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First synthesis of new polycyclic systems from *ortho*-di(heteroaryl)-substituted furazanopyrazine derivatives by the Scholl reaction

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Table of Contents

General Information.

All reagents and solvents were obtained from commercial sources and dried by using standard procedures before use. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker DRX-400, AVANCE-500 and AVANCE-600 instruments using Me_4Si as an internal standard. Elemental analysis was carried on a Eurovector EA 3000 automated analyzer. High resolution mass spectrometry was performed using a Bruker maXis Impact HD spectrometer. Melting points were determined on Boetius combined heating stages and were not corrected.

Flash-column chromatography was carried out using Alfa Aesar silica gel 0.040-0.063 mm (230–400 mesh), eluting with ethyl acetate-hexane. The progress of reactions and the purity of compounds were checked by TLC on Sorbfil plates (Russia), in which the spots were visualized with UV light (λ 254 or 365 nm).

Electrochemical behaviour of the compounds has been investigated using the Metrohm μAutolab type III potentiostat equipped with standard three electrode cell. Glassy carbon disk was used as working electrode, $Ag/AgNO_3$ a carbon rod served as a reference and counter electrodes respectively. When registering the cyclic voltammograms (CV) the anhydrous CH_2Cl_2 with 5mM of analyzed compound and 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte were used. All electrochemical measurements were carried out under N_2 atmosphere at a scan rate 100 mV/s. When HOMO-LUMO estimation, the potential of reference electrode has been calibrated by using the ferrocene/ferrocenium (Fc/Fc^+) redox couple:

$$E_{HOMO}\ (eV) = -\ [E_{ox\ onset} - E_{1/2}(Fc/Fc^+) + 5.1]$$

$$E_{LUMO}\ (eV) = -\ [E_{red\ onset} - E_{1/2}(Fc/Fc^+) + 5.1],$$

where $E_{red/Ox\ onset}$ is the peak potential of the first independent anodic or cathodic processes obtained from CVs, $E_{1/2}(Fc/Fc^+)$ is the half-wave potential of the Fc/Fc^+ couple (in this work estimated experimentally as 0.66 V) against the Ag/Ag^+ electrode.

The absorption spectra were recorded with a Shimadzu UV 2600 spectrometer.

Synthesis

General procedure for the synthesis of 5-(5-phenyl-1*H*-pyrrol-2-yl)-6-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazines (5a and 5b). To a stirred mixture of 5-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine **(1a** or **1b)** (0.5 mmol) and 2-phenyl-1*H*-pyrrole **(2)** (72 mg, 0.5 mmol)] in MeCN (4 ml) was added CF_3COOH (38 μl, 0.5 mmol). The reaction mixture was stirred at room temperature for 24 h. The solvent was distilled off *under reduced pressure*, and the residue was washed with aqueous Na_2CO_3 and air-dried. Purification by column chromatography (hexane/ethyl acetate, 1:5) led to the desired S_N^H-products **5a,b**.

5-(5-Phenyl-1*H*-pyrrol-2-yl)-6-(thiophen-2-yl)[1,2,5]oxadiazolo[3,4-*b*]pyrazine (5a). Yield 116 mg, 67%, dark red solid, mp 244 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.54 (s, 1H), 8.03 (dd, *J* = 5.0, 1.1 Hz, 1H), 8.01-7.94 (m, 2H), 7.70 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.45 (dd, *J* =10.6, 4.8 Hz, 2H), 7.34 (dd, *J* = 11.5, 4.1 Hz, 1H), 7.21 (dd, *J* = 5.0, 3.8 Hz, 1H), 6.72 (dd, *J* = 4.1, 2.5 Hz, 1H), 6.42 (dd, *J* = 4.1, 2.2 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.2, 151.4, 151.4, 150.8, 140.5, 140.1, 133.26, 132.9, 130.5, 130.5, 128.8, 128.2, 127.7, 125.8, 121.5, 109.6. Calcd. for $C_{18}H_{11}N_5OS$ (345.39): C 62.60, H 3.21, N 20.28. Found: C 62.42, H 3.30, N 20.14.

5-(5-Phenyl-1*H*-pyrrol-2-yl)-6-(thiophen-3-yl)[1,2,5]oxadiazolo[3,4-*b*]pyrazine (5b). Yield 111 mg (65%), brown solid, mp 235-237 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.12 (dd, *J* = 3.0, 1.2 Hz, 1H), 8.01–7.92 (m, 2H), 7.75 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.49–7.38 (m, 3H), 7.38–7.29 (m, 1H), 6.67 (dd, *J* = 4.2, 2.3 Hz, 1H), 5.90 (dd, *J* = 4.2, 2.1 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.8, 151.5, 151.5, 150.8, 140.7, 139.0, 130.6, 130.4, 129.6, 128.71, 128.69, 128.2, 126.7, 125.9, 121.5, 110.0. Calcd. for $C_{18}H_{11}N_5OS$ (345.39): C 62.60, H 3.21, N 20.28. Found: C 62.49, H 3.29, N 20.33.

General procedure for the synthesis of 5-(1-(2-ethylhexyl)-1*H*-indol-3-yl)-6-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazines (6a-c). To a stirred solution of 5-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine **(1a-c)** (1.0 mmol) in AcOH (10 ml) was added 1-(2-ethylhexyl)-1*H*-indole **(3)** (229 mg, 1.0 mmol). The reaction mixture was stirred at room temperature for 24 h. The solvent was distilled off under reduced pressure, and the residue was washed with aqueous Na_2CO_3 and air-dried. The residue was recrystallized from isopropanol led to the desired S_N^H-products **6a-c**.

5-(1-(2-Ethylhexyl)-1*H*-indol-3-yl)-6-(thiophen-2-yl)[1,2,5]oxadiazolo[3,4-*b*]pyrazine (6a). Yield 259 mg, 60%, bright orange solid, mp 103-105 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30–8.26 (m, 1H), 8.02 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.61–759 (m, 2H), 7.55–7.52 (m, 1H), 7.36–7.26 (m, 2H), 7.09 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.11–4.04 (m, 2H), 1.84–1.74 (m, 1H), 1.24 (td, *J* = 13.8, 12.6, 5.4 Hz, 8H), 0.86–0.80 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.7, 157.4, 151.5, 150.6, 141.0, 136.69, 136.65, 133.3, 127.7, 126.4, 123.4, 122.2, 122.0, 112.6, 111.1, 49.9, 29.7, 28.0, 23.0, 22.0, 13.9, 10.2. Calcd. for $C_{24}H_{25}N_5OS$ (431.56): C, 66.80; H, 5.84; N, 16.23. Found: C, 66.81; H, 5.86; N, 16.25.

5-(1-(2-Ethylhexyl)-1*H*-indol-3-yl)-6-(thiophen-3-yl)[1,2,5]oxadiazolo[3,4-*b*]pyrazine (6b). Yield 267 mg (62%), red solid, mp 142-145 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.55–8.50 (m, 1H), 8.10 (dd, *J* = 3.0, 1.3 Hz, 1H), 7.72 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.61–7.56 (m, 1H), 7.37 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.36–7.30 (m, 2H), 6.95 (s, 1H), 3.98 (d, *J* = 7.3 Hz, 2H), 1.69 (dt, *J* = 12.1, 6.7 Hz, 1H), 1.26–1.14 (m, 8H), 0.86–0.77 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.2,

157.7, 151.7, 150.4, 139.6, 136.82, 136.75, 130.0, 128.5, 126.5, 123.7, 122.7, 122.3, 112.6, 111.0, 49.8, 29.7, 28.0, 23.1, 22.4, 13.9, 10.2. Calcd. for $C_{24}H_{25}N_5OS$ (431.56): C, 66.80; H, 5.84; N, 16.23. Found: C, 66.82; H, 5.76; N, 16.24.

5-(1-(2-Ethylhexyl)-1*H*-indol-3-yl)-6-(1*H*-indol-3-yl)[1,2,5]oxadiazolo[3,4-*b*]pyrazine (6c). Yield 269 mg (58%), dark orange solid, mp 118-120 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.98 (s, 1H), 8.31 (dd, *J* = 8.1, 1.2 Hz, 1H), 8.25–8.12 (m, 1H), 7.82 (d, *J* = 10.2 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.54–7.50 (m, 1H), 7.35–7.18 (m, 4H), 4.09–3.95 (m, 2H), 1.69 (dq, *J* = 8.0, 4.9, 4.1 Hz, 1H), 1.27–1.04 (m, 8H), 0.82–0.73 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.3, 158.9, 151.2, 151.1, 136.8, 136.7, 136.6, 133.2, 126.5, 126.0, 123.3, 123.10, 122.4, 122.0, 121.8, 121.5, 114.7, 113.7, 112.4, 111.0, 49.6, 29.6, 27.8, 22.8, 22.4, 13.9, 10.1. Calcd. for $C_{28}H_{28}N_6O$ (464.57): C, 72.39; H, 6.08; N, 18.09. Found: C, 72.40; H, 6.12; N, 18.05.

General procedure for the synthesis of 5-(6-bromo-9-(2-ethylhexyl)-9*H*-carbazol-3-yl)-6-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (7a,b).

To a stirred mixture of 5-(heteroaryl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine **(1a,b)** (1.0 mmol) and 3-bromo-9-(2-ethylhexyl)-9*H*-carbazole **(4)** (358 mg, 1.0 mmol) in MeCN (10 ml) was added $BF_3{\cdot}Et_2O$ (124 μl, 1.0 mmol). The reaction mixture was stirred at room temperature for 24 h. The solvent was distilled off under reduced pressure, and the residue was washed with aqueous Na_2CO_3 and air-dried. The residue was recrystallized from isopropanol led to the desired S_N^H-products **7a,b**.

5-(6-Bromo-9-(2-ethylhexyl)-9*H*-carbazol-3-yl)-6-(thiophen-2-yl)[1,2,5]oxadiazolo-[3,4-*b*]pyrazine (7a). Yield 314 mg, 56%, orange solid, mp 127-129 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.63 (t, *J* = 1.2 Hz, 1H), 8.48 (t, *J* = 1.1 Hz, 1H), 7.94 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.72 (d, *J* = 1.4 Hz, 2H), 7.64 (d, *J* = 1.7 Hz, 2H), 6.92 (dd, *J* = 5.0, 4.0 Hz, 1H), 6.77 (dd, *J* = 3.9, 1.1 Hz, 1H), 4.35 (d, *J* = 7.6 Hz, 2H), 2.03–1.96 (m, 1H), 1.35–1.13 (m, 8H), 0.87 (t, *J* = 7.4 Hz, 3H), 0.76 (t, *J* = 7.1 Hz, 3H). The ^{13}C NMR spectra of **7a** could not be obtained due to the poor solubility of this compound in deuteriated solvents. Calcd. for $C_{28}H_{26}BrN_5OS$ (560.51): C, 60.00; H, 4.65; N, 12.49. Found: C, 60.05; H, 4.68; N, 12.46.

5-(6-Bromo-9-(2-ethylhexyl)-9*H*-carbazol-3-yl)-6-(thiophen-3-yl)[1,2,5]oxadiazolo-[3,4-*b*]pyrazine (7b). Yield 381 mg, 68%, dark red solid, mp 113-115 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.55 (d, *J* = 1.7 Hz, 1H), 8.42 (d, *J* = 1.7 Hz, 1H), 7.71 (dd, *J* = 2.9, 1.3 Hz, 1H), 7.66–7.60 (m, 3H), 7.58 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.52 (dd, *J* = 5.1, 2.9 Hz, 1H), 7.14 (dd, *J* = 5.1, 1.3 Hz, 1H), 4.32 (d, *J* = 7.6 Hz, 2H), 1.98 (dt, *J* = 13.1, 6.3 Hz, 1H), 1.33–1.13 (m, 8H), 0.85 (t, *J* = 7.5 Hz, 3H), 0.75 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.0, 157.7, 151.23, 151.16, 142.7, 140.1, 131.7, 129.3, 128.8, 128.3, 128.1, 126.0, 124.4, 123.3, 123.0,

121.8, 112.9, 111.0, 109.1, 47.8, 39.3, 30.9, 28.7, 24.4, 23.0, 14.0, 10.9. Calcd. for $C_{28}H_{26}BrN_5OS$ (560.51): C, 59.95; H, 4.68; N, 12.49. Found: C, 60.05; H, 4.69; N, 12.52.

General procedure for the synthesis of polycyclic systems (8-10) from *ortho*-di(heteroaryl)-containing furazanopyrazine derivatives (5-7). The corresponding *ortho*-di(heteroaryl)-containing furazanopyrazine derivatives **5-7** (0.5 mmol) were dissolved in dry $CHCl_3$ (10 ml). Then, iron(III) chloride (649 mg, 4.0 mmol) were added to this solution. The reaction mixture was stirred at room temperature for 10 h. The solvent was distilled off under reduced pressure, and the residue was washed with water and air-dried. Purification by column chromatography (CH_2Cl_2) afforded the desired polycycles **8-10**.

5-Phenyl-6*H*-[1,2,5]oxadiazolo[3,4-*b*]pyrrolo[2,3-*f*]thieno[3,2-*h*]quinoxaline (8a). Yield 55 mg, 32%, black needles, mp >300 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.39 (s, 1H), 8.30 (d, *J* = 5.1 Hz, 1H), 8.12–8.09 (m, 2H), 7.81 (d, *J* = 5.1 Hz, 1H), 7.52 (dd, *J* = 8.3, 6.9 Hz, 2H), 7.47 (s, 1H), 7.44–7.40 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 151.6, 150.9, 149.2, 143.4, 140.9, 137.4, 131.14, 131.06, 129.2, 129.1, 127.9, 127.4, 126.6, 126.5, 125.3, 105.0. Calcd. for $C_{18}H_9N_5OS$ (343.36): C, 62.96; H, 2.64; N, 20.40. Found: C, 62.92; H, 2.70; N, 20.38. HRMS (APCI): m/z calcd. for $C_{18}H_{10}N_5OS$: 344.0601 $[M+H]^+$; found: 344.0597.

2-Phenyl-1*H*-[1,2,5]oxadiazolo[3,4-*b*]pyrrolo[2,3-*f*]thieno[2,3-*h*]quinoxaline (8b). Yield 110 mg, 64%, violet solid, mp >300 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 13.47 (s, 1H), 8.19–8.14 (m, 2H), 8.10 (d, *J* = 5.2 Hz, 1H), 7.79 (d, *J* = 5.2 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.46–7.41 (m, 2H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 151.3, 151.2, 149.3, 143.6, 142.6, 141.8, 132.2, 130.8, 129.4, 129.3, 126.9, 126.6, 126.3, 126.1, 104.2. Calcd. for $C_{18}H_9N_5OS$ (343.36): C, 62.96; H, 2.64; N, 20.40. Found: C, 63.01; H, 2.68; N, 20.41. HRMS (APCI): m/z calcd. for $C_{18}H_{10}N_5OS$: 344.0601 $[M+H]^+$; found: 344.0595.

8-(2-Ethylhexyl)-8*H*-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-*c*]thieno[3,2-*a*]carbazole (9a). Yield 129 mg, 60%, black solid, mp 237-239 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.79–8.72 (m, 1H), 8.51–8.44 (m, 1H), 8.07–8.00 (m, 1H), 7.91–7.83 (m, 1H), 7.53–7.38 (m, 2H), 4.76–4.62 (m, 2H), 2.61–1.96 (m, 1H), 1.45–1.03 (m, 9H), 0.92–0.71 (m, 5H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 152.2, 150.6, 149.5, 148.2, 148.1, 139.9, 138.8, 137.7, 137.5, 134.1, 125.1, 124.8, 124.1, 122.6, 112.7, 111.0, 49.2, 30.1, 29.5, 28.2, 23.7, 22.9, 14.2, 11.1. Calcd. for $C_{24}H_{23}N_5OS$ (429.54): C, 67.11; H, 5.40; N, 16.30. Found: C, 67.05; H, 5.45; N, 16.32.

