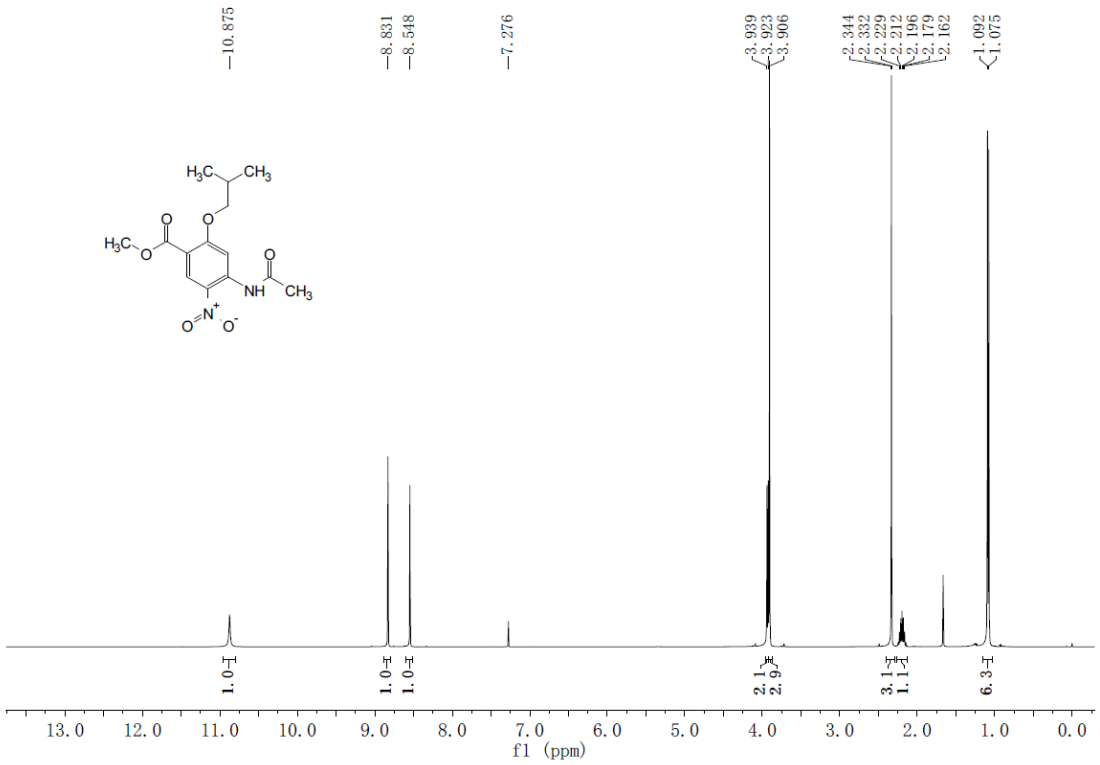


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8** at 25 °C.

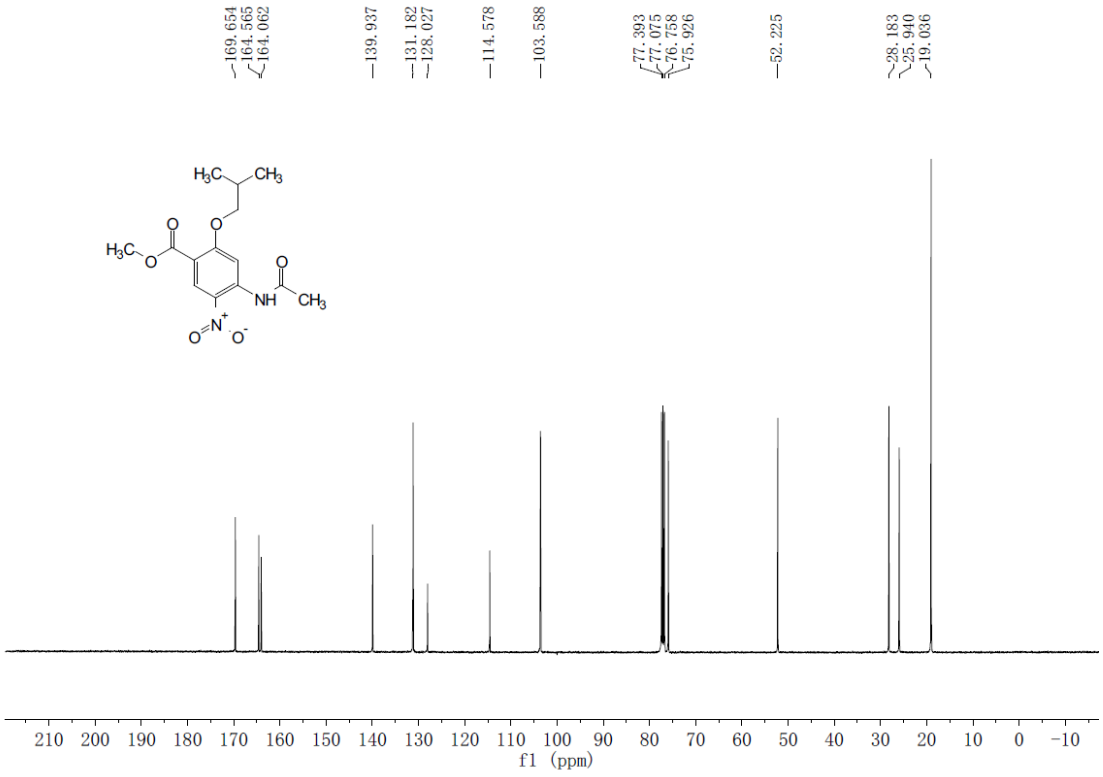


Figure S4. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8** at 25 °C.

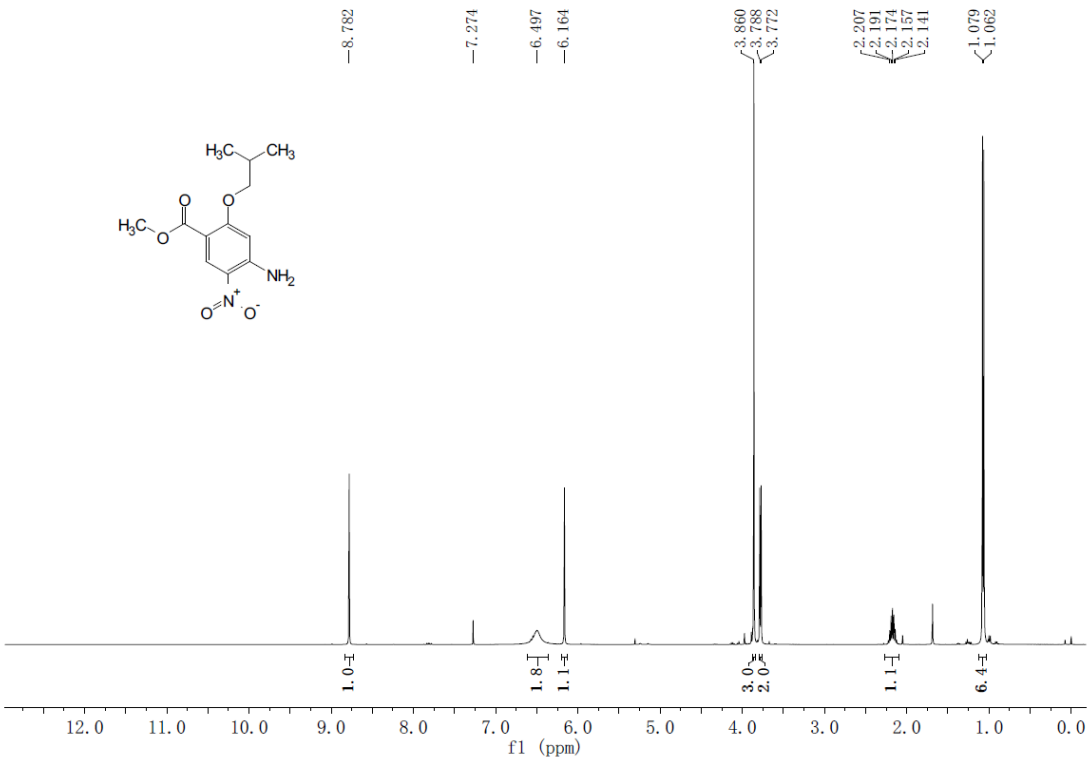


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9** at 25 °C.

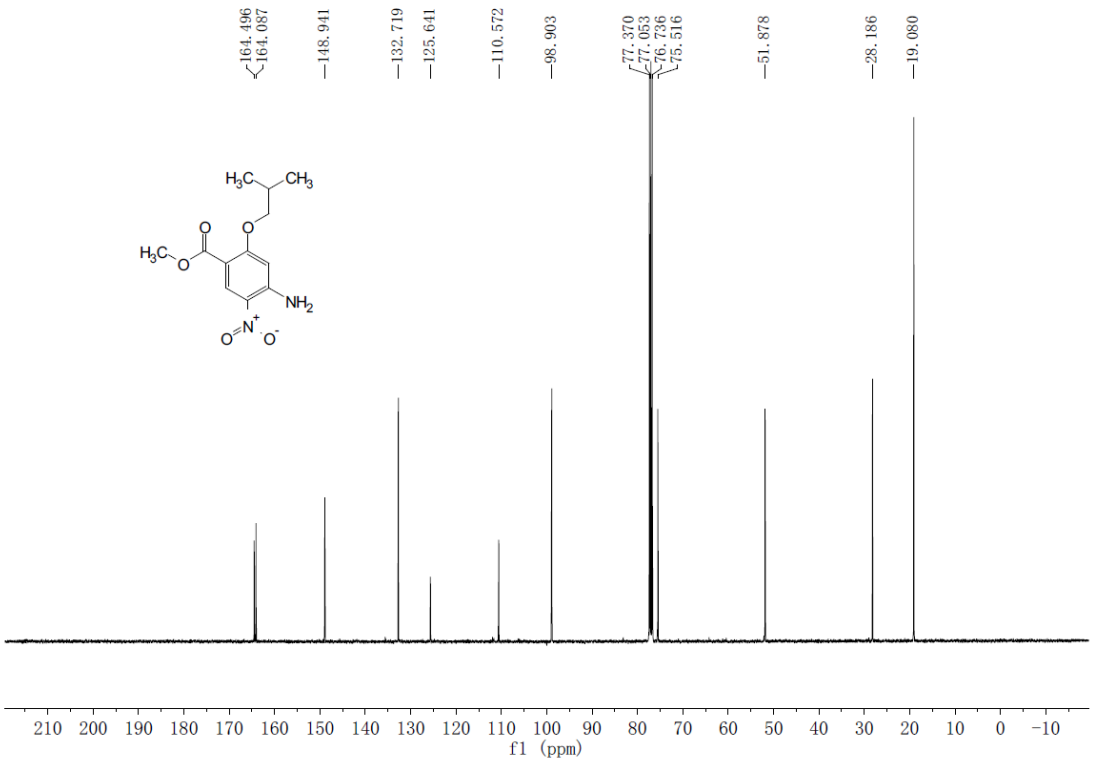


Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **9** at 25 °C.