8-(2-Ethylhexyl)-8*H*-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-*c*]thieno[2,3-*a*]carbazole (9b). Yield 183 mg, 85%, black solid, mp 208-210 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.73 (d, *J* = 7.6 Hz, 1H), 8.30 (d, *J* = 5.0 Hz, 1H), 8.12 (d, *J* = 5.2 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.47 (dt, *J* = 19.9, 7.2 Hz, 2H), 4.57 (d, *J* = 7.8 Hz, 2H), 2.15–2.10 (m, 1H), 1.50–1.42 (m, 2H), 1.32–1.18

(m, 6H), 0.89–0.76 (m, 6H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 151.8, 150.9, 149.3, 148.5, 139.9, 138.4, 137.4, 133.53, 129.6, 126.7, 125.5, 124.8, 124.2, 122.7, 112.7, 110.2, 49.8, 30.4, 29.5, 28.3, 23.9, 22.9, 14.2, 11.1. Calcd. for $C_{24}H_{23}N_5OS$ (429.54): C, 67.11; H, 5.40; N, 16.30. Found: C, 67.11; H, 5.50; N, 16.24.

9-(2-Ethylhexyl)-9,10-dihydro-[1,2,5]oxadiazolo[3',4':5,6]pyrazino[2,3-*c*]indolo-[2,3-*a*]carbazole (9c). Yield 203 mg (88%), black solid, mp 285-287 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 8.81–8.78 (m, 1H), 8.70 (dd, *J* = 6.1, 3.1 Hz, 1H), 7.72 (dd, *J* = 6.1, 3.1 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.52–7.44 (m, 2H), 7.41 (dd, *J* = 6.1, 3.1 Hz, 2H), 4.62 (d, *J* = 7.7 Hz, 2H), 1.95–1.86 (m, 1H), 1.31–1.09 (m, 8H), 0.78 (t, *J* = 7.4 Hz, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 150.6, 150.5, 148.9, 148.7, 139.1, 138.9, 134.4, 132.2, 125.5, 125.4, 125.3, 124.8, 123.9, 123.6, 122.9, 122.4, 113.6, 113.2, 112.3, 111.7, 49.1, 30.1, 28.6, 23.8, 22.8, 14.2, 11.5. Calcd. for $C_{28}H_{26}N_6O$ (462.56): C, 72.71; H, 5.67; N, 18.17. Found: C, 72.73; H, 5.62; N, 18.20. HRMS (APCI): m/z calcd. for $C_{28}H_{27}N_6O$: 463.2241 $[M+H]^+$; found: 463.2229.

12-Bromo-9-(2-ethylhexyl)-9*H*-[1,2,5]oxadiazolo[3',4':2,3]thieno[3',2':7,8]quinoxalino-[6,5-*b*]carbazole (10a). Yield 142 mg, 51%, deep red solid, mp 197-199 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.80 (d, *J* = 1.9 Hz, 1H), 7.57 (d, *J* = 5.1 Hz, 1H), 7.45 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.28 (d, *J* = 5.2 Hz, 1H), 7.04 (d, *J* = 8.6 Hz, 1H), 3.98–3.91 (m, 2H), 1.98–1.93 (m, 1H), 1.40–1.30 (m, 8H), 0.98 (d, *J* = 7.3 Hz, 3H), 0.90 (d, *J* = 7.2 Hz, 3H). The ^{13}C NMR spectra of **10a** could not be obtained due to the poor solubility of this compound in deuteriated solvents. Calcd. for $C_{28}H_{24}BrN_5OS$ (558.50): C, 60.22; H, 4.33; N, 12.54. Found: C, 60.23; H, 4.36; N, 12.59.

12-Bromo-9-(2-ethylhexyl)-9*H*-[1,2,5]oxadiazolo[3',4':2,3]thieno[2',3':7,8]quinoxalino-[6,5-*b*]carbazole (10b). Yield 184 mg, 66%, violet solid, mp 205-207 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.19 (d, *J* = 1.5 Hz, 1H), 8.03 (d, *J* = 5.1 Hz, 1H), 7.57 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.50 (s, 1H), 7.40 (d, *J* = 5.2 Hz, 1H), 7.19 (d, *J* = 8.6 Hz, 1H), 4.11 (dd, *J* = 7.0, 3.8 Hz, 2H), 2.00 (dd, *J* = 12.7, 7.1 Hz, 1H), 1.41–1.29 (m, 8H), 0.97 (t, *J* = 7.4 Hz, 3H), 0.91 (d, *J* = 7.1 Hz, 3H). The ^{13}C NMR spectra of **10a** could not be obtained due to the poor solubility of this compound in deuteriated solvents. Calcd. for $C_{28}H_{24}BrN_5OS$ (558.50): C, 60.22; H, 4.33; N, 12.54. Found: C, 60.26; H, 4.29; N, 12.56.

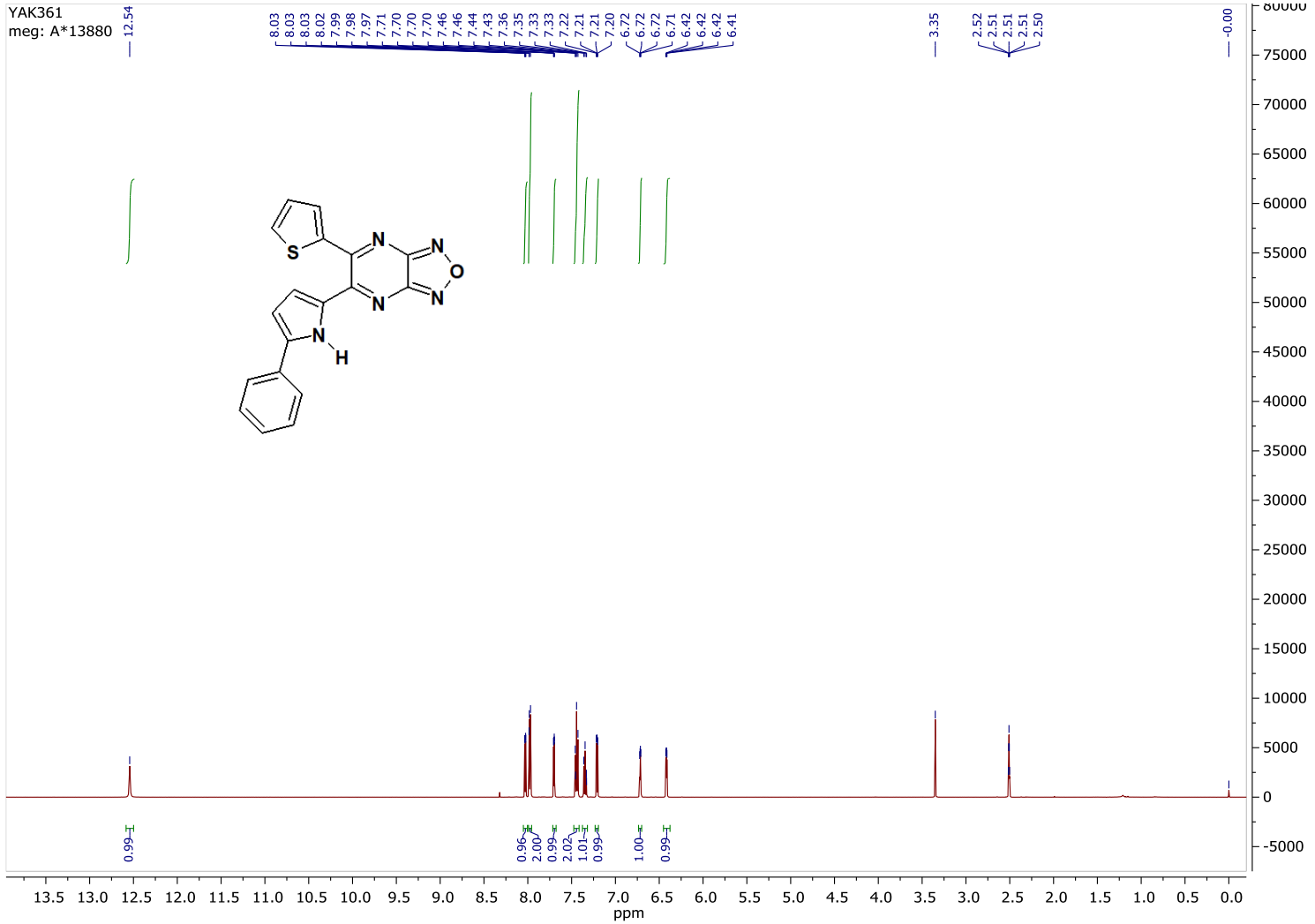

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **5a**.

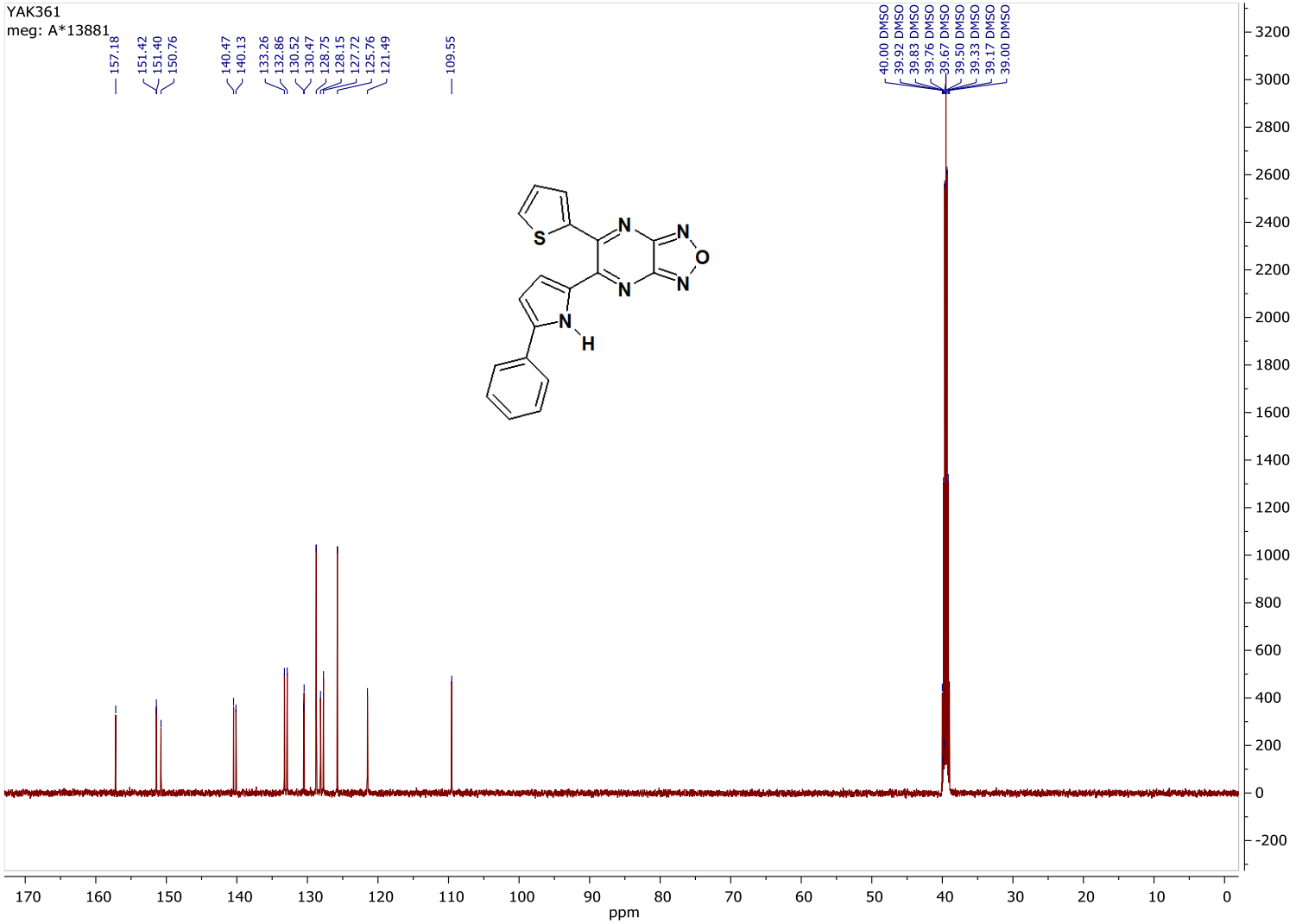

Figure S2. ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **5a**.

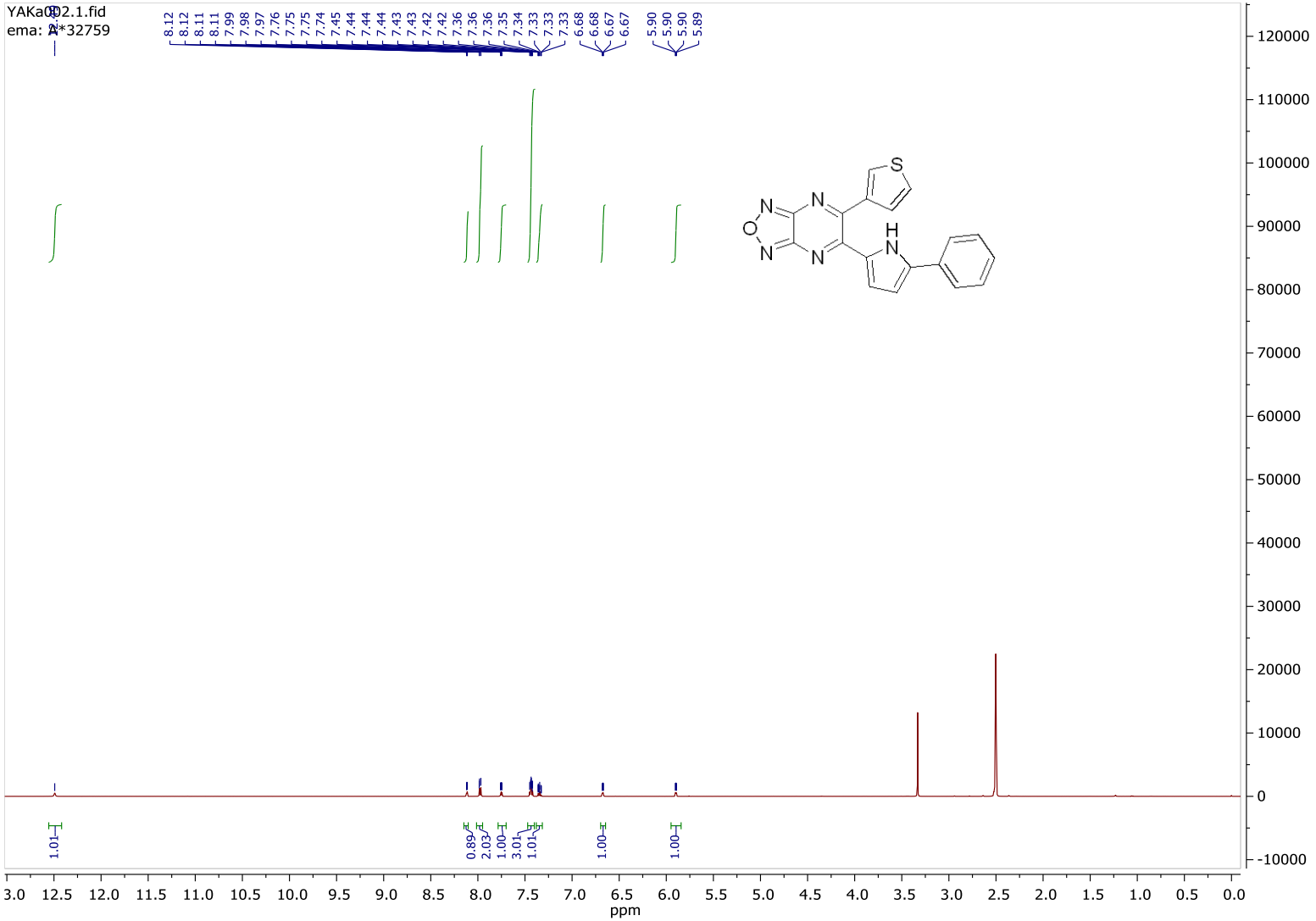

Figure S3. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **5b**.

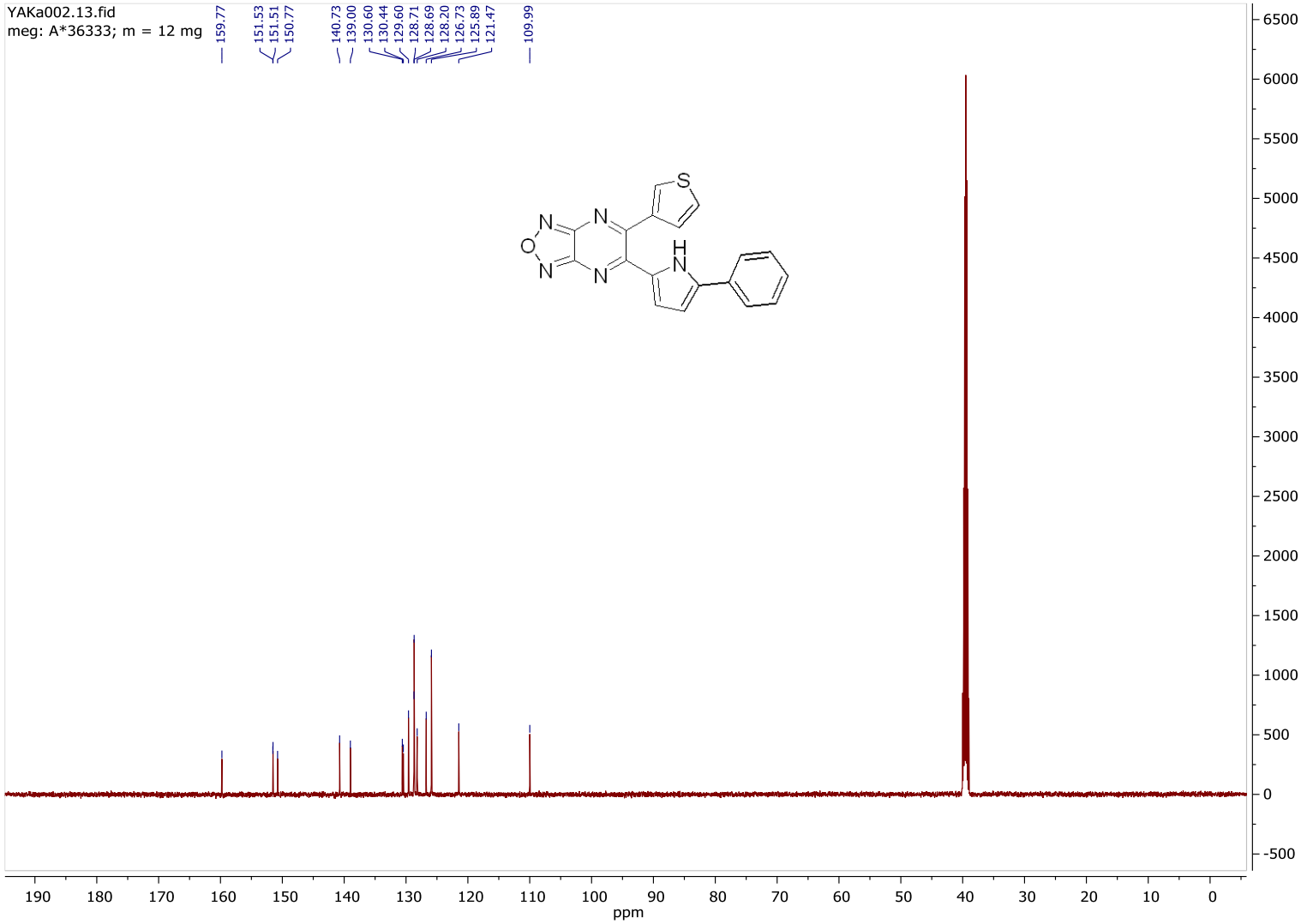

Figure S4. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **5b**.

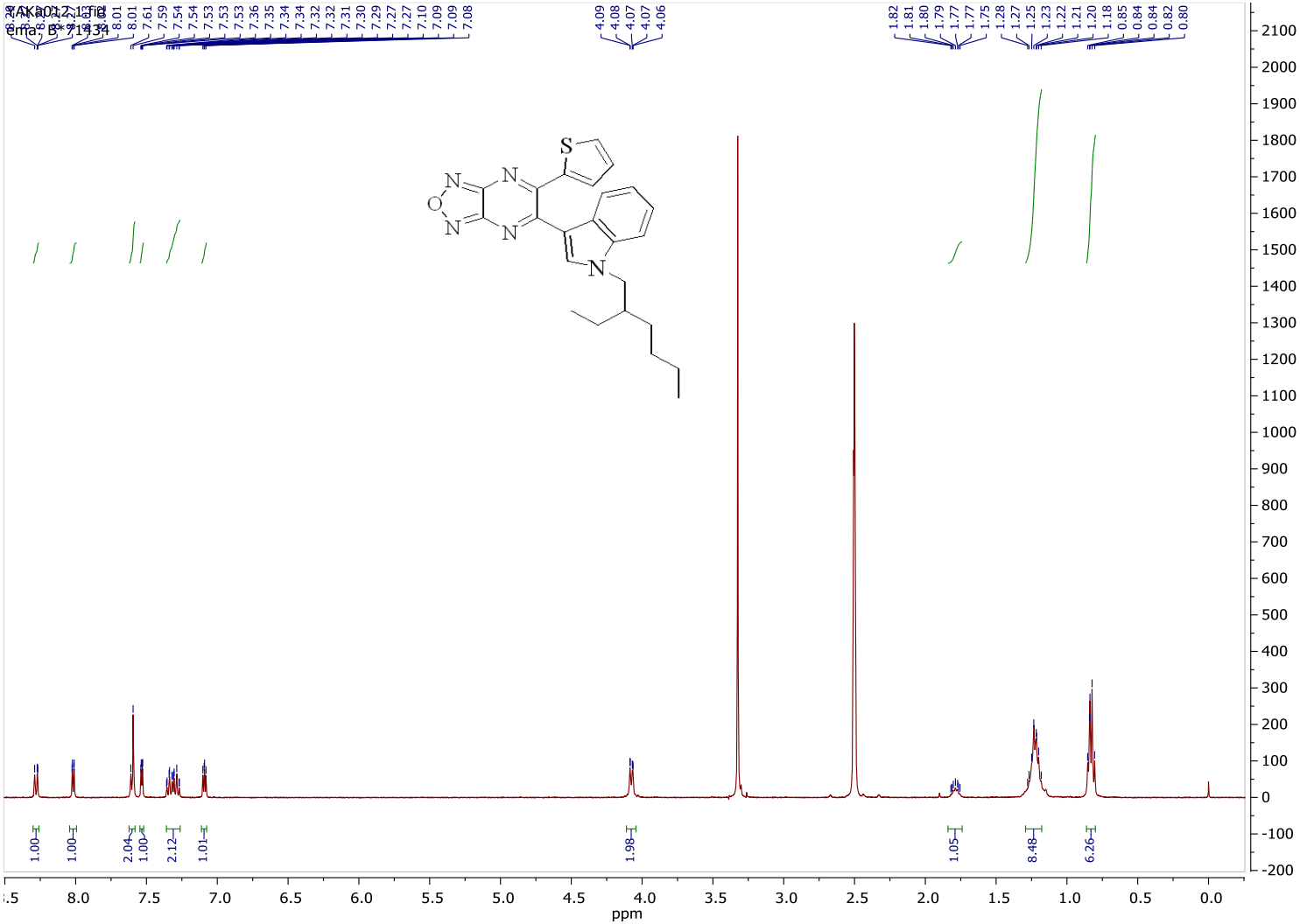

Figure S5. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **6a**.

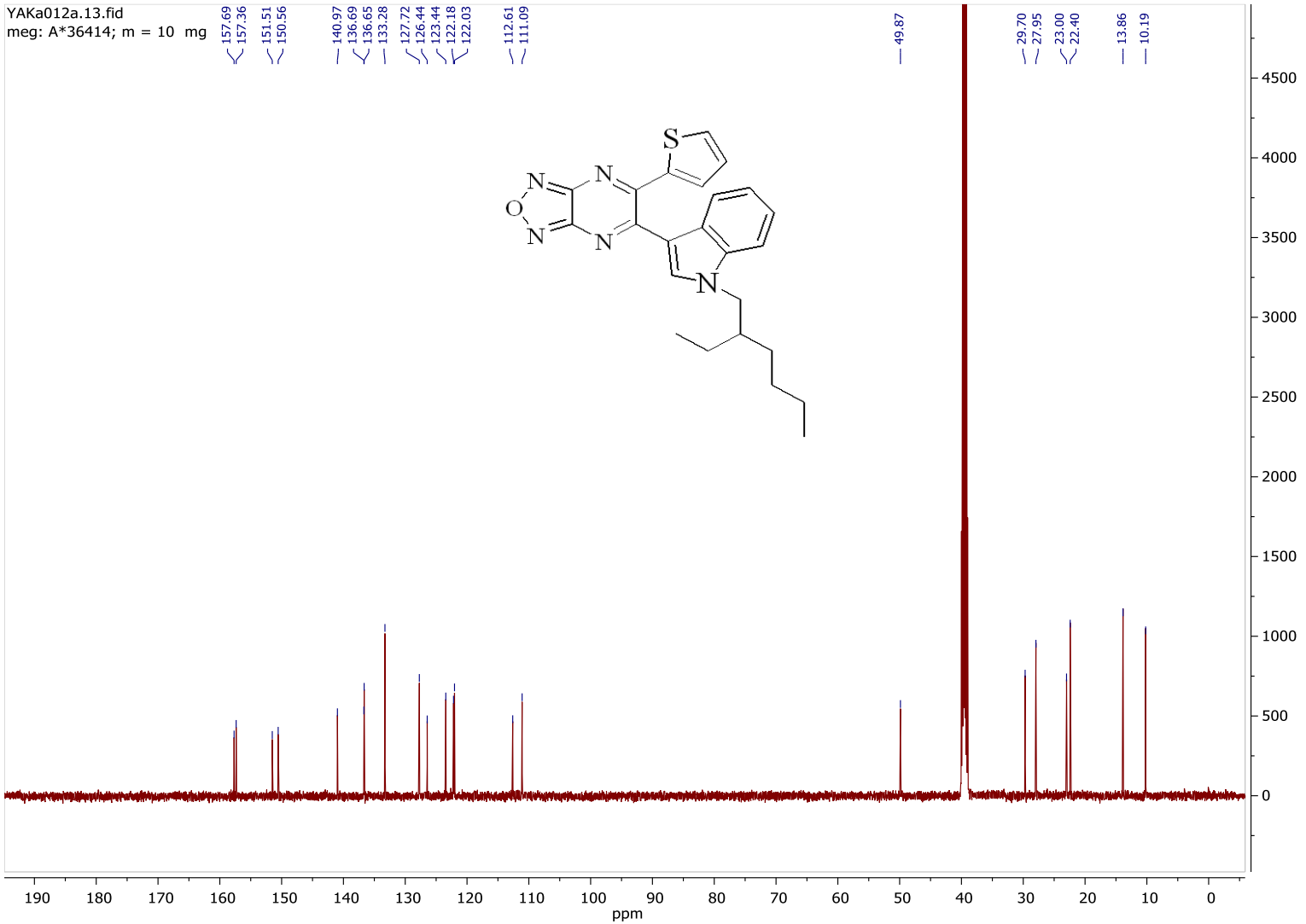

Figure S6. ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **6a**.

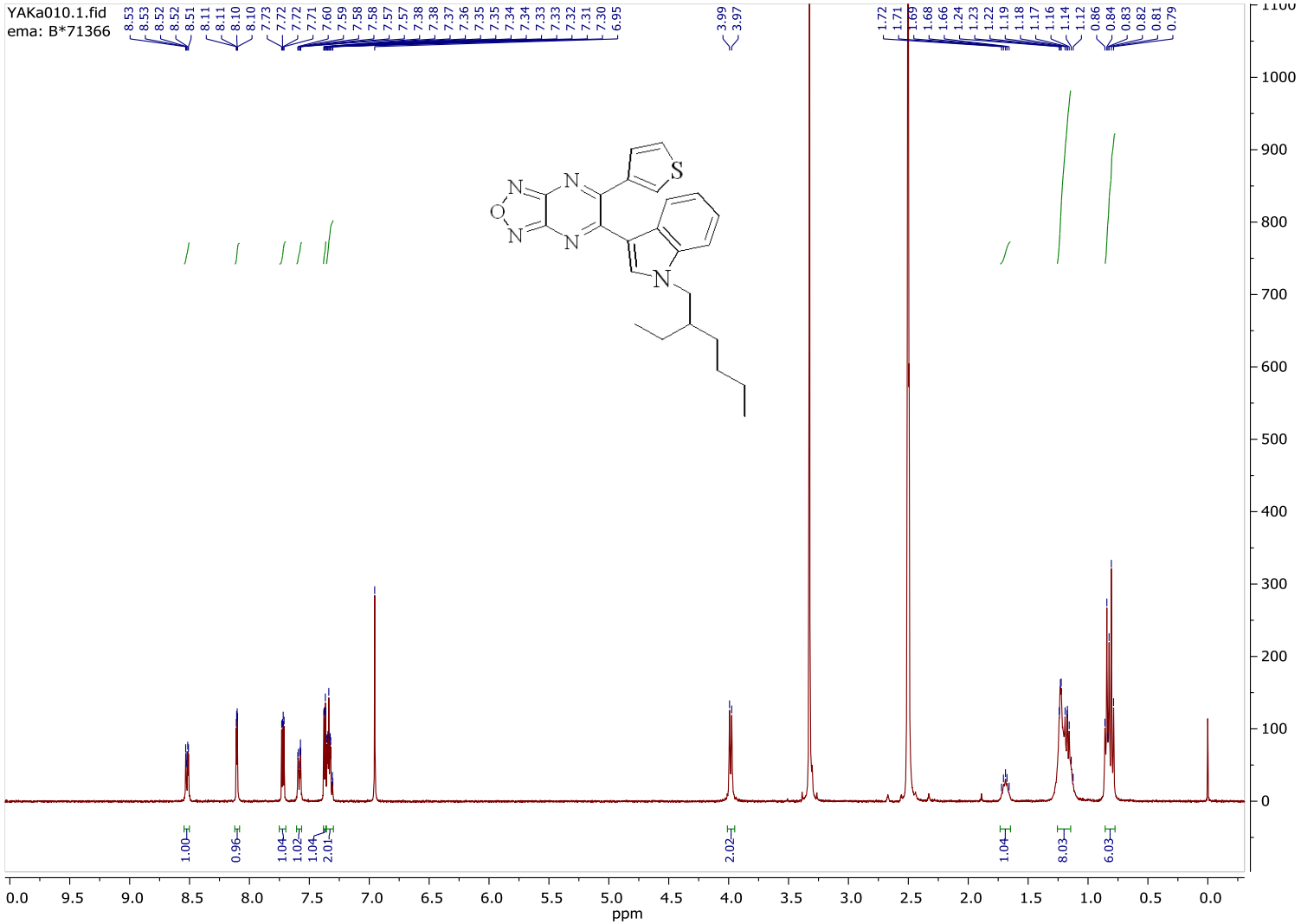

Figure S7. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **6b**.