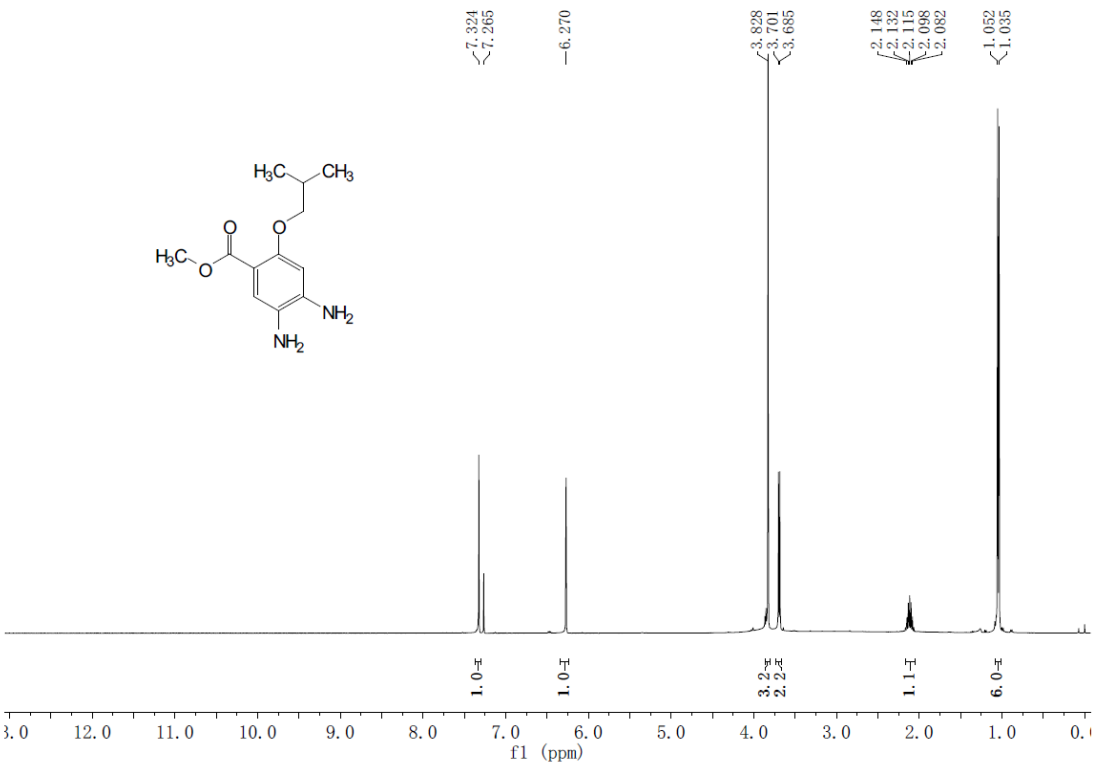


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10** at 25 °C.

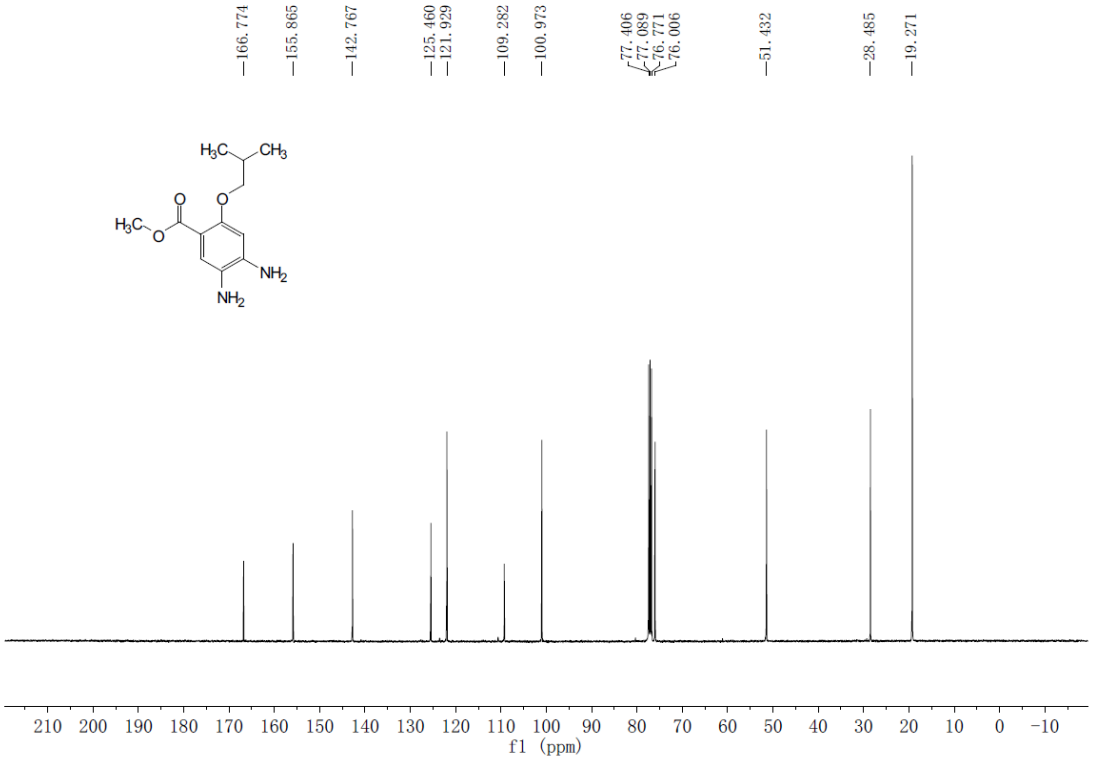


Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **10** at 25 °C.

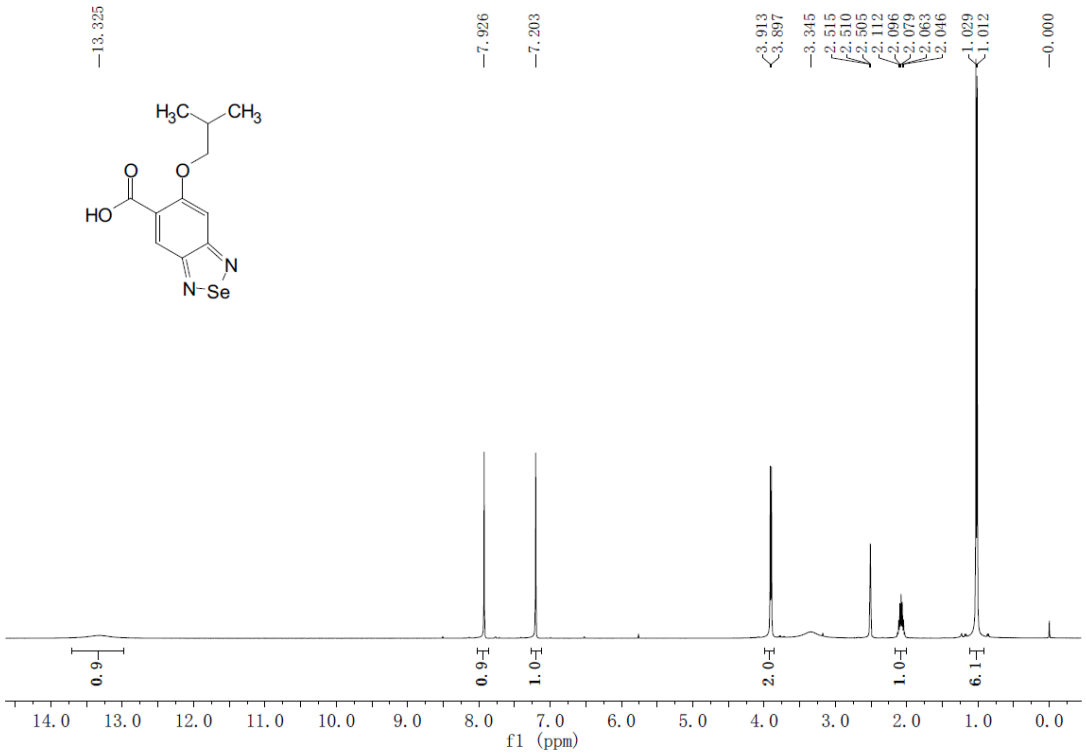


Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11** at 25 °C.

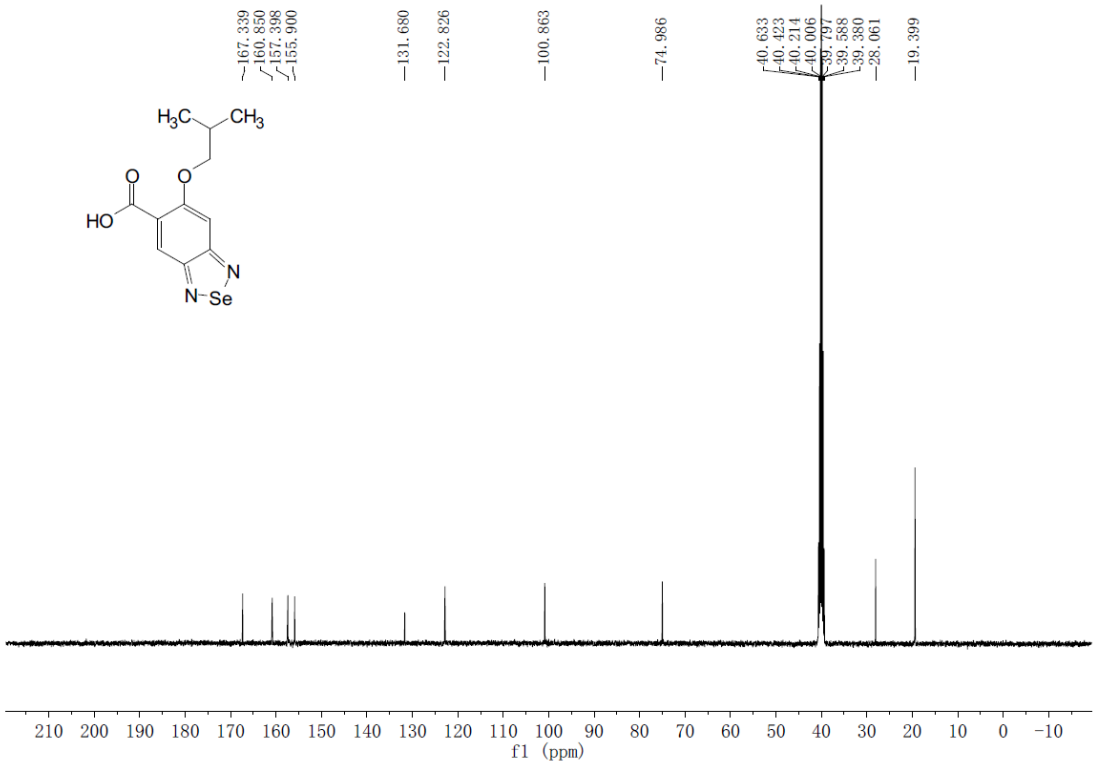


Figure S10. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **11** at 25 °C.