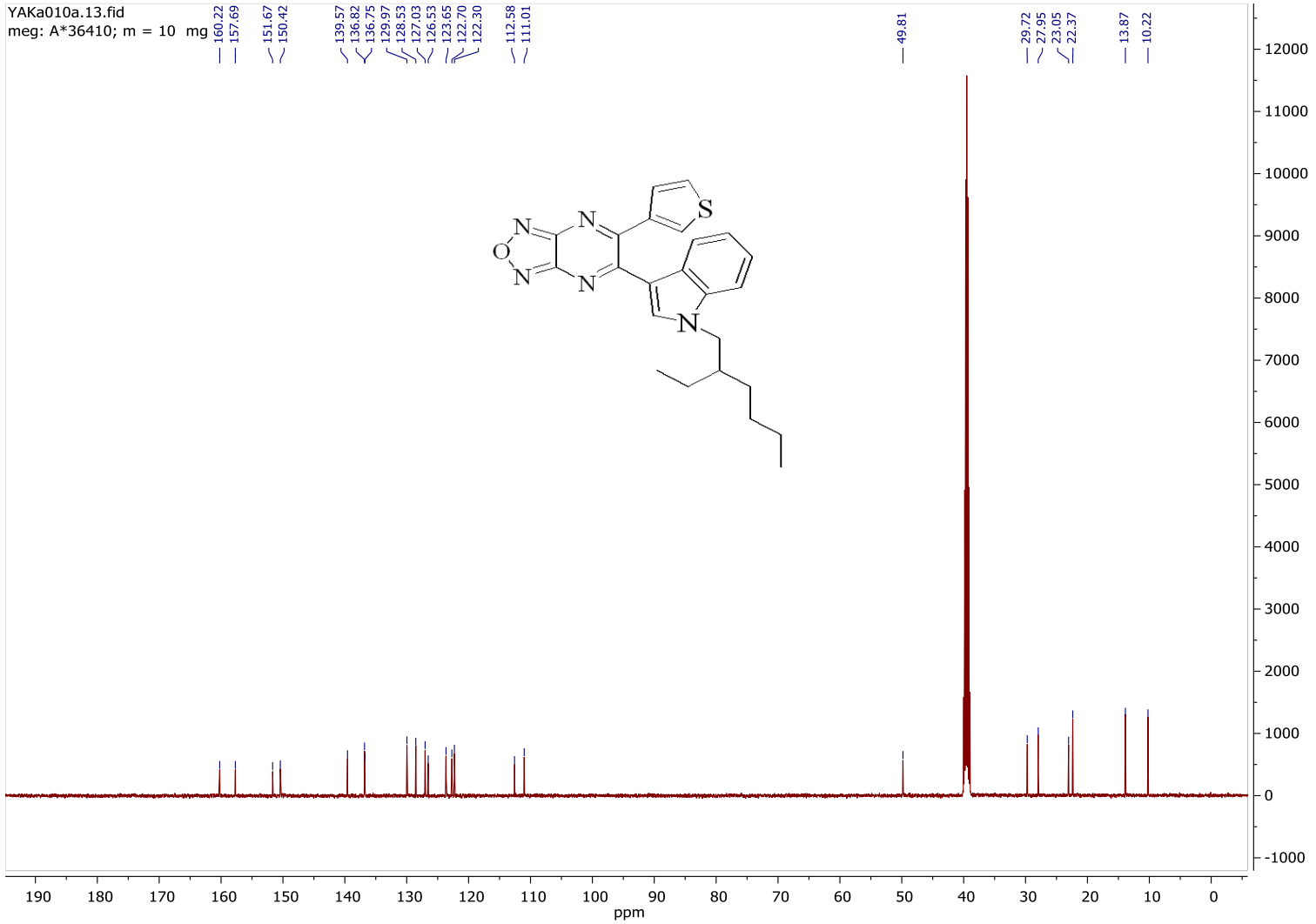

Figure S8. ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **6b**.

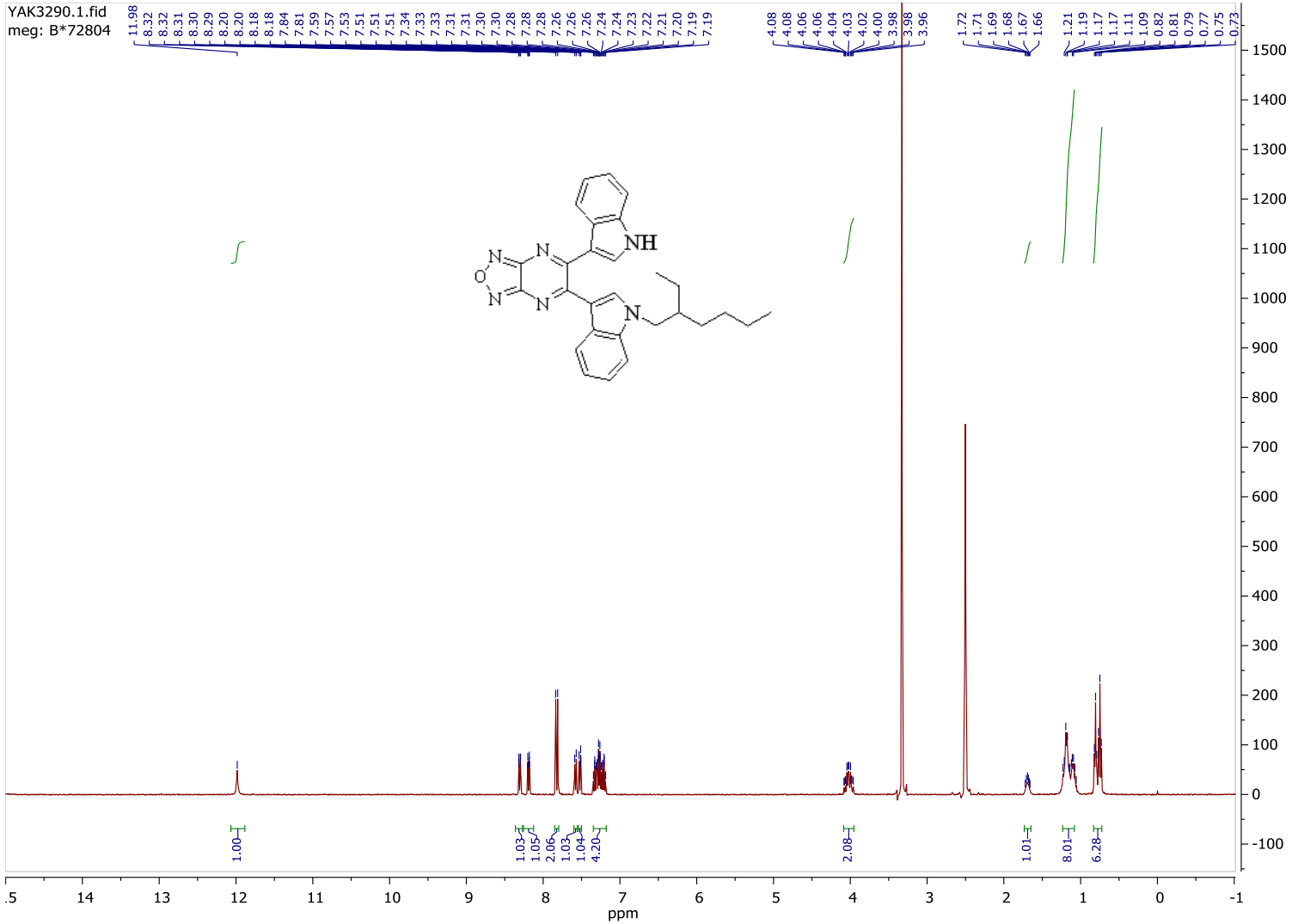

Figure S9. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **6c**.

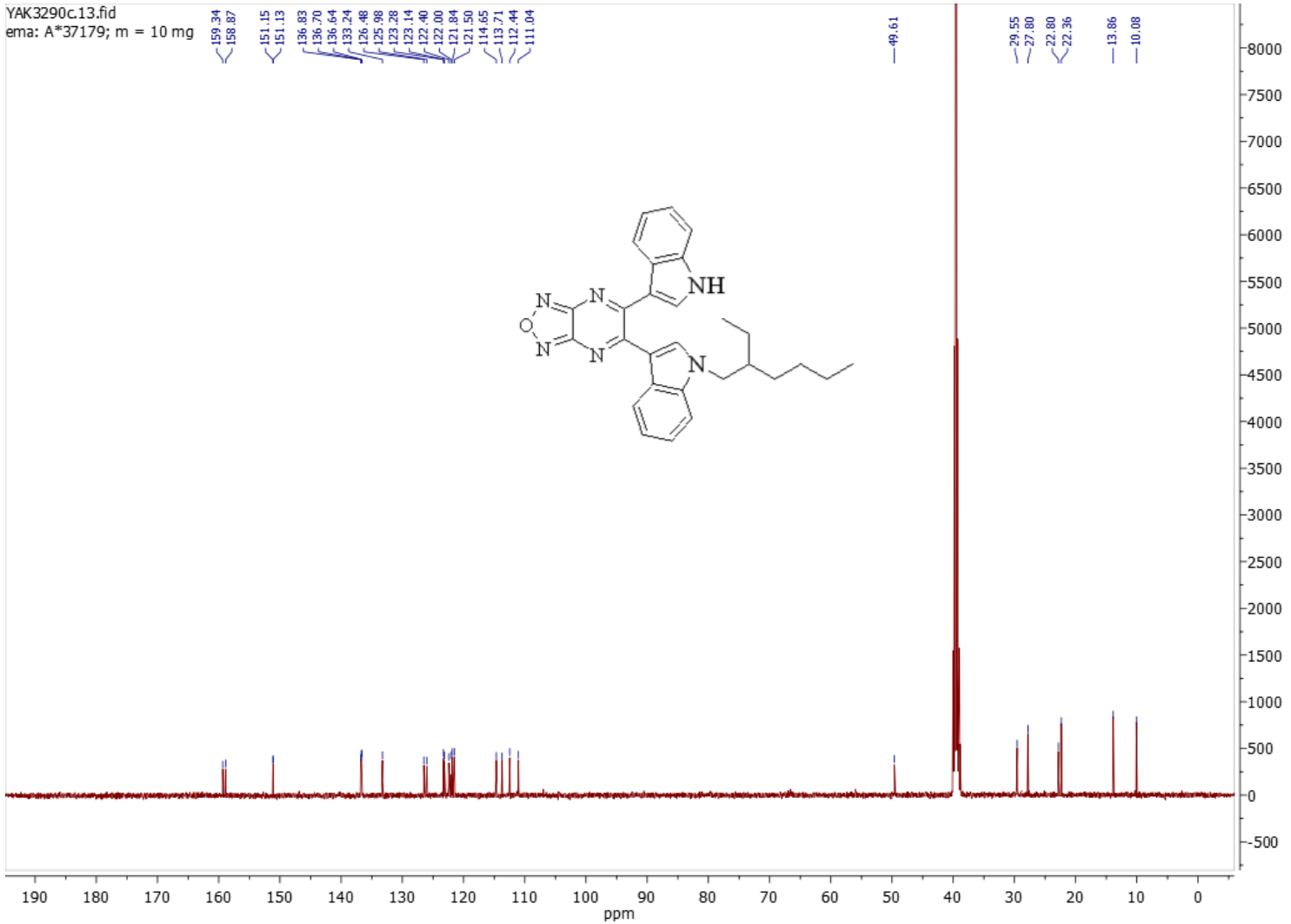

Figure S10. ^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **6c**.

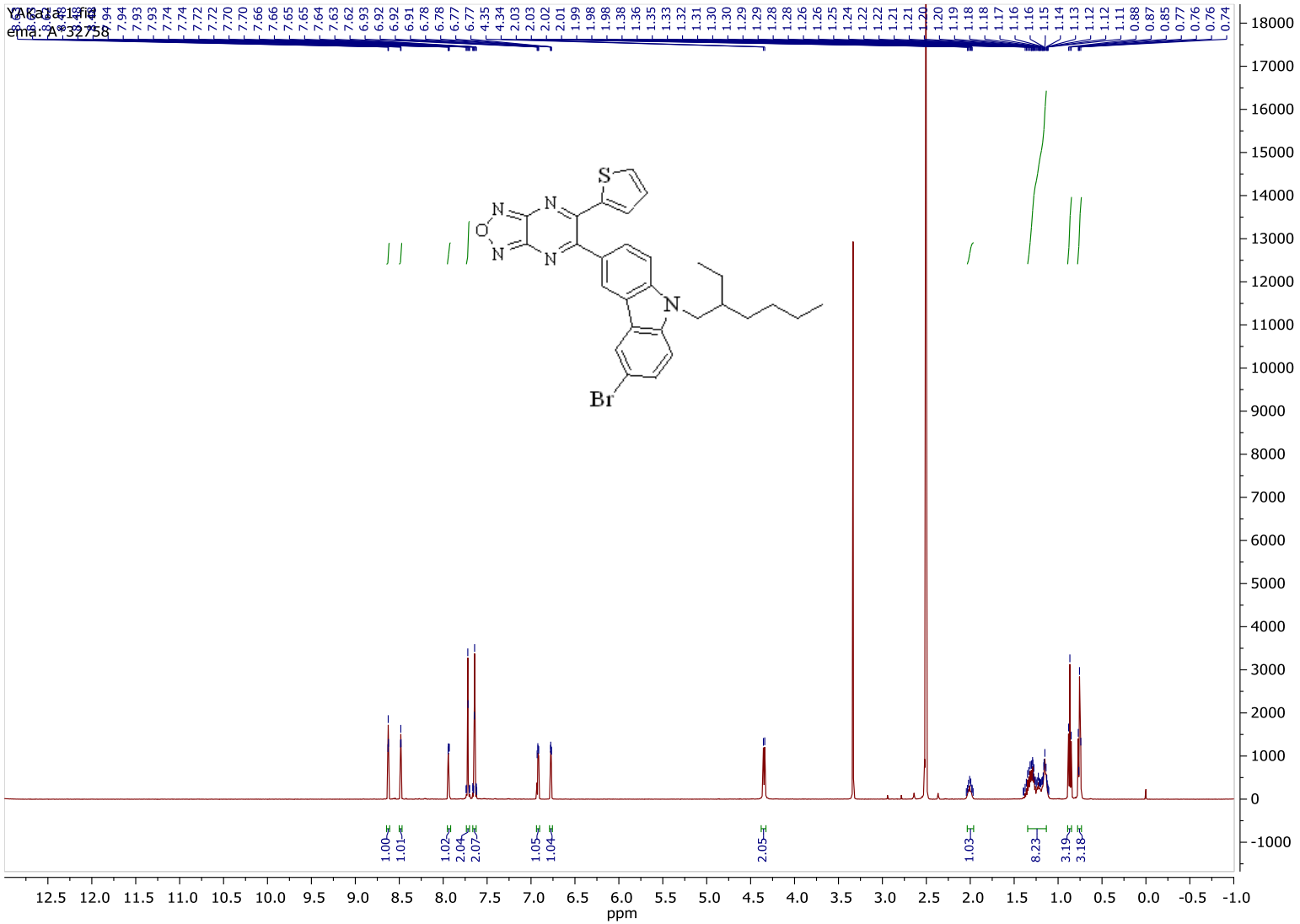

Figure S11. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **7a**.