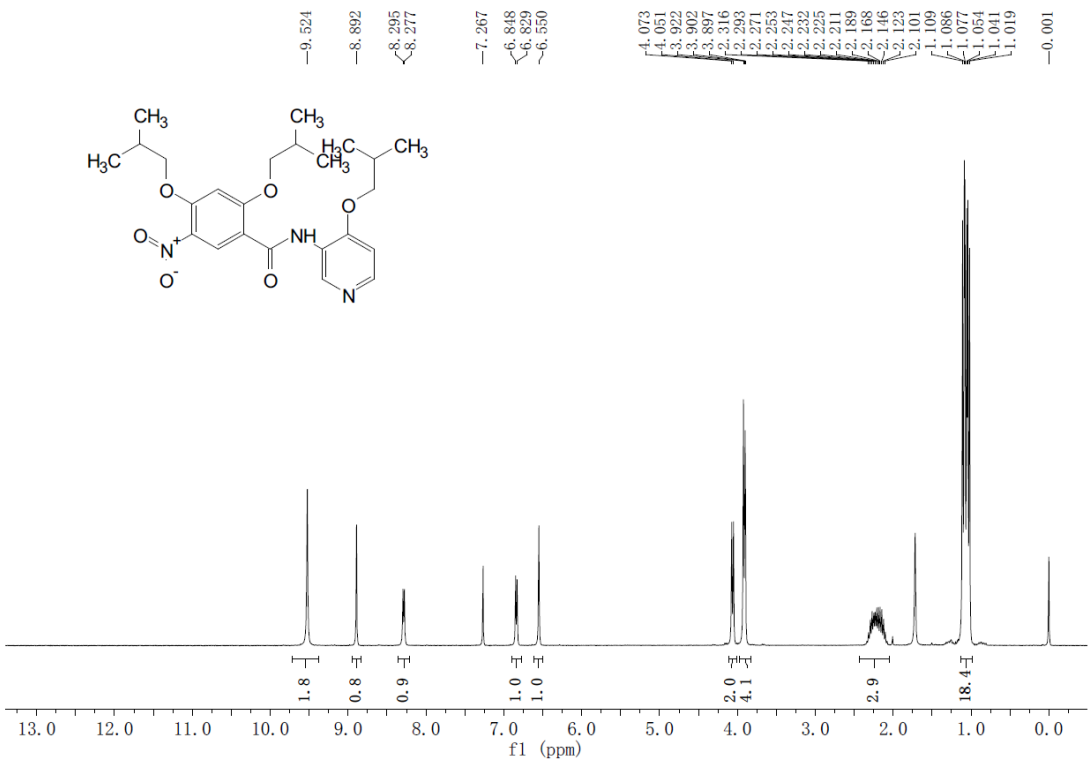


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **14** at 25 °C.

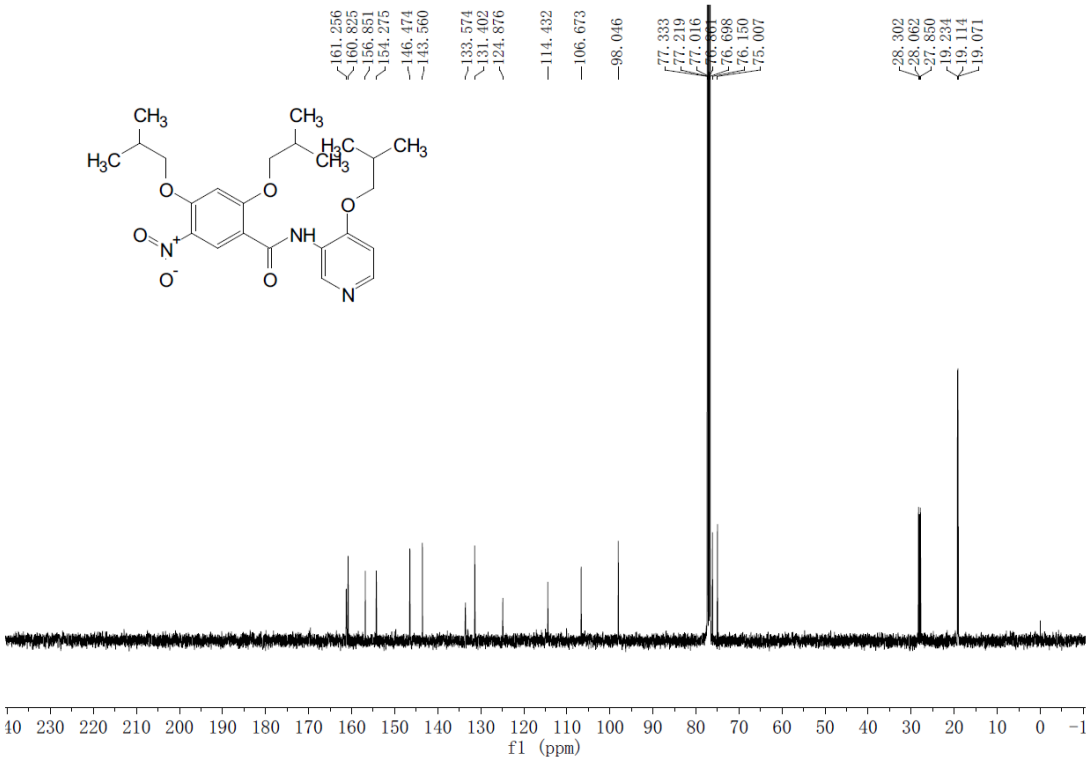


Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **14** at 25 °C.

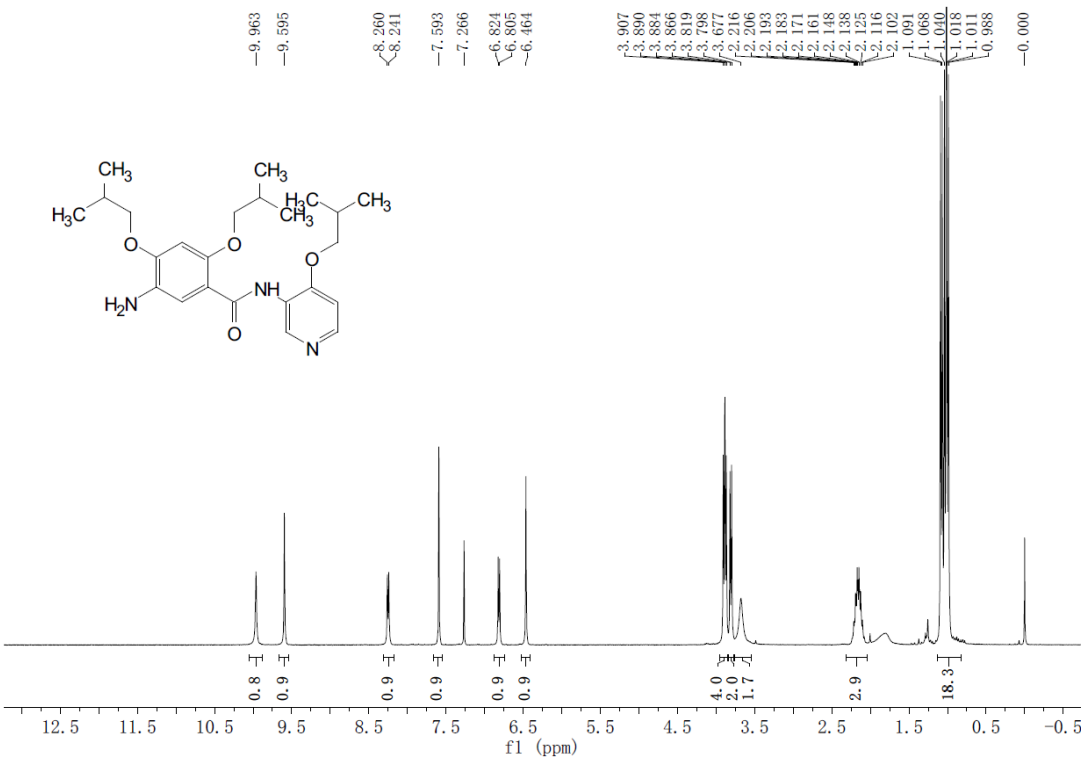


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **15** at 25 °C.

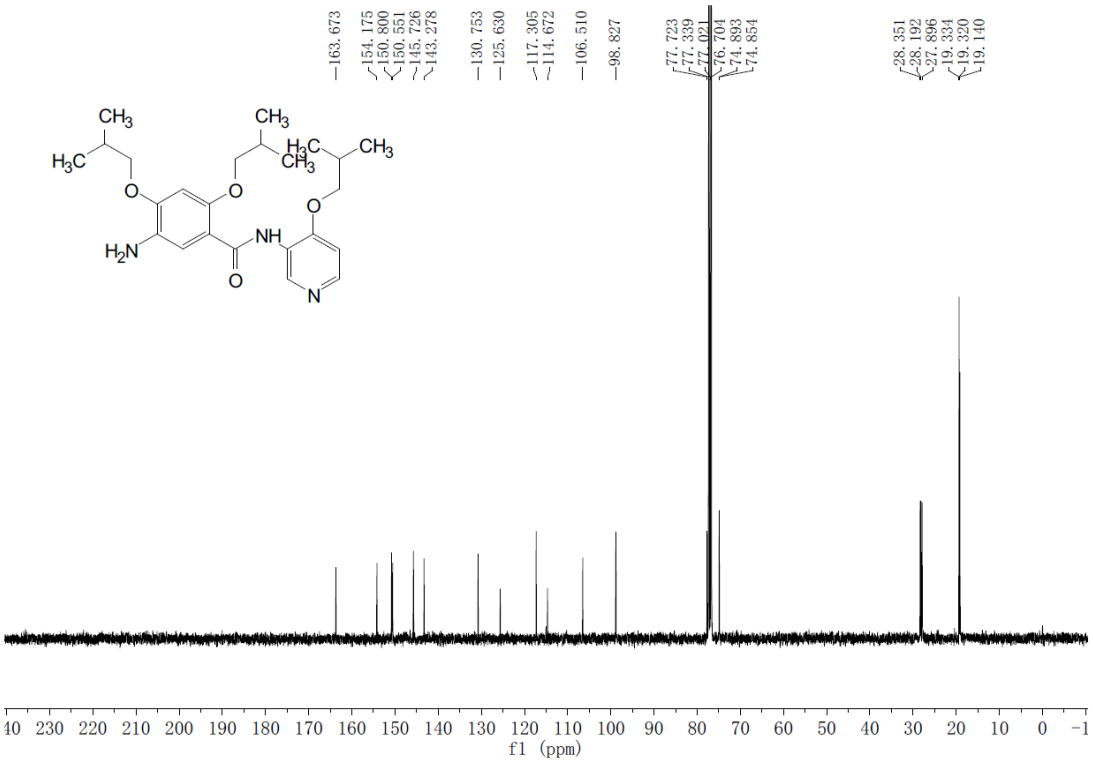


Figure S14. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **15** at 25 °C.

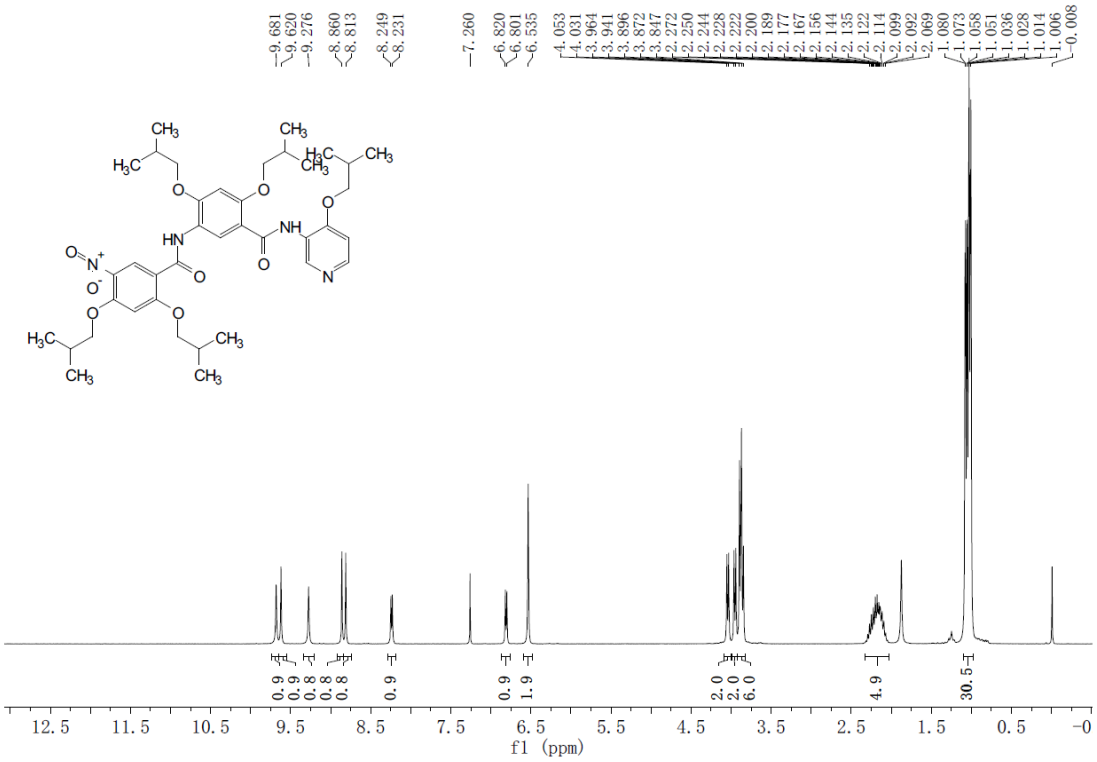


Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **16** at 25 °C.