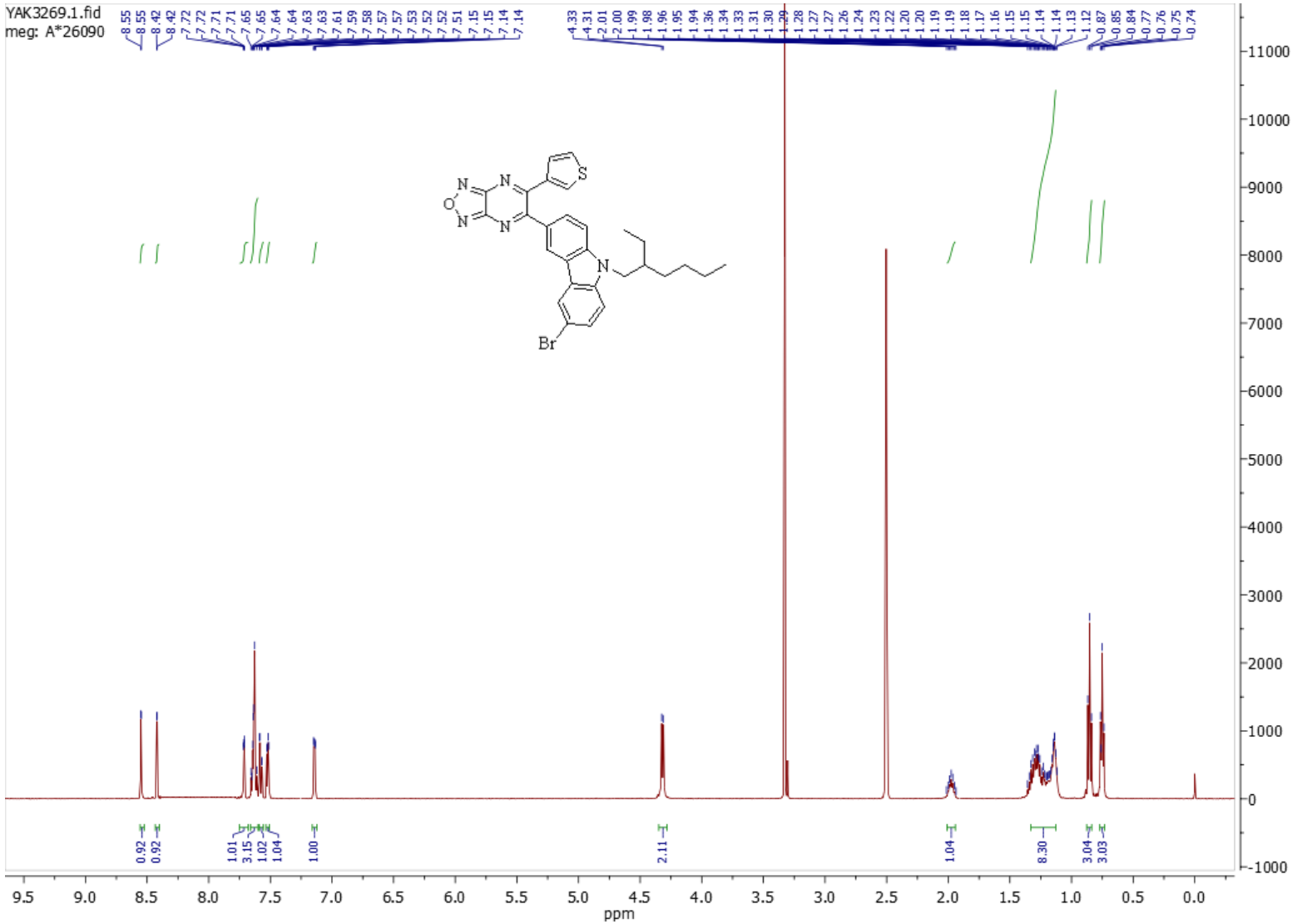

Figure S12. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **7b**.

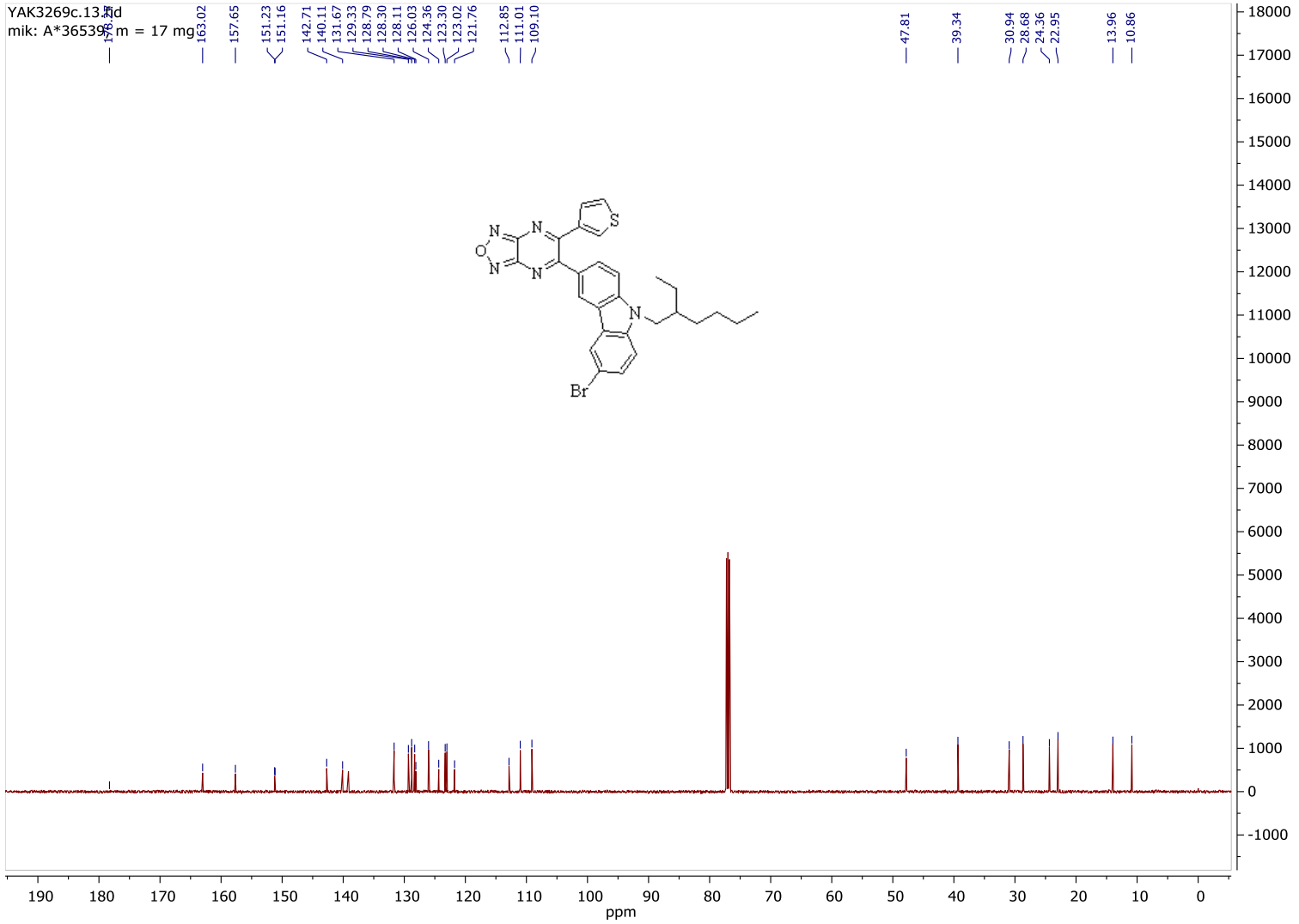

Figure S13. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **7b**.

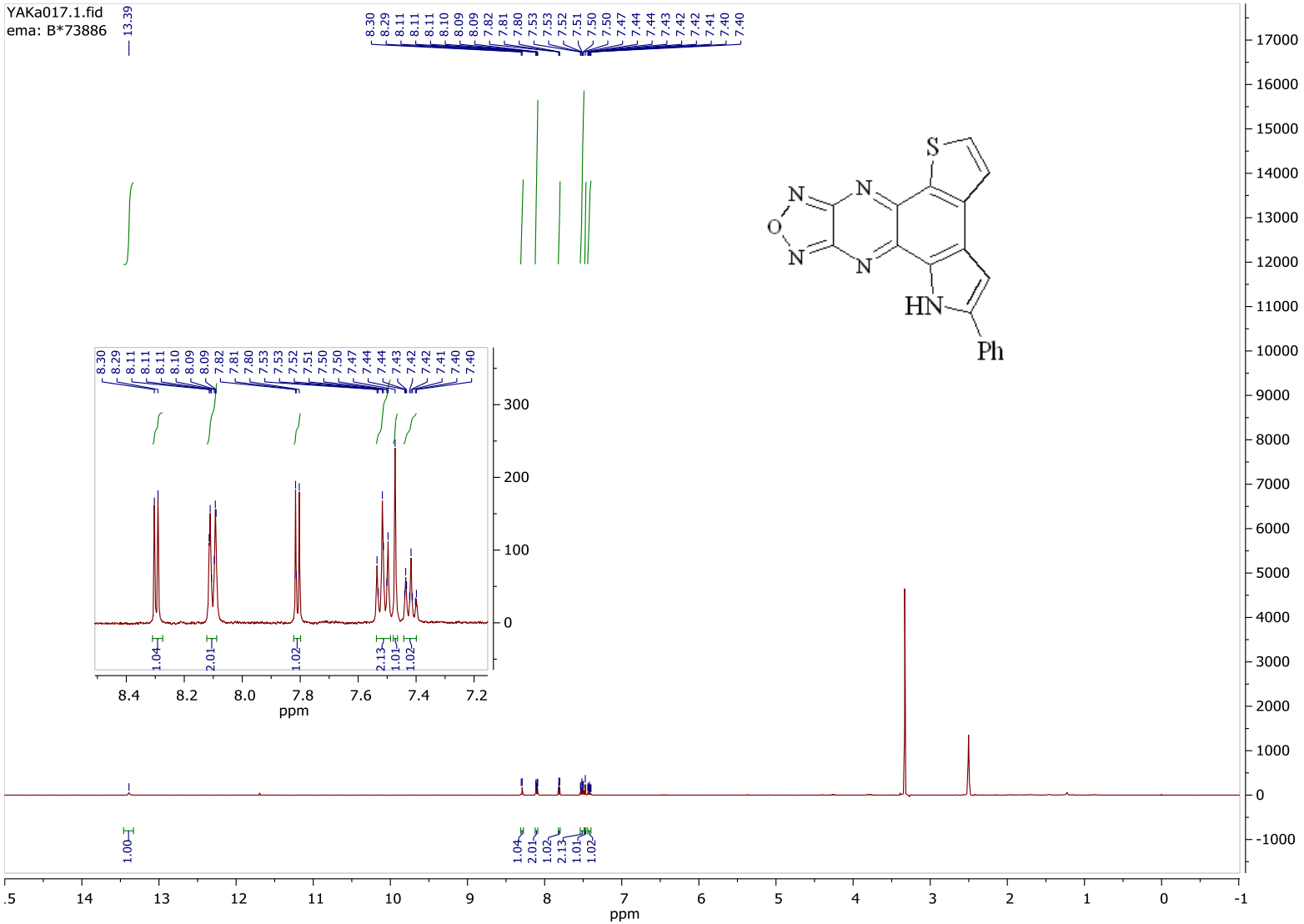

Figure S14. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **8a**.

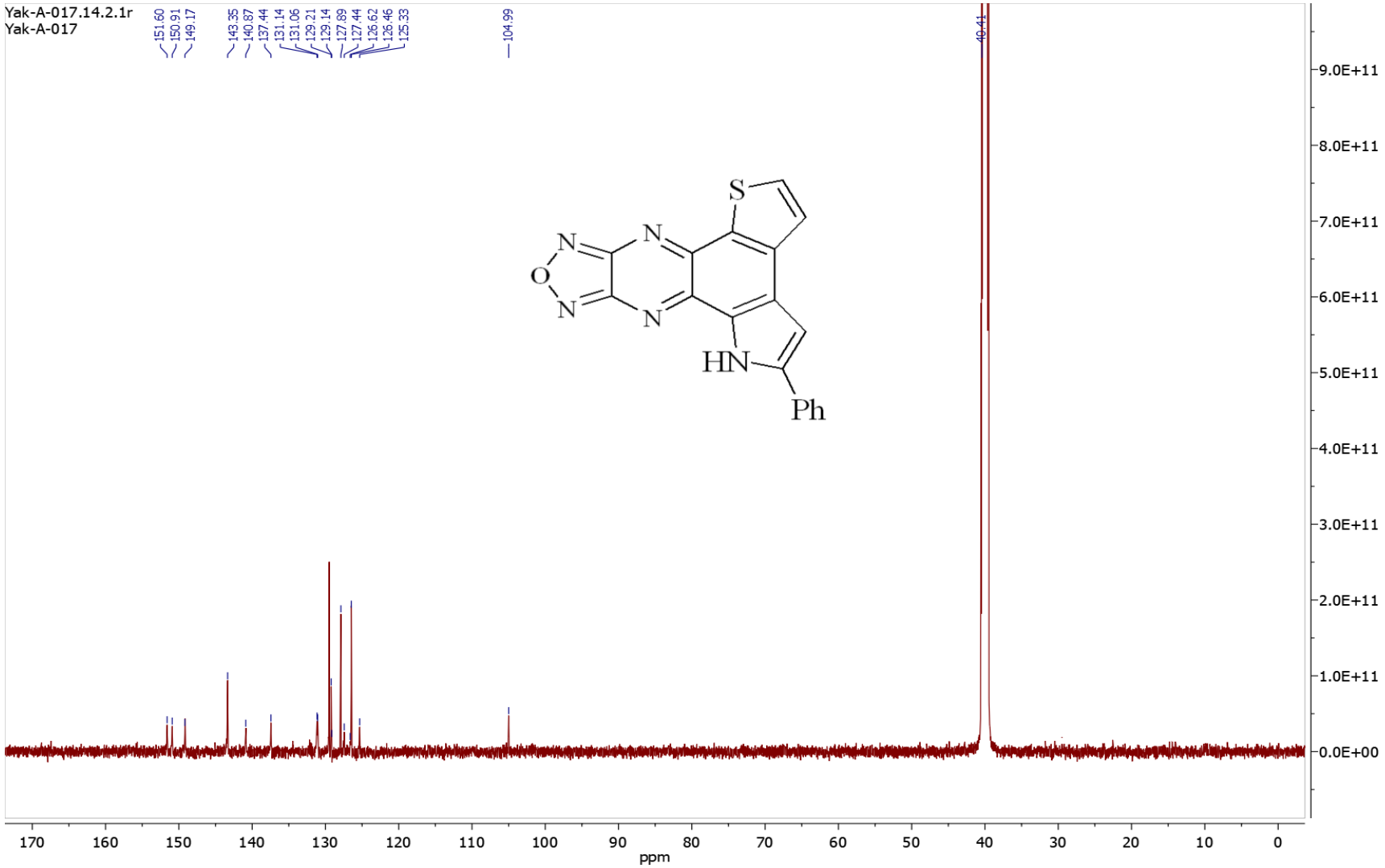

Figure S15. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **8a**.

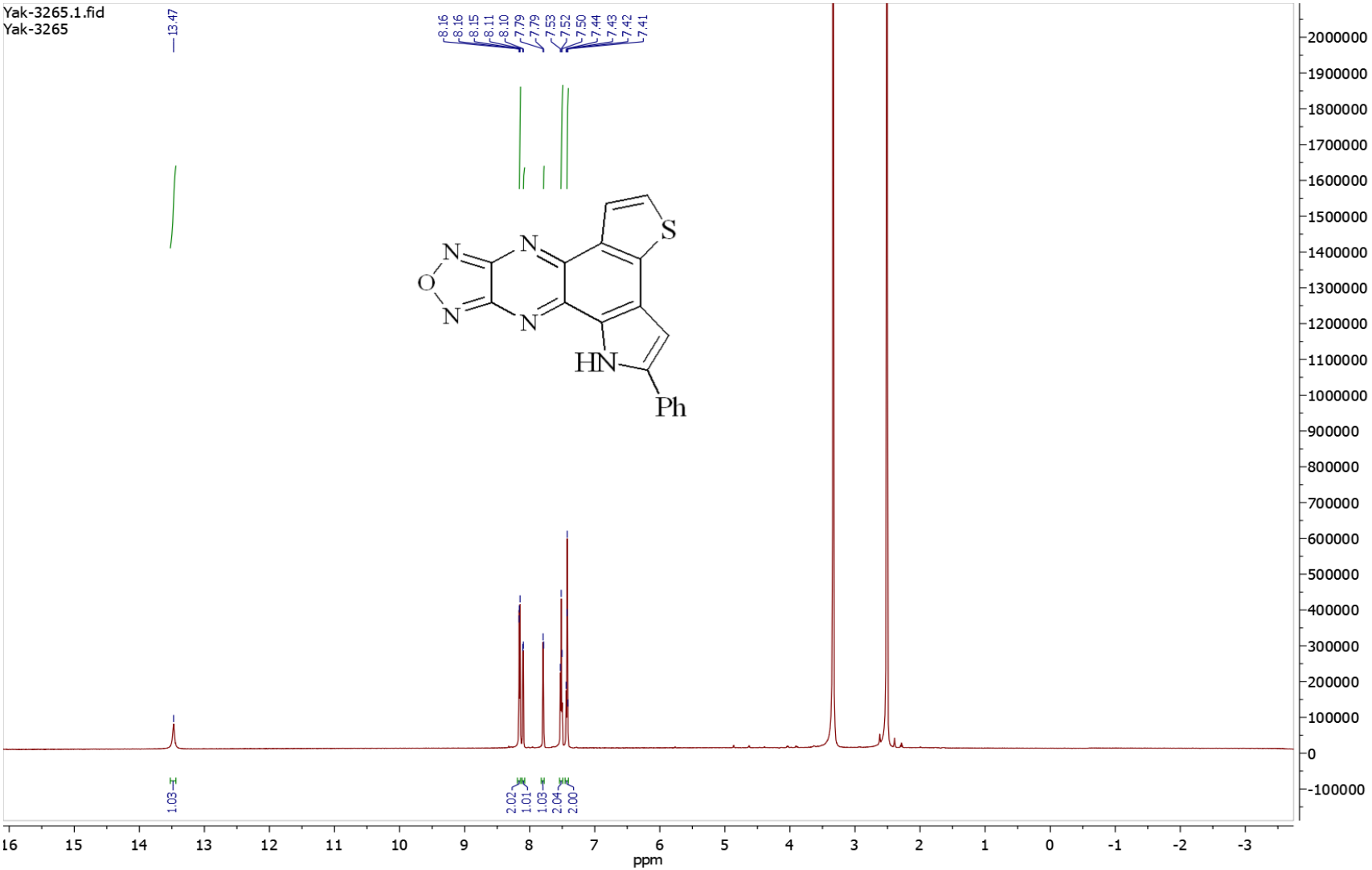

Figure S16. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **8b**.

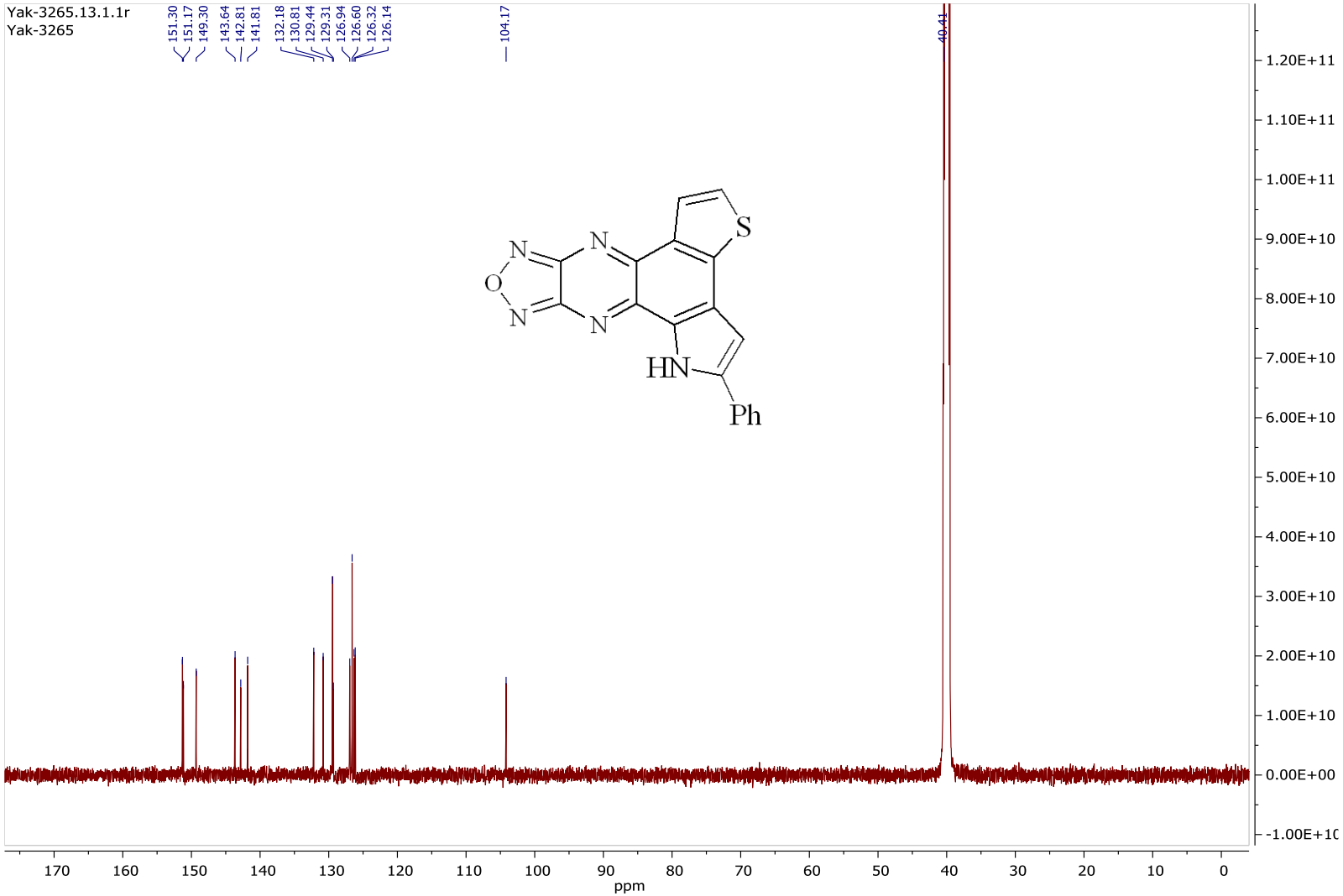

Figure S17. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **8b**.

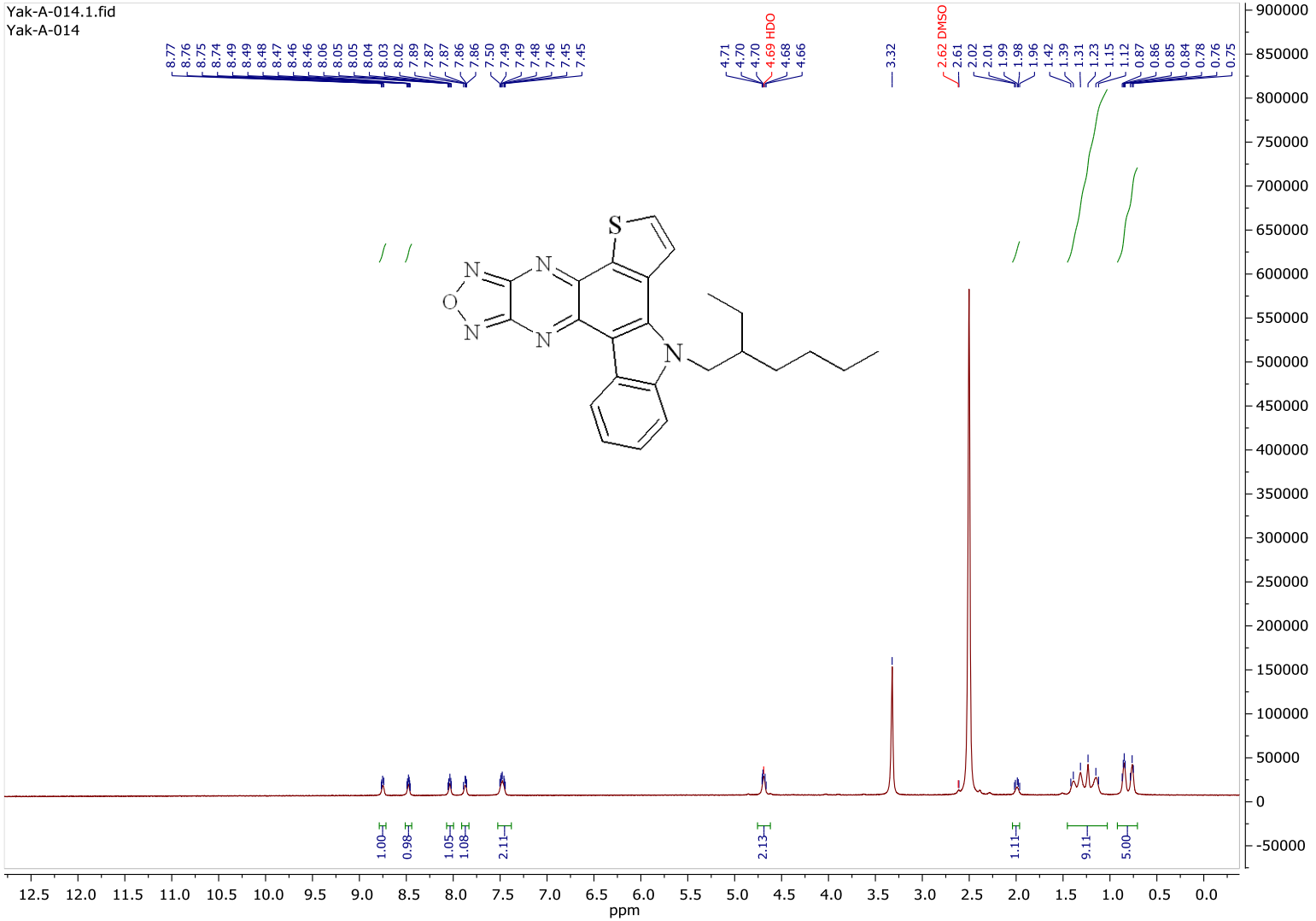

Figure S18. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **9a**.

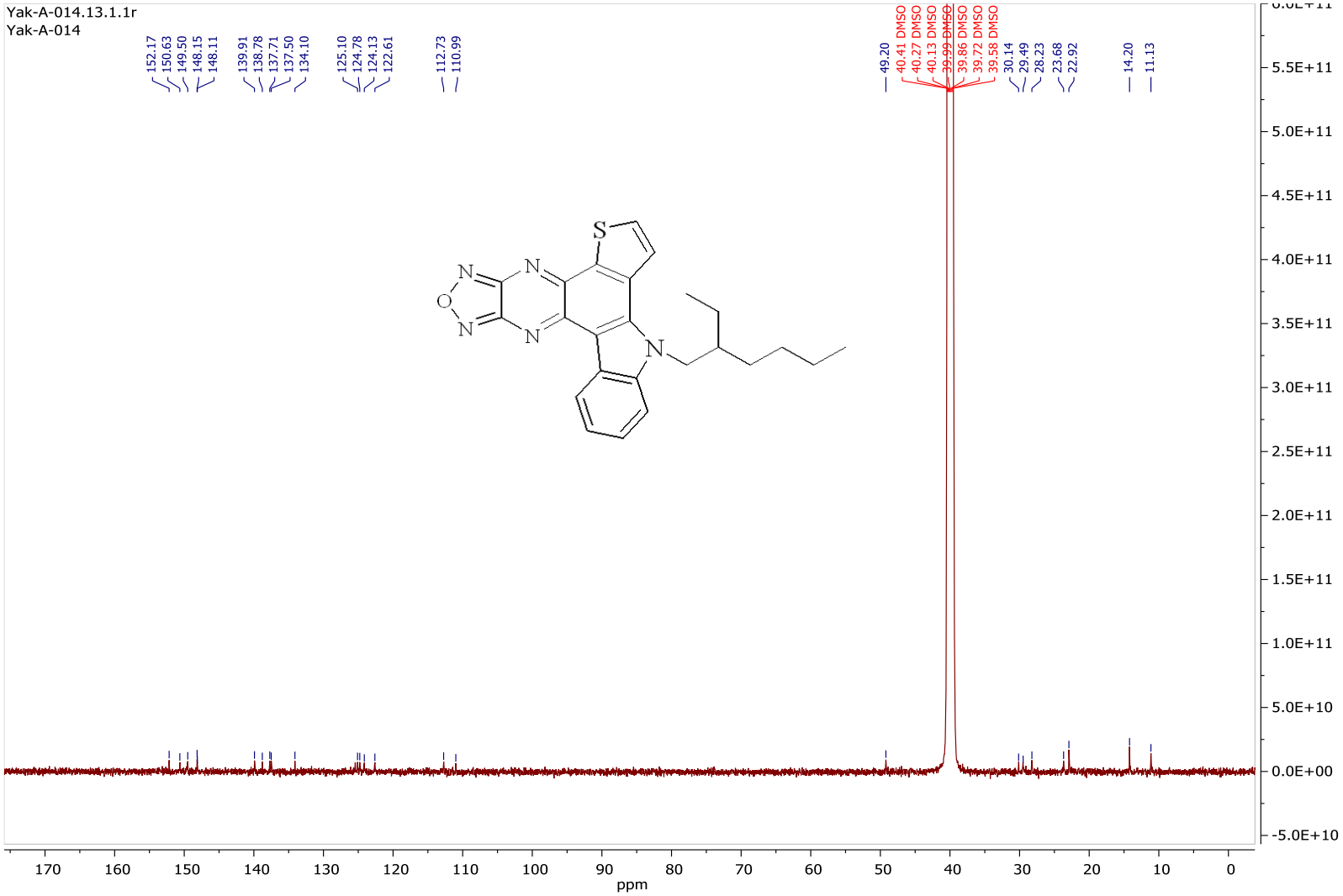

Figure S19. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **9a**.

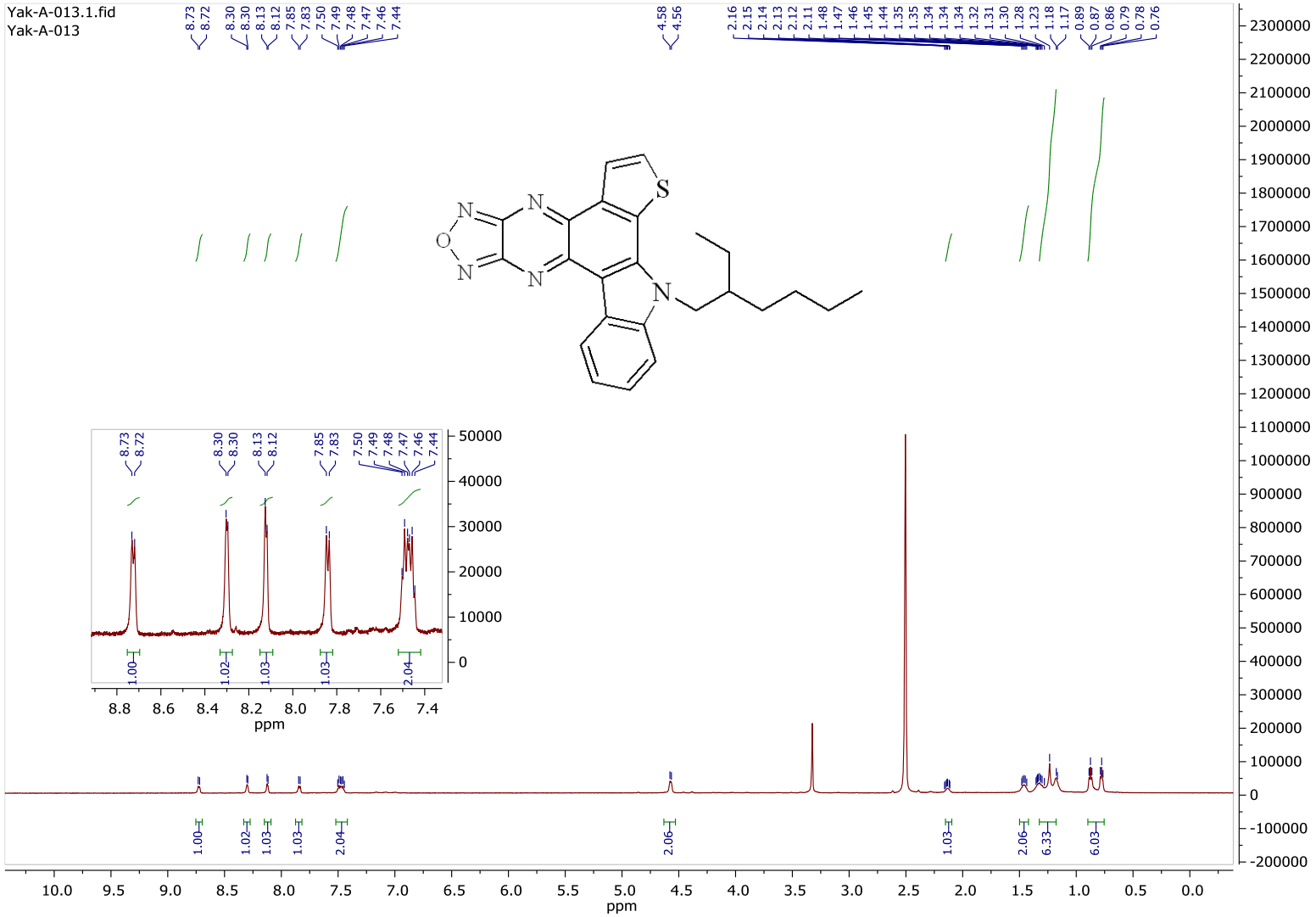

Figure S20. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **9b**.