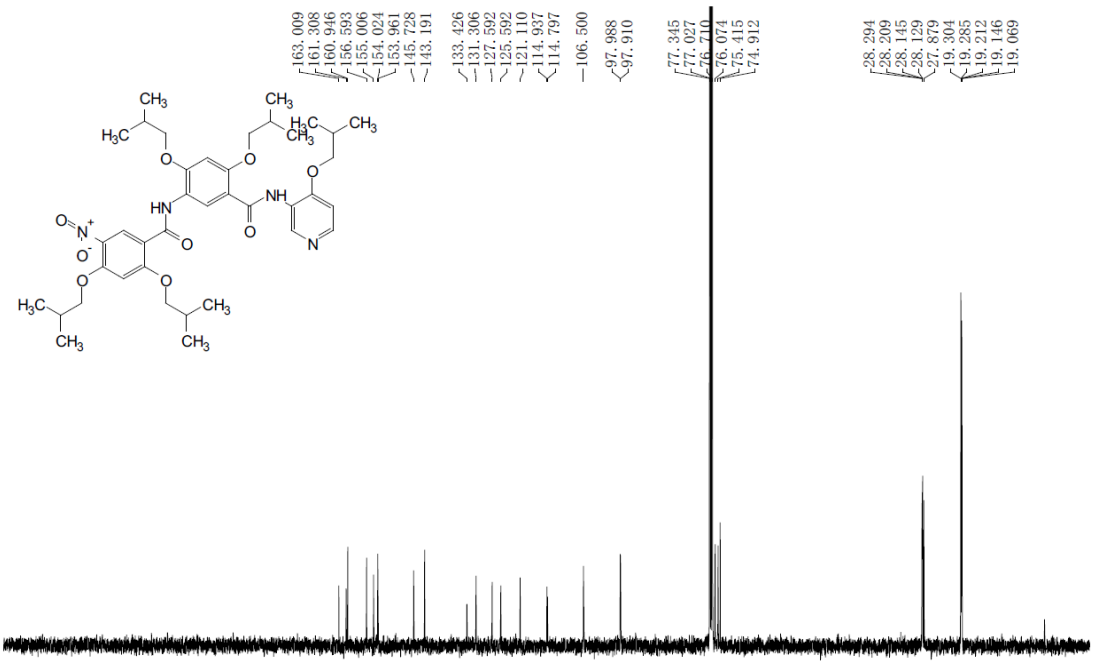


Figure S16. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **16** at 25 °C.

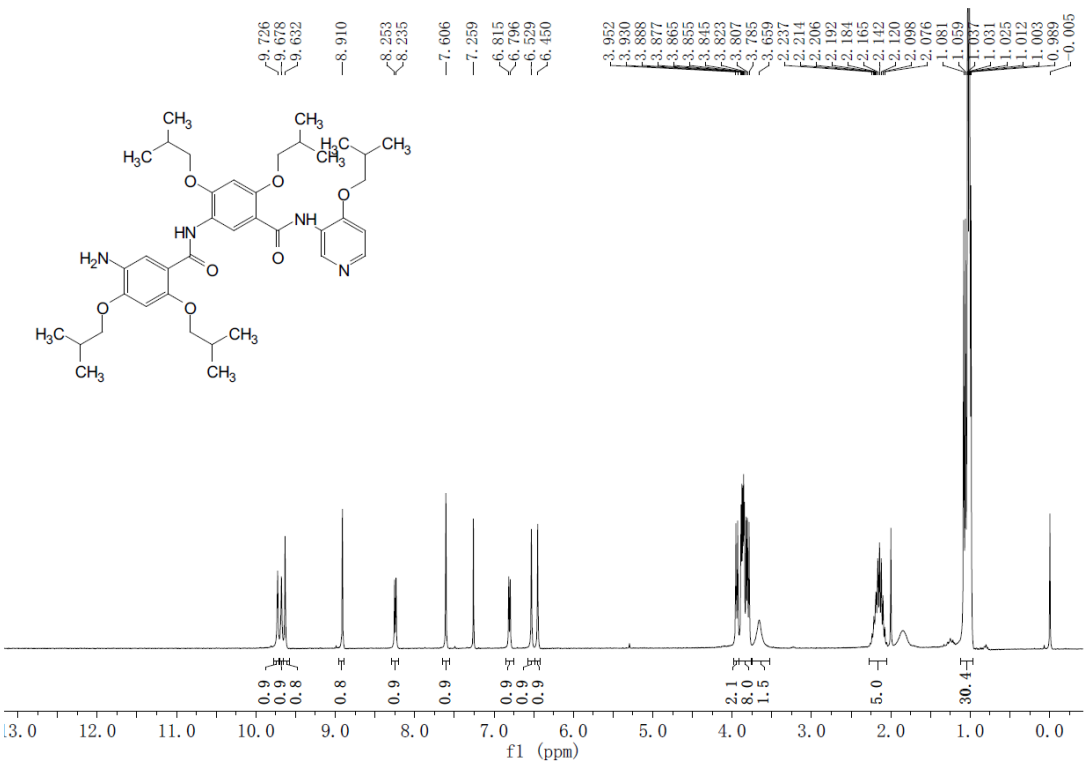


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **17** at 25 °C.

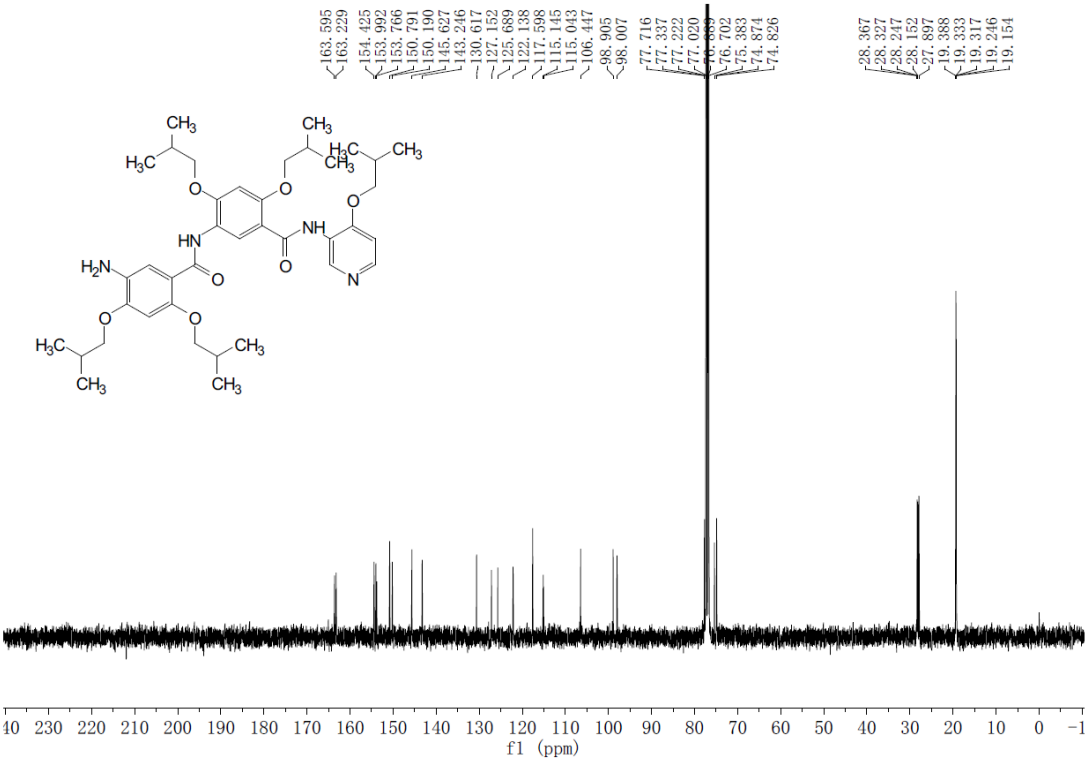


Figure S18. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **17** at 25 °C.

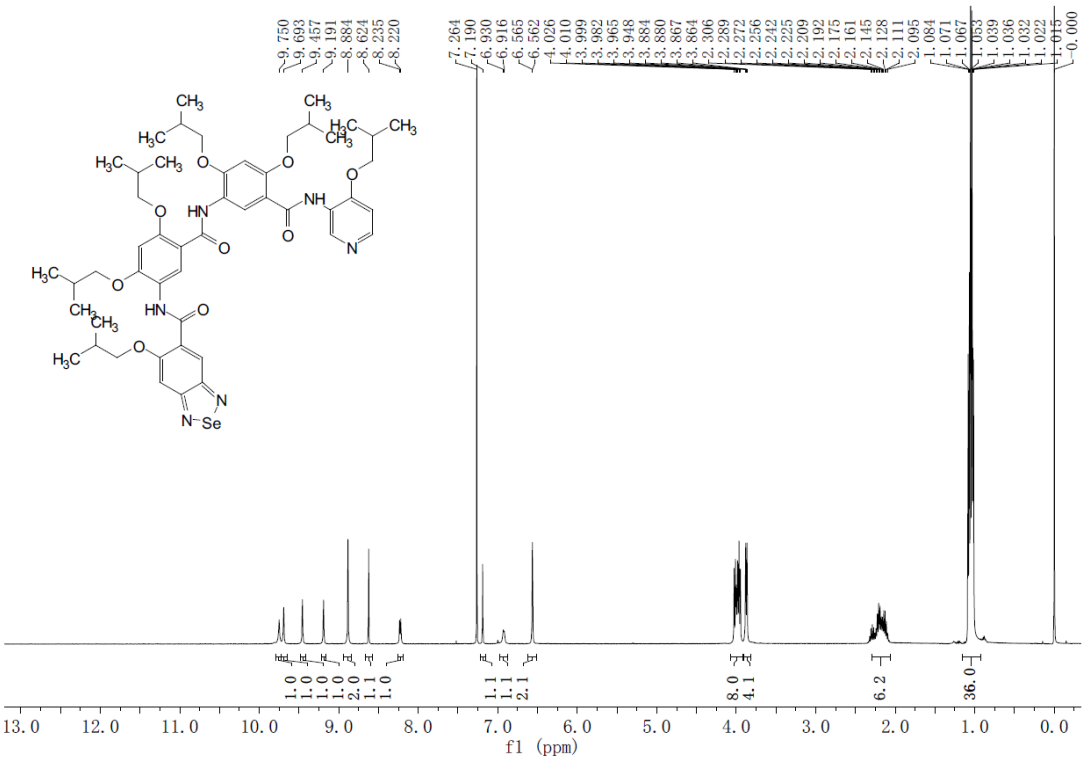


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1** at 25 °C.

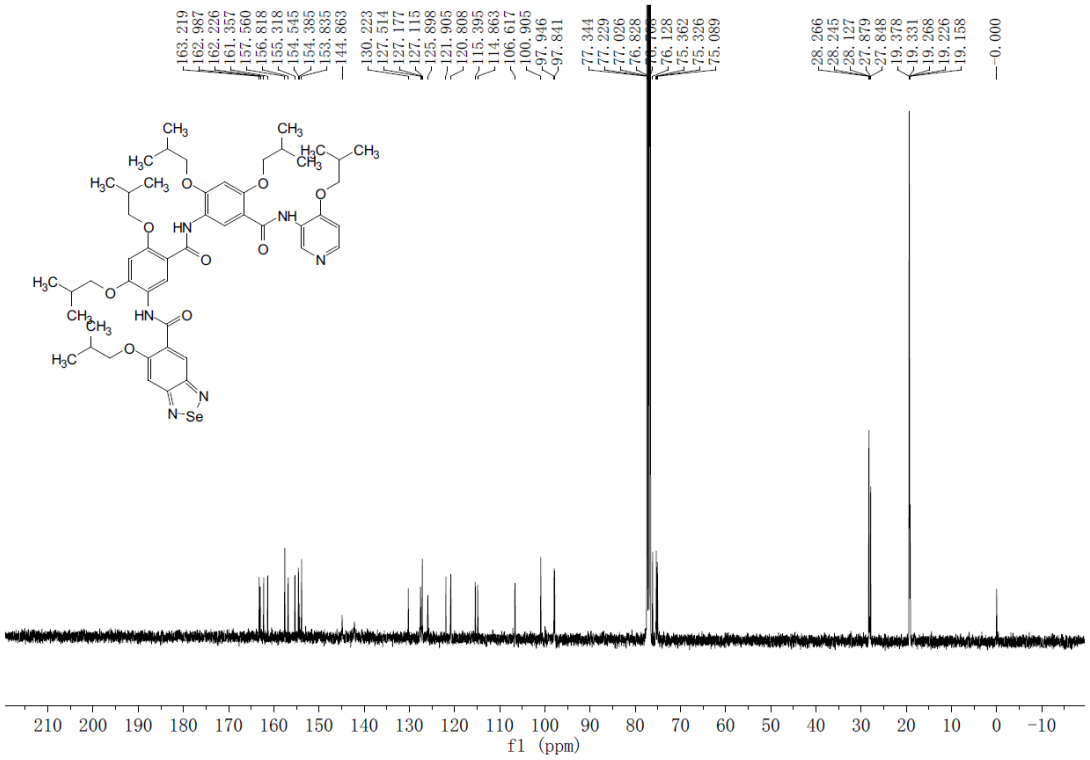


Figure S20. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **1** at 25 °C.

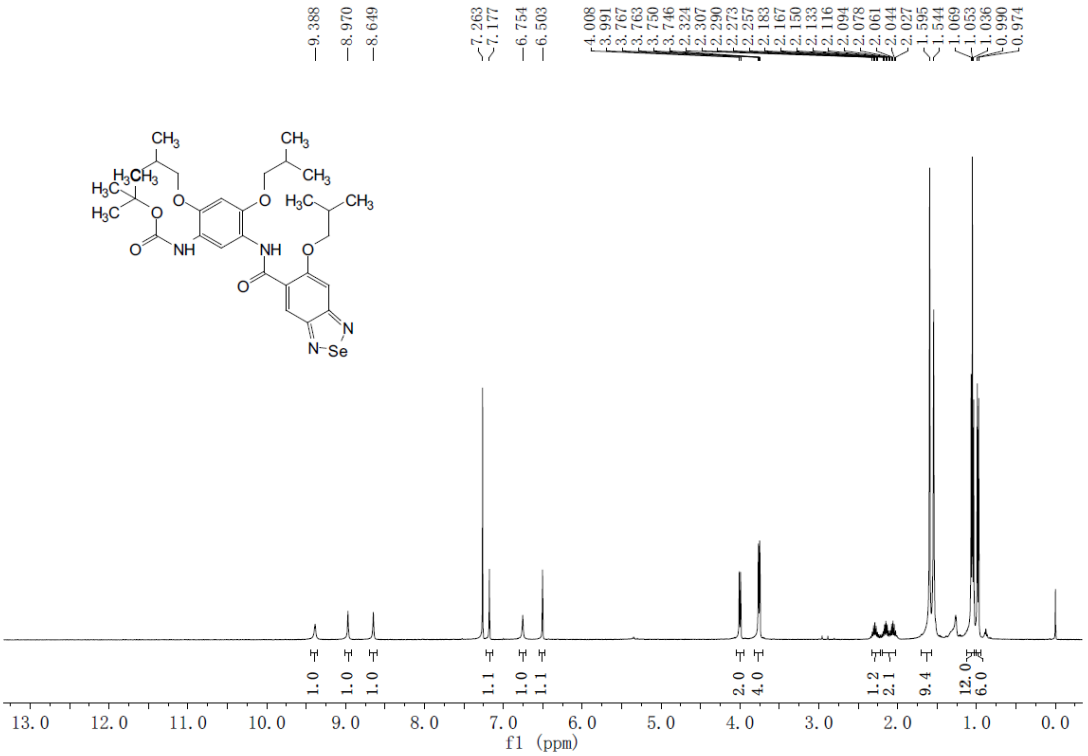


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **19** at 25 °C.

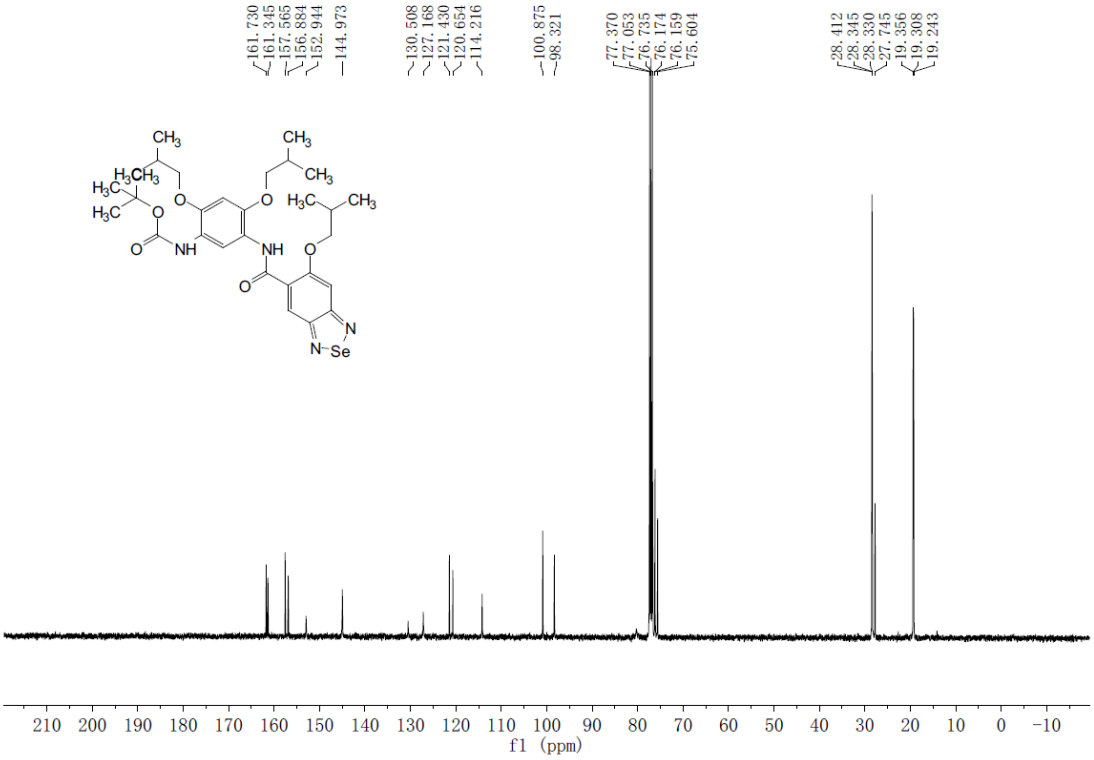


Figure S22. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **19** at 25 °C.

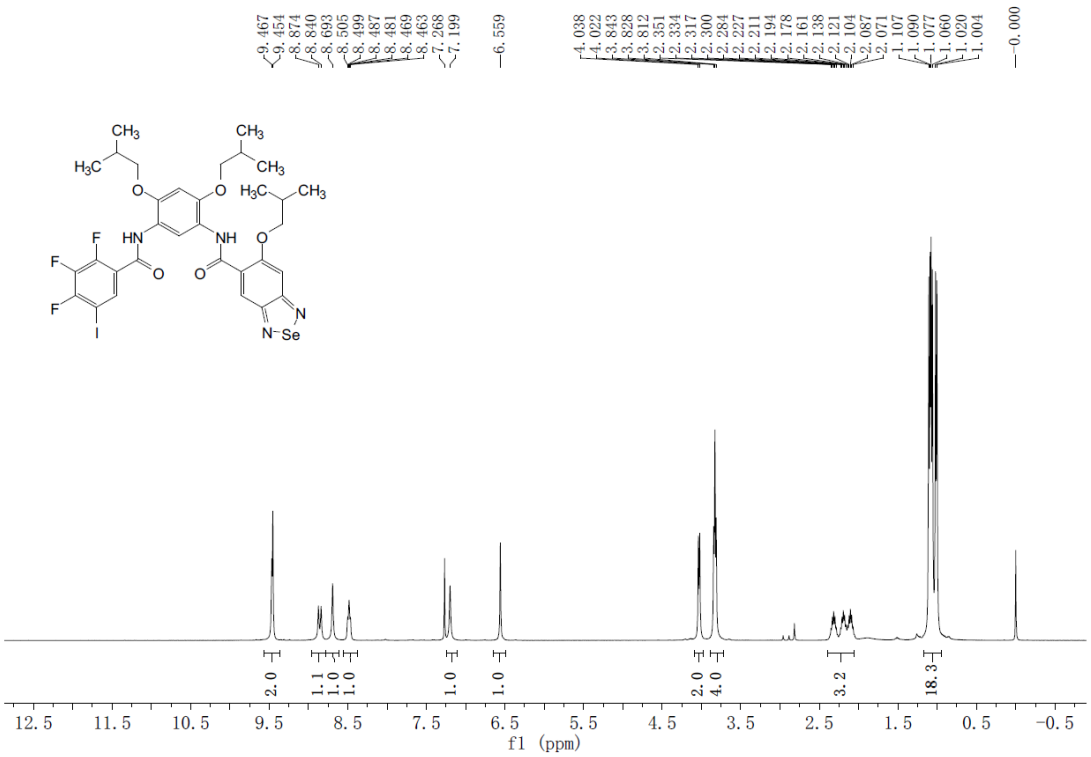


Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3** at 25 °C.