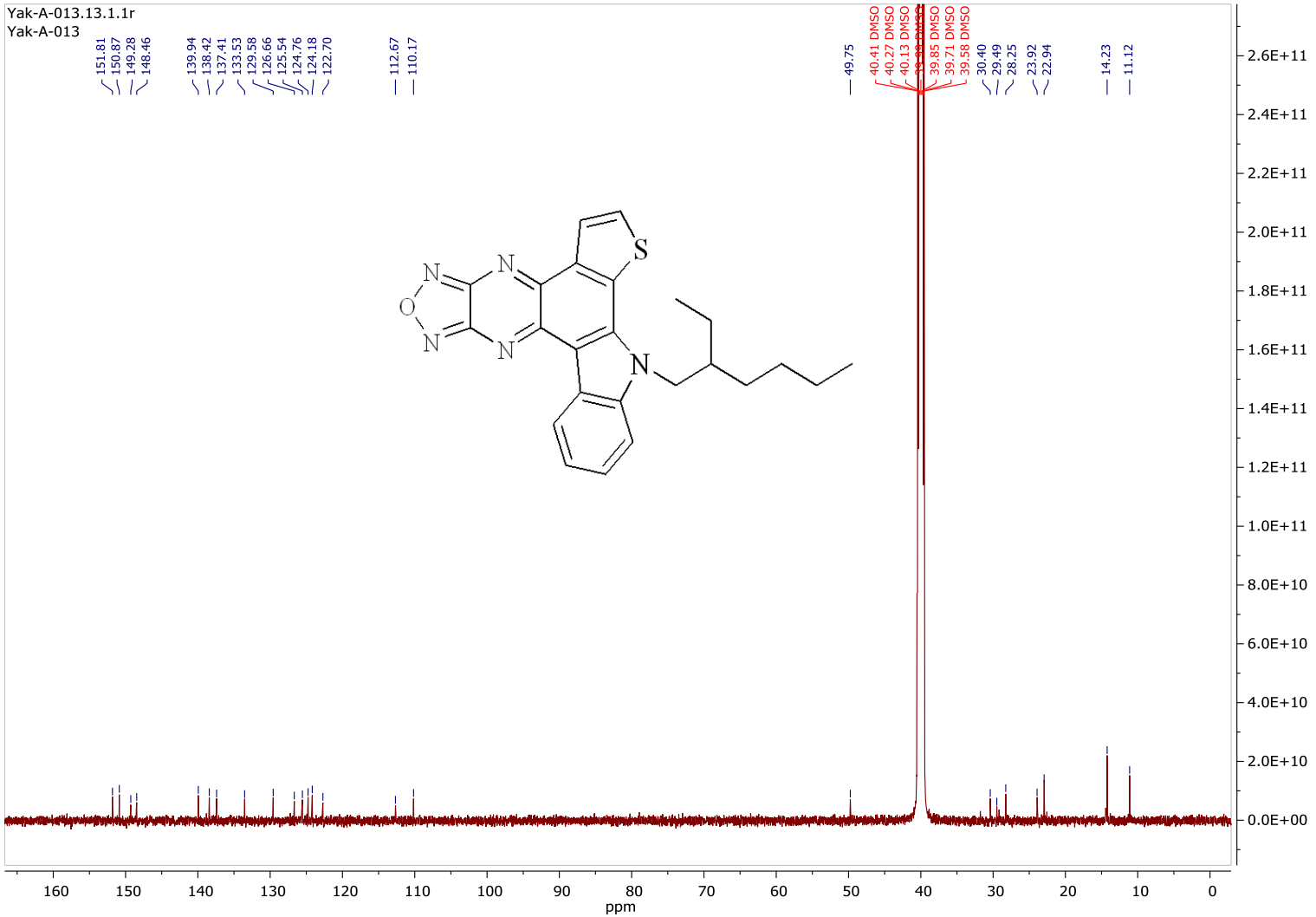

Figure S21. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **9b**.

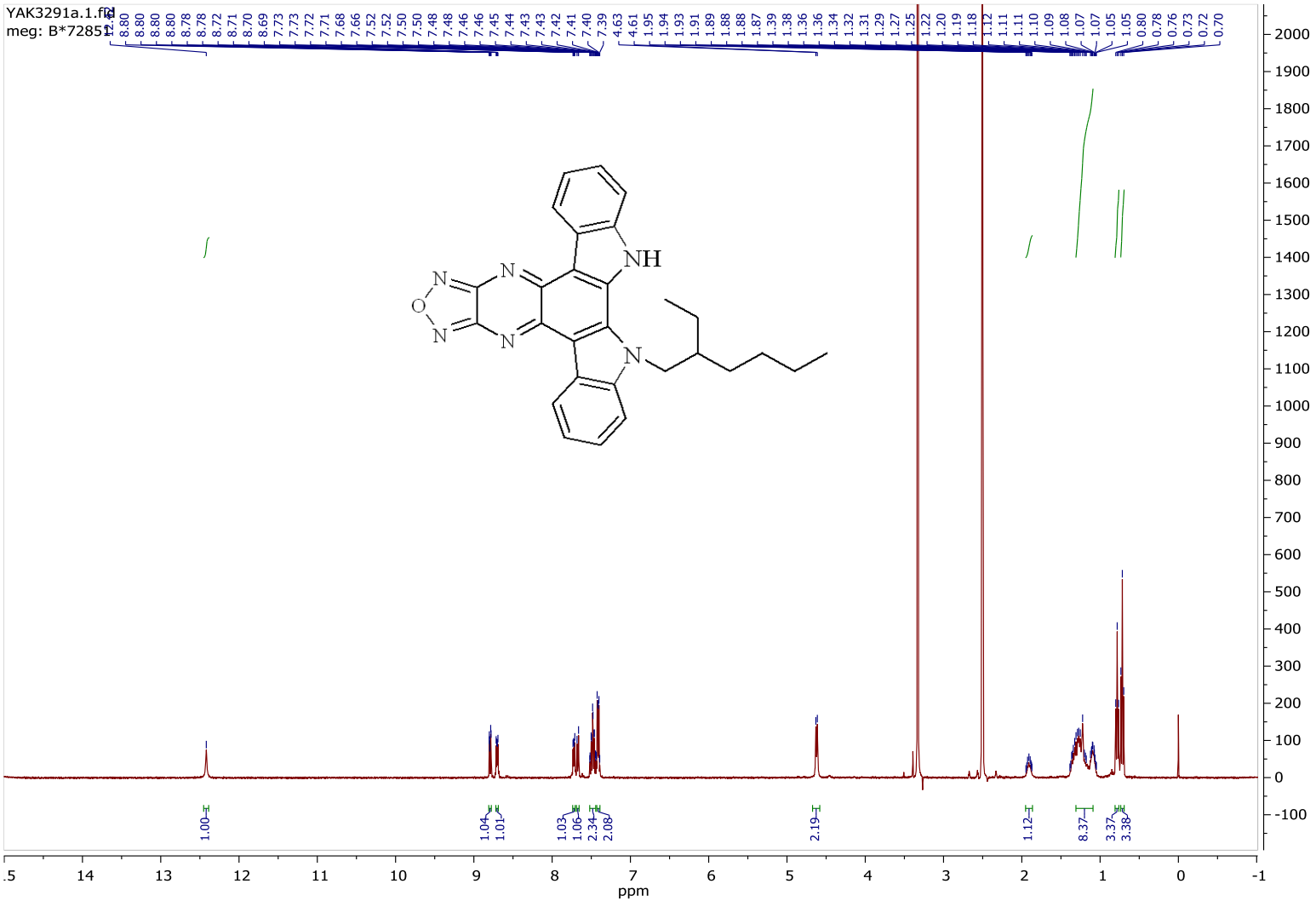

Figure S22. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **9c**.

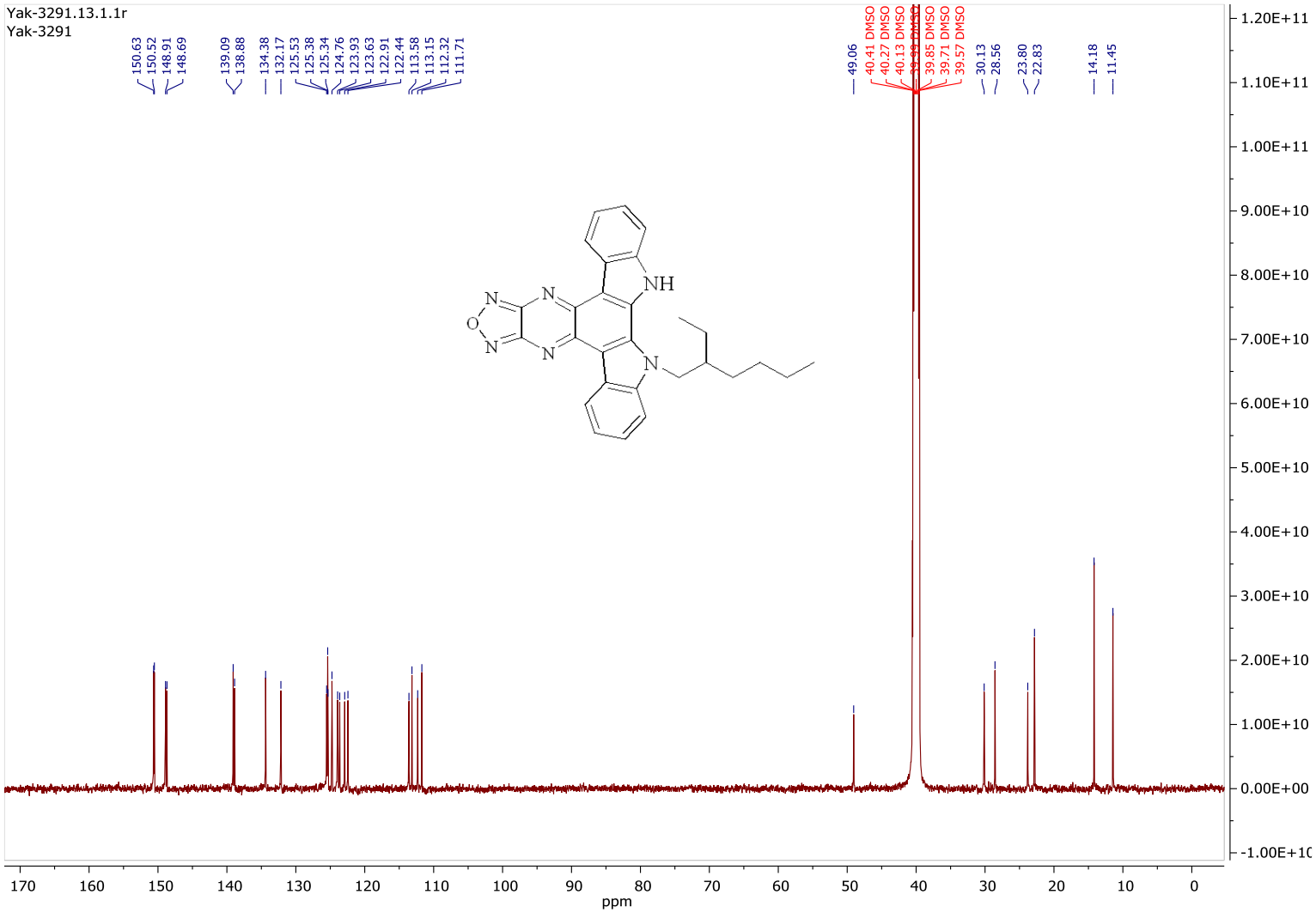

Figure S23. ^{13}C NMR (151 MHz, DMSO-d_6) spectrum of **9c**.

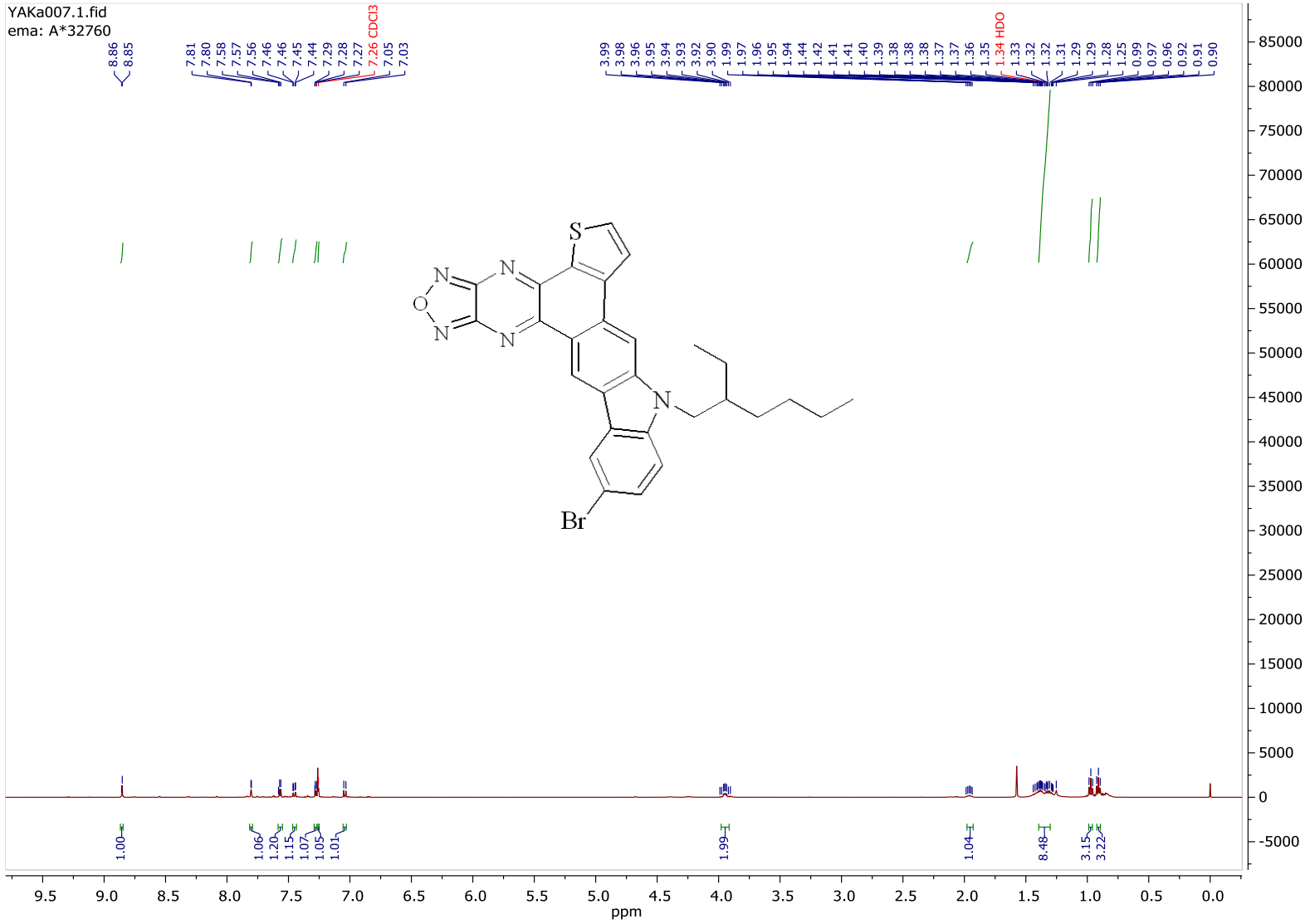

Figure S24. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10a**.