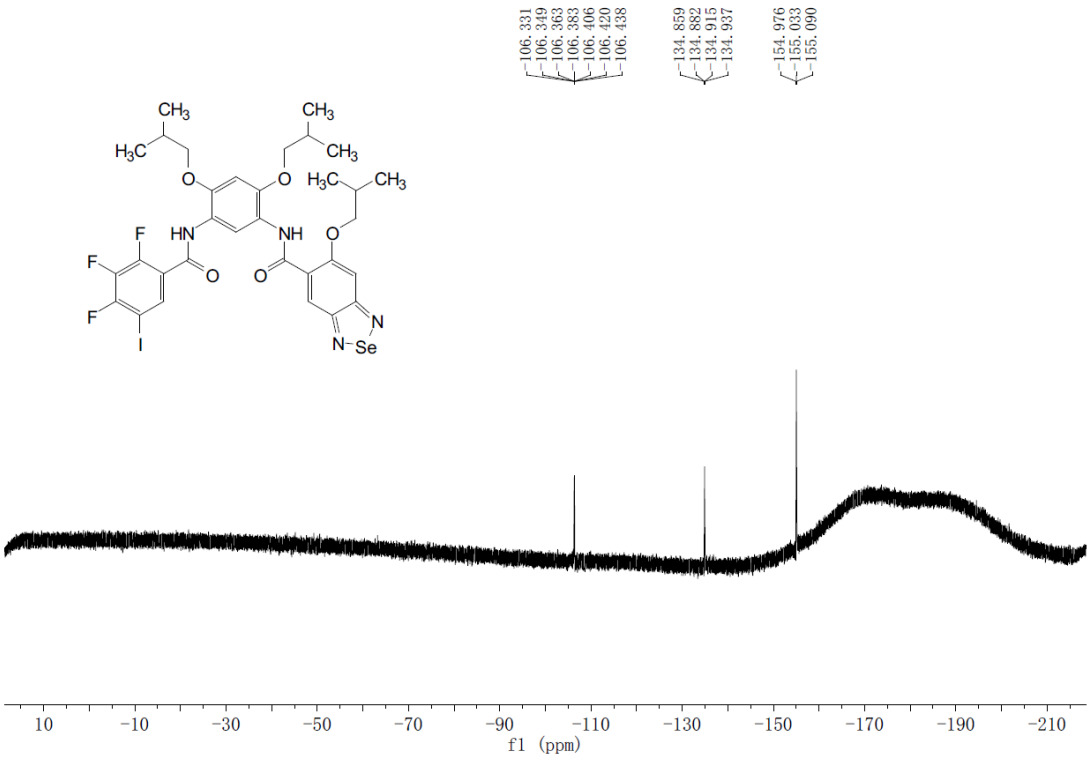


Figure S24. ^{19}F NMR (300 MHz, $CDCl_3$) spectrum of compound **3** at 25 °C.

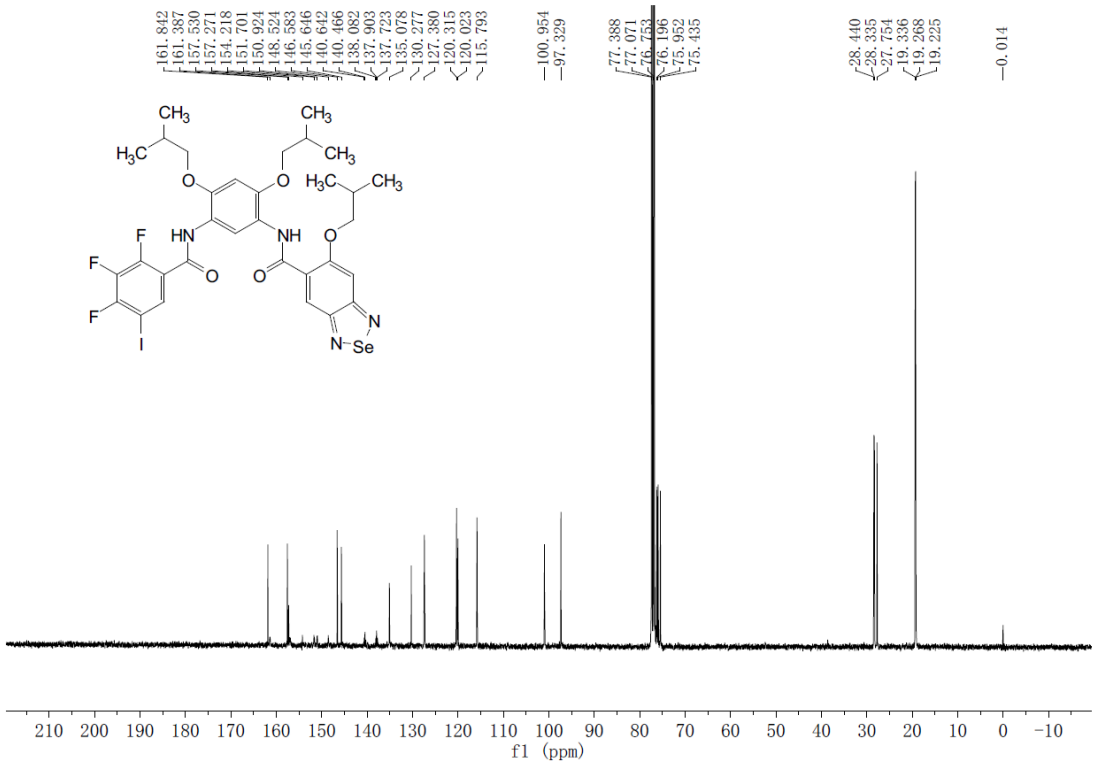


Figure S25. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3** at 25 °C.

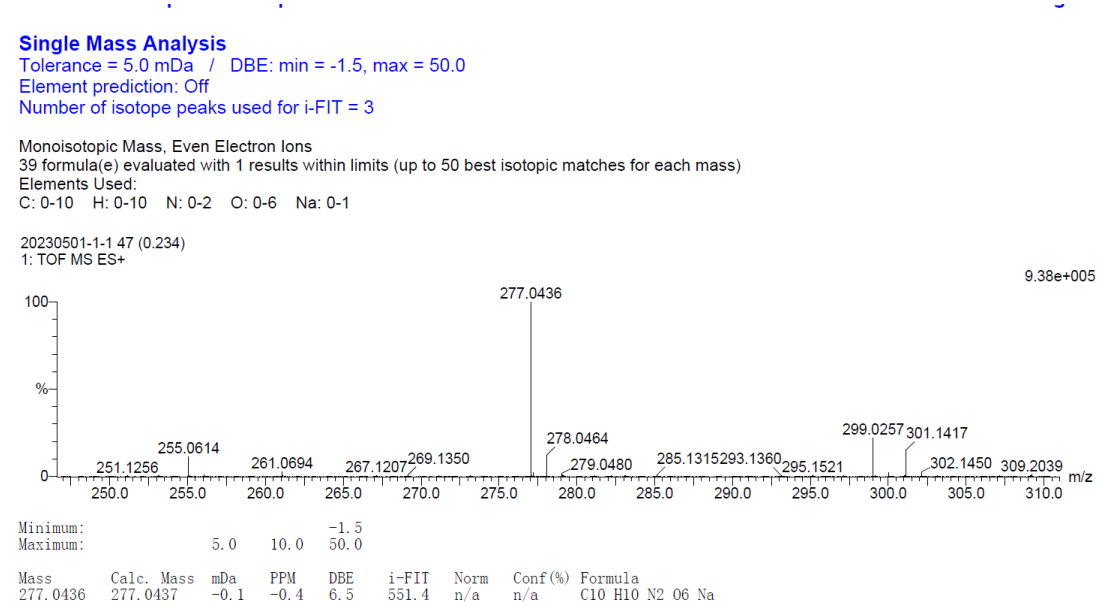


Figure S39. HR-MS (ESI) of compound **7**.

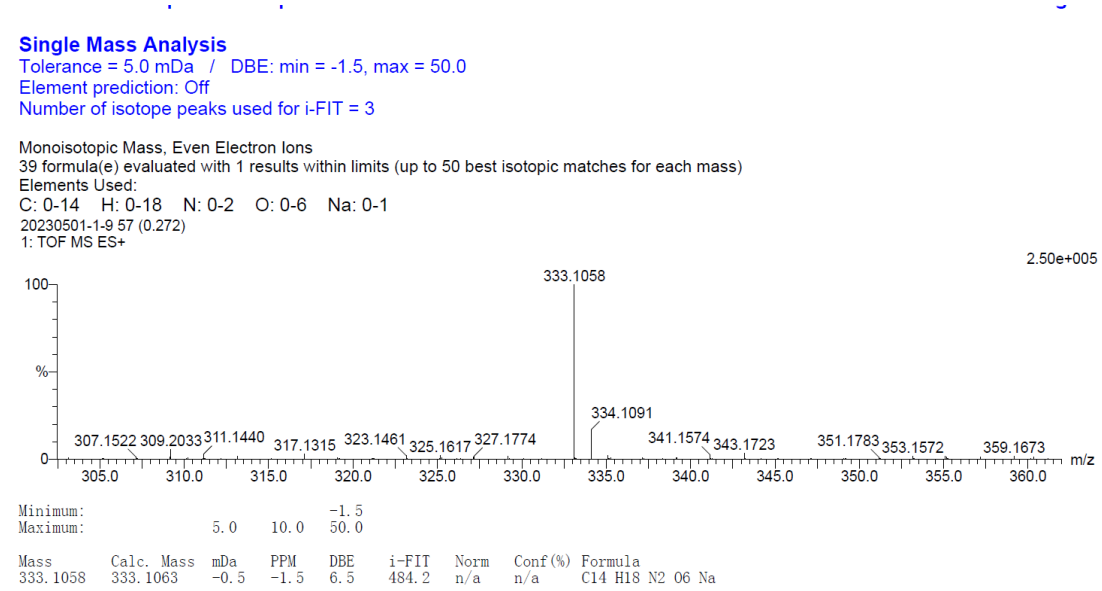
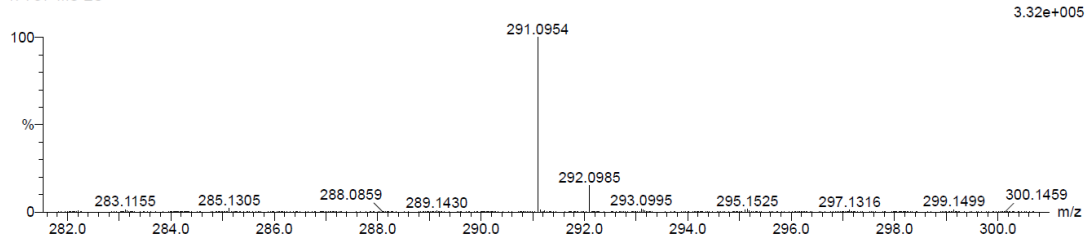


Figure S40. HR-MS (ESI) of compound **8**.

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
38 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-16 N: 0-2 O: 0-6 Na: 0-1
20230501-1-10 49 (0.241)
1: TOF MS ES+



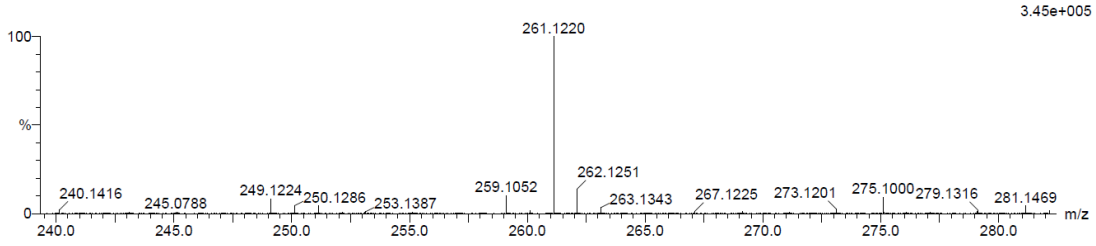
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
291.0954	291.0957	-0.3	-1.0	5.5	542.3	n/a	n/a	C12 H16 N2 O5 Na

Figure S41. HR-MS (ESI) of compound **9**.