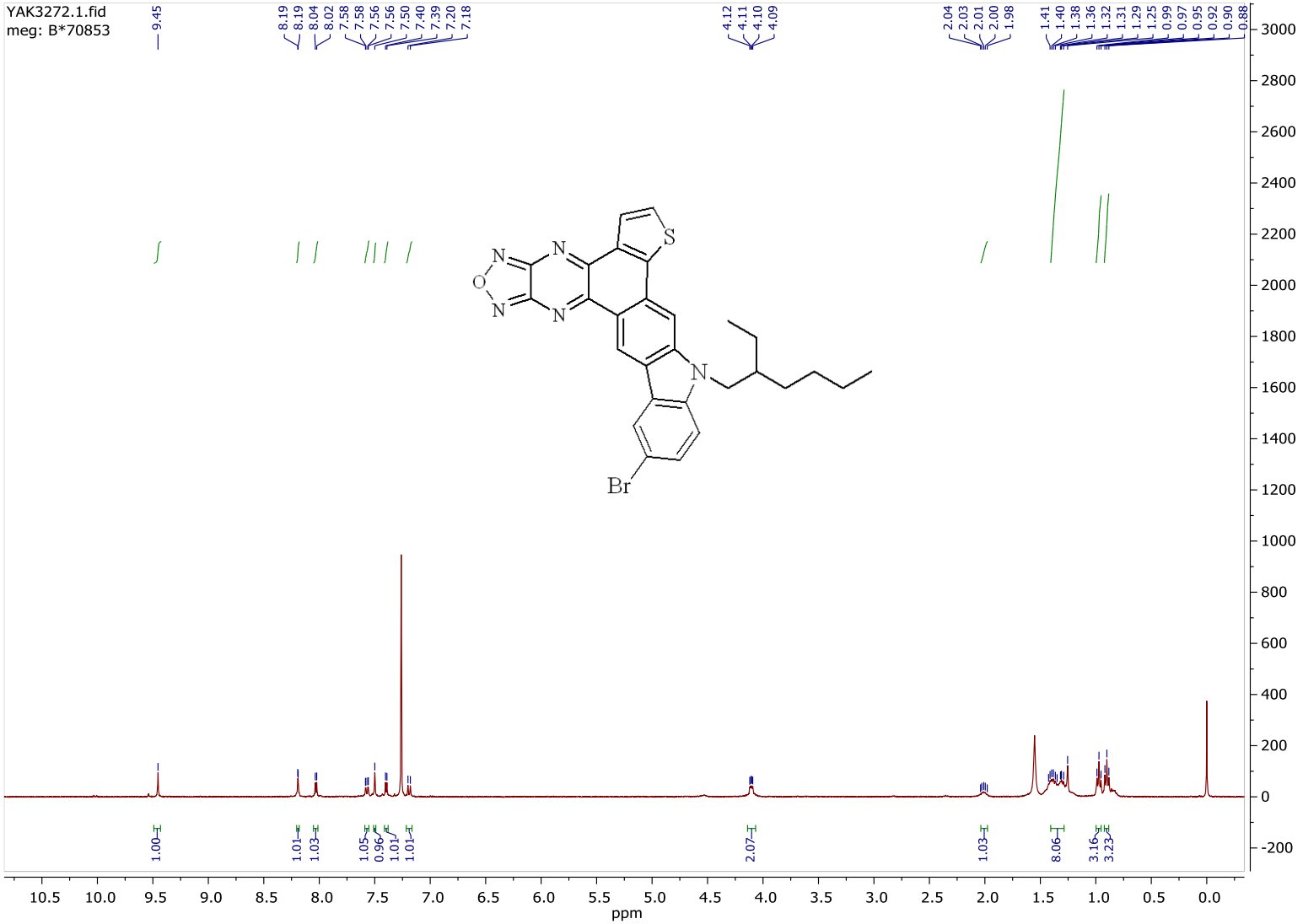

Figure S25. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10b**.

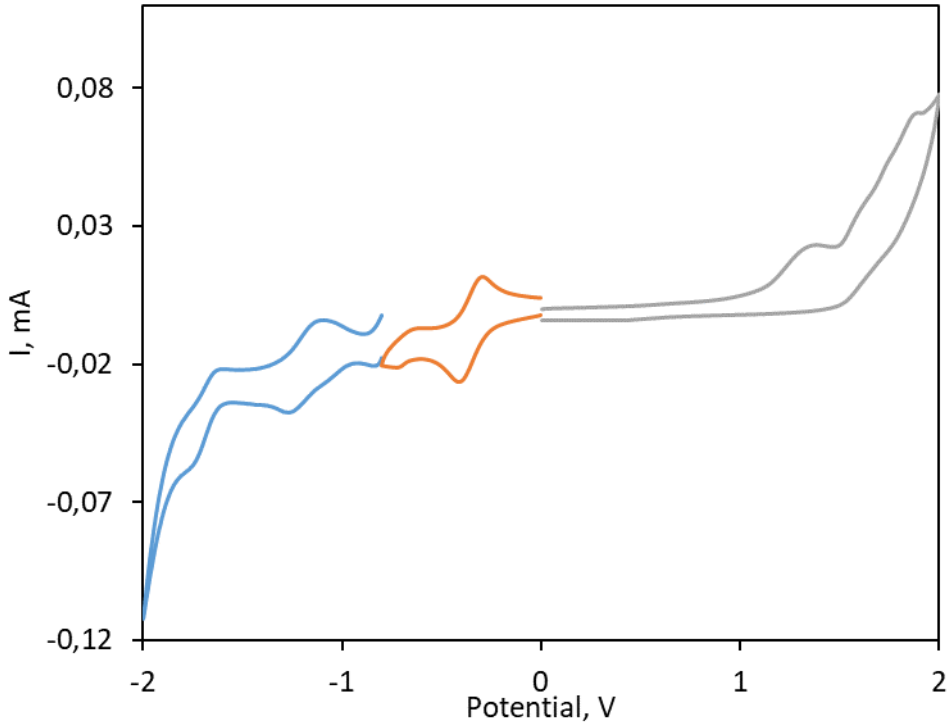

Figure S26. Cyclic voltammograms of **8a** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

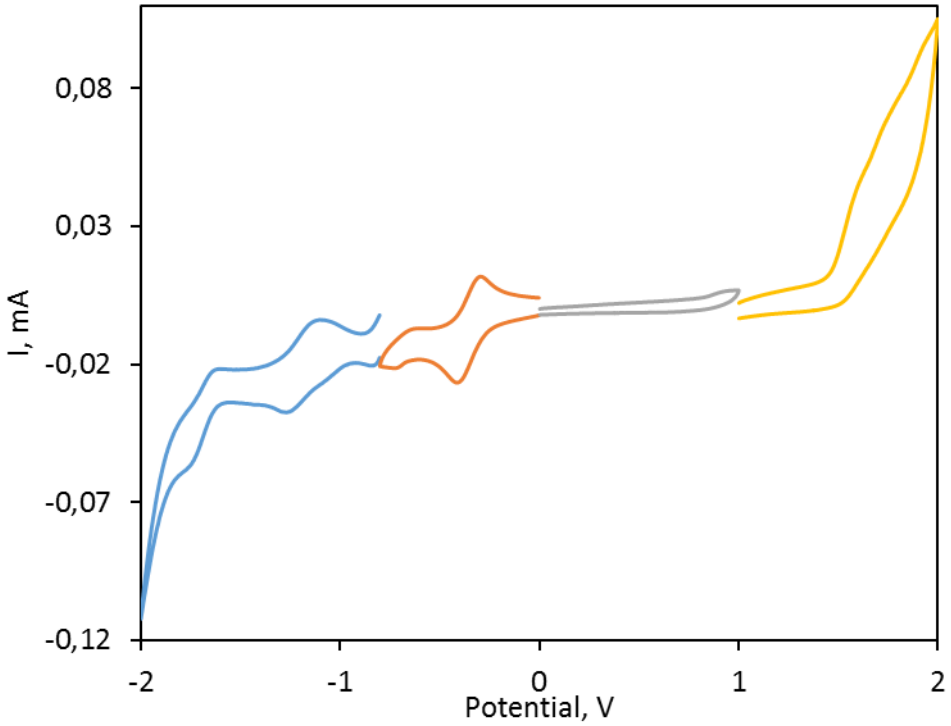

Figure S27 Cyclic voltammograms of **8b** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

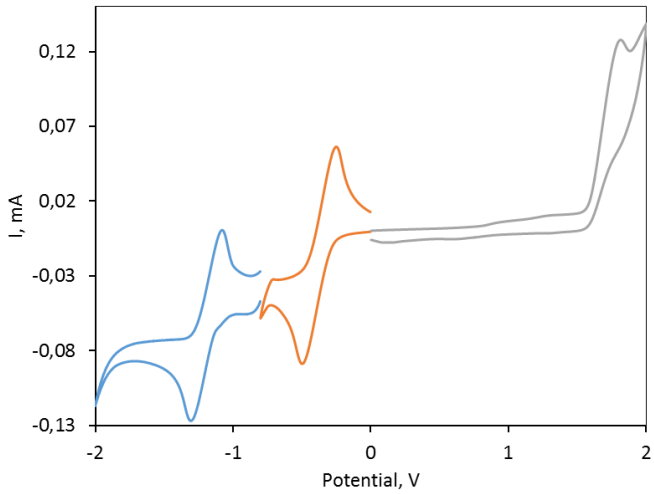

Figure S28. Cyclic voltammograms of **9a** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

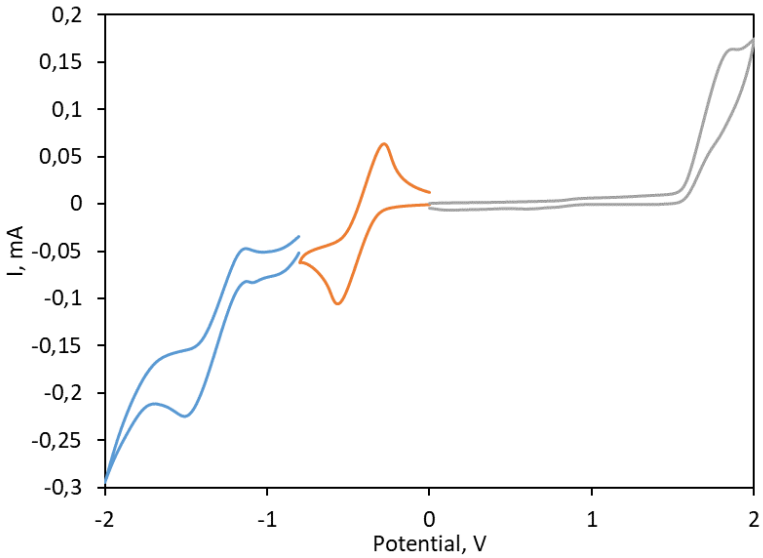

Figure S29 Cyclic voltammograms of **9b** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

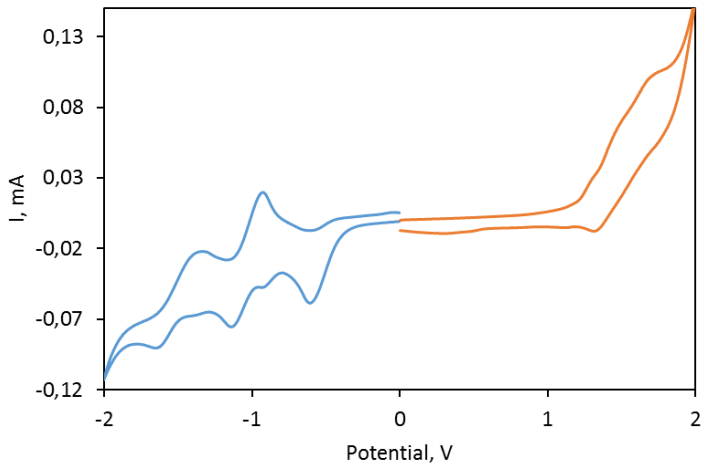

Figure S30 Cyclic voltammograms of **9c** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

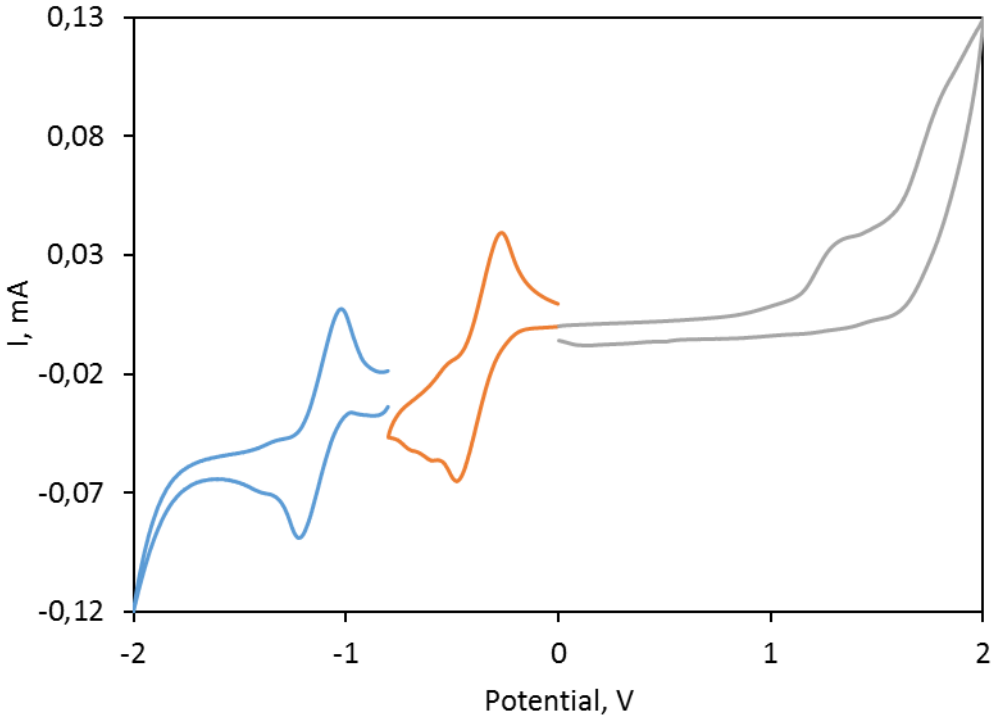

Figure S31 Cyclic voltammograms of **10a** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).

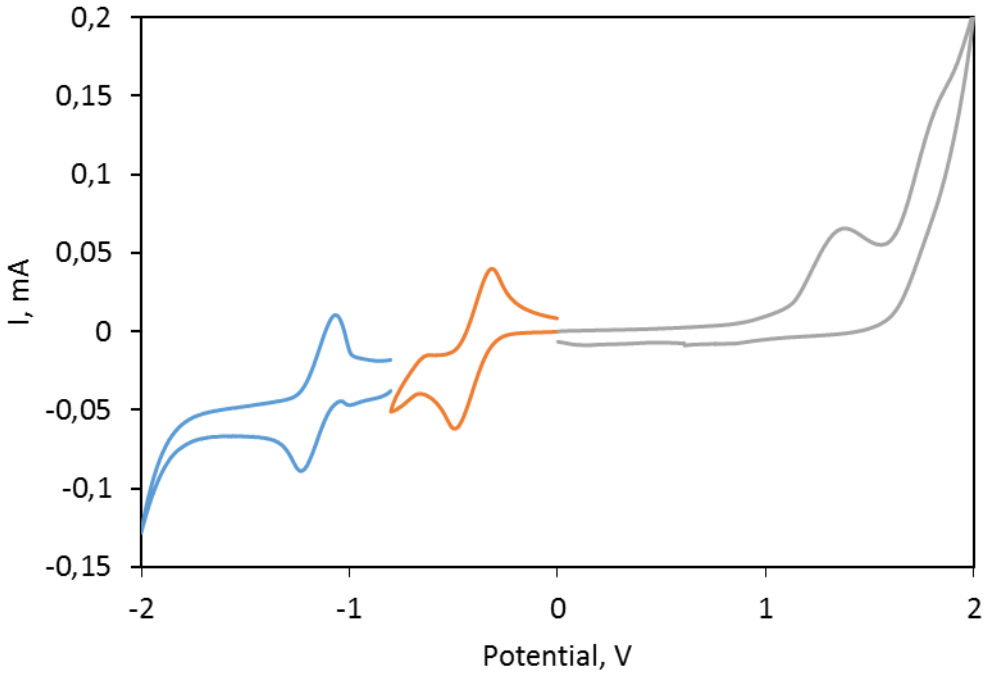

Figure S32 Cyclic voltammograms of **10b** measured in anhydrous CH_2Cl_2 with Bu_4NBF_4 (0.1 M) at 100 mV/s ($Ag/AgNO_3$ reference electrode).