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
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-18 N: 0-2 O: 0-3 Na: 0-1

20230501-1-8 47 (0.234)
1: TOF MS ES+



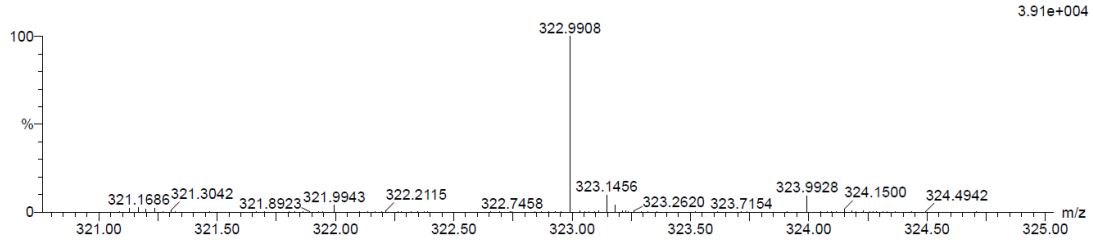
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
261.1220	261.1215	0.5	1.9	4.5	524.6	n/a	n/a	C12 H18 N2 O3 Na

Figure S42. HR-MS (ESI) of compound **10**.

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
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-11 H: 0-12 N: 0-2 O: 0-3 Se: 0-1 Na: 0-1

20230501-1-11 130 (0.589)
1: TOF MS ES+



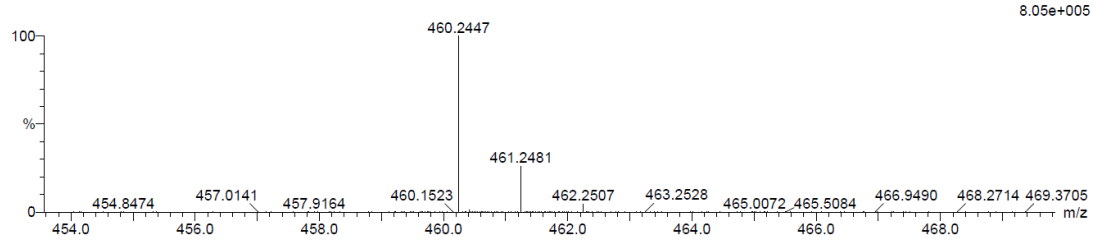
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
322.9908	322.9911	-0.3	-0.9	7.5	359.9	n/a	n/a	C11 H12 N2 O3 Se Na

Figure S43. HR-MS (ESI) of compound **11**.

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
235 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-24 H: 1-34 N: 1-3 O: 0-6 Na: 0-1 Se: 0-2

20240329-4-6-Pos 58 (0.245)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
460.2447	460.2448	-0.1	-0.2	9.5	573.2	n/a	n/a	C24 H34 N3 O6

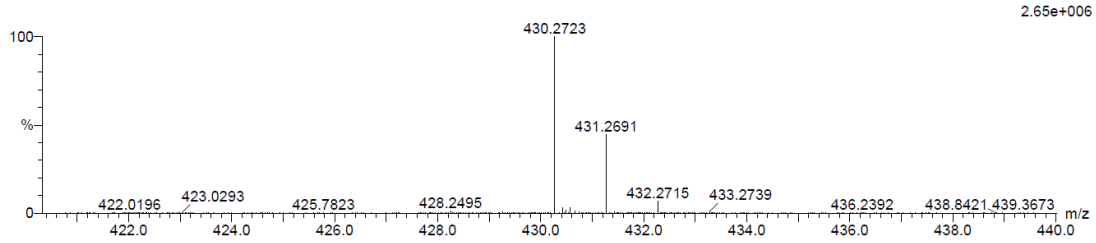
Figure S44. HR-MS (ESI) of compound **14**.

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
287 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-24 H: 1-36 N: 1-3 O: 0-6 Na: 0-1 Se: 0-2

20240329-4-7-Pos 44 (0.192)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
430.2723	430.2706	1.7	4.0	8.5	758.2	n/a	n/a	C24 H36 N3 04

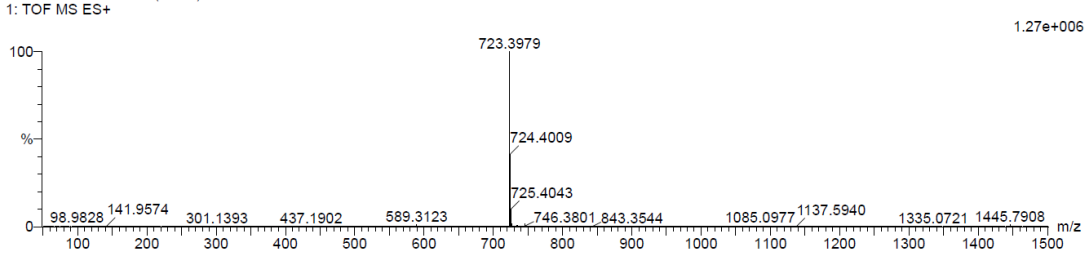
Figure S45. HR-MS (ESI) of compound **15**.

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
537 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-39 H: 1-55 N: 1-4 O: 0-9 Na: 0-1 Se: 0-2

20240329-4-8-Pos 70 (0.291)
1: TOF MS ES+



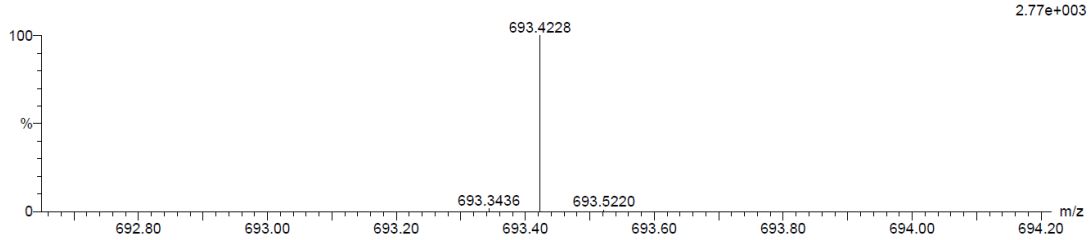
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
723.3979	723.3969	1.0	1.4	14.5	567.6	n/a	n/a	C39 H55 N4 09

Figure S46. HR-MS (ESI) of compound **16**.

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
674 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-39 H: 1-57 N: 1-4 O: 0-9 Na: 0-1 Se: 0-2
20240329-4-9-Pos 86 (0.352)
1: TOF MS ES+



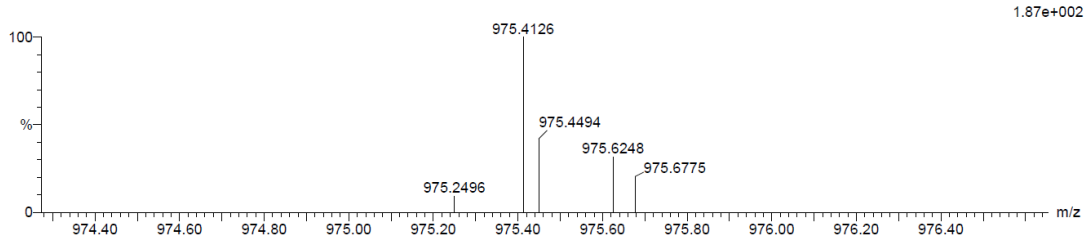
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
693.4228	693.4227	0.1	0.1	13.5	33.6	n/a	n/a	C39 H57 N4 O7

Figure S47. HR-MS (ESI) of compound **17**.

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
418 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-50 H: 1-67 N: 1-6 O: 0-9 Na: 0-1 Se: 0-2
20240329-4-11-Pos 106 (0.433)
1: TOF MS ES+



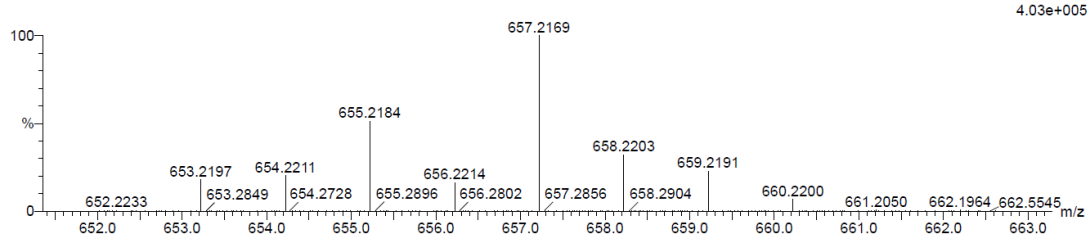
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
975.4126	975.4135	-0.9	-0.9	21.5	49.1	n/a	n/a	C50 H67 N6 O9 Se

Figure S48. HR-MS (ESI) of compound **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
731 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-42 N: 0-4 O: 0-6 Na: 0-1 Se: 0-4

20230728-2-lcz-136 109 (0.444)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
657.2169	657.2167	0.2	0.3	12.5	547.9	n/a	n/a	C30 H42 N4 O6 Na Se

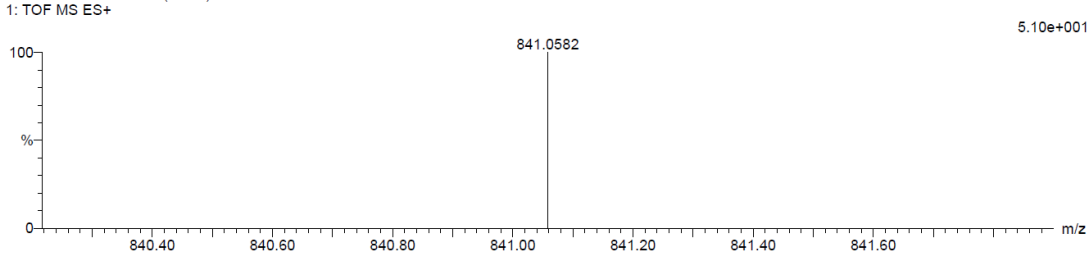
Figure S49. HR-MS (ESI) of compound **19**.

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
5338 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-32 H: 1-36 N: 1-4 O: 0-5 Na: 0-1 S: 0-1 Br: 0-1 F: 0-3 I: 0-1 Se: 0-2

20240329-3-1-Pos 197 (0.789)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
841.0582	841.0589	-0.7	-0.8	16.5	22.1	n/a	n/a	C32 H34 N4 O5 Na F3 I Se

Figure S50. HR-MS (ESI) of compound **3**.

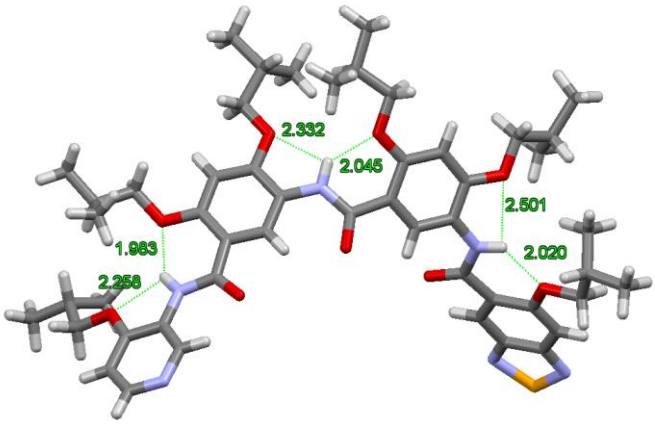


Figure S51. Three sets of intramolecular three-center hydrogen bonding (O···H···O, the N-H protons with oxygen atoms in nearby alkoxy groups) were formed in the crystal state of compound **1**. (The unit of length of hydrogen bond is "Å").

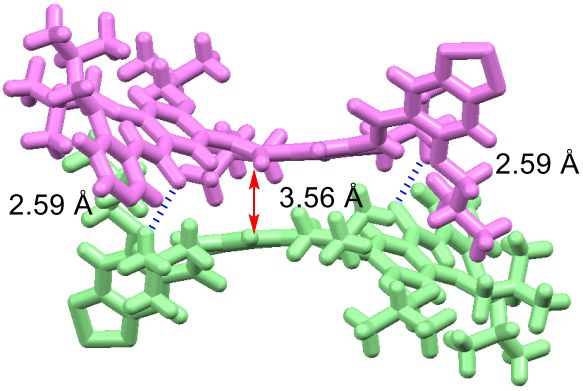


Figure S52. The detailed stacking pattern between P-helix and M-helix. The driving force came from the dual hydrogen bonding (O atom of carbonyl group near pyridine end) O···H (H of the *t*-BuO- on the aromatic ring near the benzoselenadiazole end) (O···H distance: 2.59 Å, the sum of the van der Waals radium of O and H: 2.62 Å). There were no effective π-π interaction between two molecule (the distance between two nearly parallel aromatic rings was 3.56 Å), although it seemed to exist.

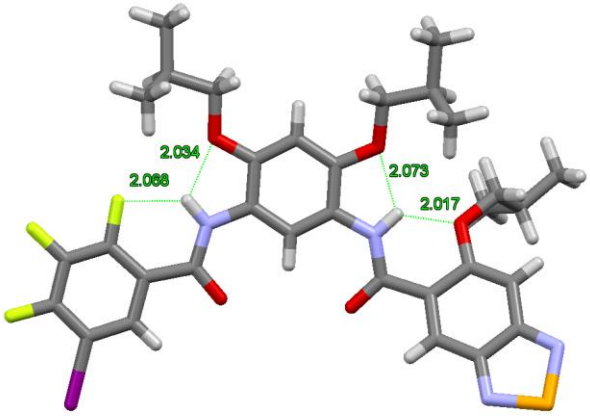


Figure S53. Two sets of intramolecular three-center hydrogen bonding (F···H···O and O···H···O, the N-H protons with oxygen atoms in nearby F atom or alkoxy

groups) were formed in the crystal state of compound **3**. (The unit of length of hydrogen bond is “Å”).

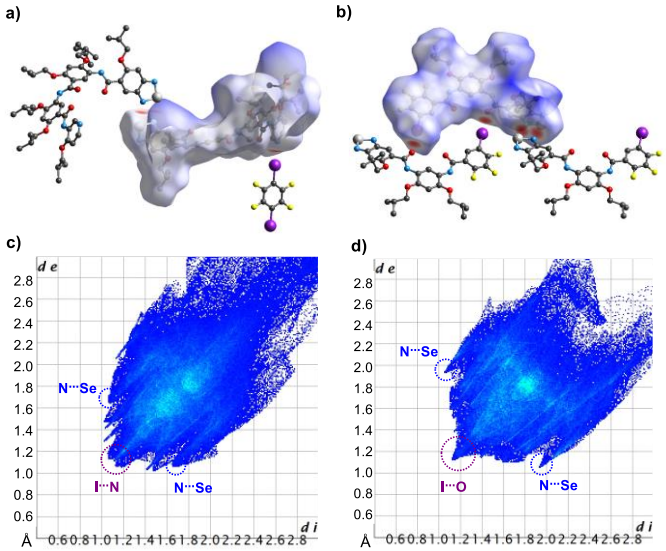


Figure S54. The Hirshfeld surfaces of the molecule of compound **1** in co-crystal of compound **1** and **2** (a) and the molecule of compound **3** in crystal (b). c) and d) 2D fingerprint plot generated by Hirshfeld surface of a) and b).

The interaction sites of XB and ChB can be clearly observed from the Hirshfeld surfaces of the molecules of compound **1** and **3** (red circle dot; the clarity of the circle dot is related to the strength of the interaction. Fig. 5a and 5b). From the 2D fingerprint plot generated by Hirshfeld surface of co-crystal of compound **1** and **2** (Fig. 5c), the numerous and complex peak patterns indicated that molecular surface of compound **1** exhibits a diverse range of intermolecular interactions. Therefore, the regions of Se···N ChB and I···N XB can only be roughly determined. However, the 2D fingerprint plot of crystal 3 presented relatively clear intermolecular interactions, including Se···N ChB and I···O XB (Fig. 5d). The discrimination of intermolecular XB and ChB base on Hirshfeld analysis has been further demonstrated.

Cifreport：co-crystal of **1** and **2**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3820_auto

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_3820_auto

Bond precision: C-C = 0.0071 A Wavelength=1.54184

Cell: a=21.6338(3) b=28.0204(3) c=21.9354(3)
alpha=90 beta=98.596(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	13147.6(3)	13147.6(3)
Space group	I 2/a	I 1 2/a 1
Hall group	-I 2ya	-I 2ya
Moiety formula	C50 H66 N6 O9 Se, C6 F4 I2 [+ solvent]	C6 F4 I2, C50 H66 N6 O9 Se, 2.062[CH2CL2]
Sum formula	C56 H66 F4 I2 N6 O9 Se [+ solvent]	C58.06 H70.12 Cl4.12 F4 I2 N6 O9 Se
Mr	1375.91	1550.85
Dx,g cm-3	1.390	1.567
Z	8	8
Mu (mm-1)	8.686	10.261
F000	5536.0	6228.0
F000'	5540.58	
h,k,lmax	25,33,26	25,33,26
Nref	11738	11715
Tmin,Tmax	0.077,0.105	0.267,1.000
Tmin'	0.020	

Correction method= # Reported T Limits: Tmin=0.267 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 67.077

R(reflections)= 0.0560(10139) wR2(reflections)= 0.1582(11715)

S = 1.036 Npar= 751

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.93Ang From I1 2.95 eA-3

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.09 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.7 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C32 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.4 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.040 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 19 Report
1 3 0, 2 1 1, -5 2 1, -1 2 1, 0 3 1, 4 3 1,
1 4 1, -4 2 2, 3 3 2, -2 4 2, -2 1 3, 1 1 4,
-3 3 4, -2 1 5, 2 1 5, 4 30 6, 11 28 7, 14 0 14,
6 0 24,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From I2 1.67 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C58.06 H70.12 Cl4.12 F4 I2 N6 O9
Atom count from the _atom_site data: C56 H66 F4 I2 N6 O9 Se1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C58.06 H70.12 Cl4.12 F4 I2 N6 O9 S
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	464.48	448.00	16.48
H	560.96	528.00	32.96
Cl	32.96	0.00	32.96
F	32.00	32.00	0.00
I	16.00	16.00	0.00
N	48.00	48.00	0.00
O	72.00	72.00	0.00
Se	8.00	8.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
H2 H3 H4
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

```
             Calc: C56 H66 F4 I2 N6 O9 Se
             Rep.: C58.06 H70.12 Cl4.12 F4 I2 N6 O9 Se
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C50 H66 N6 O9 Se, C6 F4 I2
             Rep.: C6 F4 I2, C50 H66 N6 O9 Se, 2.062[CH2CL2]
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      15.35 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      40.76 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         5% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H16      ..H43B     .       2.13 Ang.
                                                    x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  I1       ..N1       .       2.73 Ang.
                                       1/2+x,1/2+y,1/2+z  =      3_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  I1       ..C5       .       3.39 Ang.
                                       1/2+x,1/2+y,1/2+z  =      3_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I2       ..F4       .       3.34 Ang.
                                          3/2-x,y,2-z  =      2_657 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         96 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        75% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
               1  1  0,   0  2  0,   0  1  1,   0  0  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         19 Note
              -5  2  1,  -4  2  2,  -3  3  4,  -2  1  3,  -2  1  5,  -2  4  2,
              -1  2  1,   0  0  2,   0  1  1,   0  2  0,   0  3  1,   1  1  0,
               1  1  4,   1  3  0,   1  4  1,   2  1  1,   2  1  5,   3  3  2,
               4  3  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.25 Note
             Predicted wR2: Based on SigI**2  7.04 or SHELX Weight 15.79
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 31 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
 12 ALERT type 3 Indicator that the structure quality may be low
  5 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

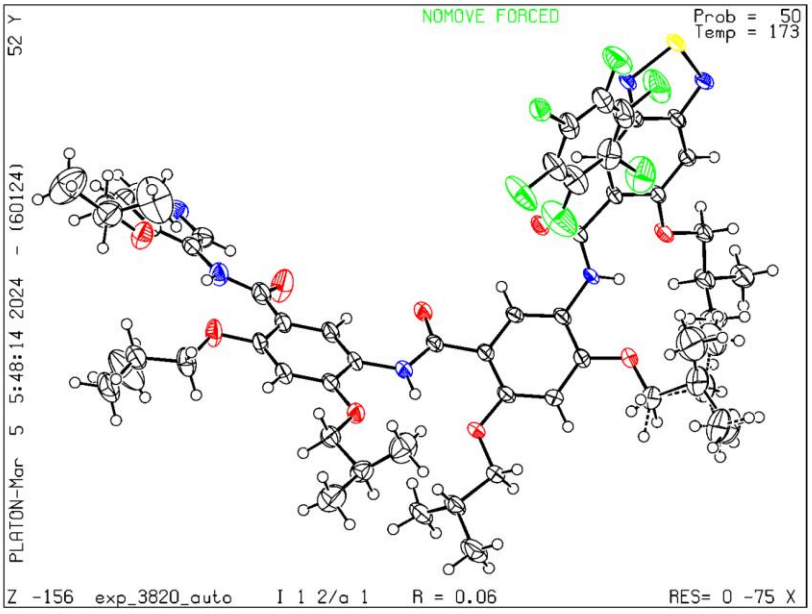
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock exp_3820_auto - ellipsoid plot



Cifreport：crystal of **3**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3698_auto

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: exp_3698_auto

```
Bond precision:   C-C = 0.0051 A          Wavelength=1.54184

Cell:           a=9.5768(5)       b=10.0412(3)      c=18.3416(5)
                alpha=96.600(3)   beta=101.321(3)   gamma=98.752(3)
Temperature:    173 K

                 Calculated                Reported
Volume           1690.13(12)               1690.13(11)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C32 H34 F3 I N4 O5 Se     C32 H34 F3 I N4 O5 Se
Sum formula      C32 H34 F3 I N4 O5 Se     C32 H34 F3 I N4 O5 Se
Mr               817.49                    817.49
Dx,g cm-3        1.606                     1.606
Z                2                         2
Mu (mm-1)        9.207                     9.207
F000             816.0                     816.0
F000'            816.15
h,k,lmax         11,11,21                  11,11,21
Nref             6040                      6014
Tmin,Tmax        0.137,0.276               0.368,1.000
Tmin'            0.061

Correction method= # Reported T Limits: Tmin=0.368 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 67.066

R(reflections)= 0.0339( 5418)                    wR2(reflections)=
                                                 0.0918( 6014)
S = 1.088                 Npar= 421
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 26 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 1 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT431_ALERT_2_G Short Inter HL..A Contact I1 ..O4 . 2.93 Ang.
-x,2-y,1-z = 2_576 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 80% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock exp_3698_auto - ellipsoid plot