

Supporting Information

Ruthenium-catalyzed oxidative coupling of 2-aryl-4-quinazolinones with olefins: synthesis of pyrrolo[2,1-b]quinazolin-9(1H)-one motifs

Yong Zheng, Wei-Bin Song, Shu-Wei Zhang, Li-Jiang Xuan*

State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 501 Haik Road, Zhangjiang Hi-Tech Park, Shanghai 201203, PR China

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1. Experimental Section

1.1 General

^1H and ^{13}C NMR spectra were recorded on a Bruker NMR spectrometer with CDCl_3 as the solvent and TMS as an internal standard. HRESIMS was measured on an Agilent G6224A TOF spectrometer. TLC was performed on precoated silica gel GF254 plates (Qingdao Marine Chemical Factory). Column chromatography was performed on silica gel (200–300 mesh, Qingdao Marine Chemical Factory). Petroleum was distilled prior to use.

1.2 General procedure for synthesis of 3a-3s:

1 (0.25 mmol), **2** (0.5 mmol), $[\text{RuCl}_2(\text{pcymene})]_2$ (5 % mol), $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$ (2.2 equiv) and DCE (2 ml) were added in a sealed tube. The reaction mixture was allowed to stir at 100°C for 10 h. After cooling at room temperature, the mixture was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to afford the pure product.

2. Data Characterisation:

Methyl 2-(10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3a).

¹H NMR (400 MHz, CDCl₃) δ 8.37 (ddd, *J* = 7.9, 1.6, 0.7 Hz, 1H), 8.19 (dt, *J* = 7.1, 1.2 Hz, 1H), 7.87 – 7.77 (m, 2H), 7.66 – 7.58 (m, 3H), 7.51 (ddd, *J* = 8.2, 6.8, 1.6 Hz, 1H), 5.89 (dd, *J* = 7.9, 3.7 Hz, 1H), 3.72 (dd, *J* = 16.5, 3.8 Hz, 1H), 3.69 (s, 3H), 3.01 (dd, *J* = 16.5, 7.9 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.4, 160.8, 154.4, 151.5, 149.3, 143.3, 134.4, 132.7, 129.4, 127.4, 126.6, 126.5, 123.5, 123.2, 121.0, 58.5, 52.0, 35.8. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₅N₂O₃, 307.1077; found: 307.1086.

Methyl 2-(2-methyl-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3b).

¹H NMR (400 MHz, CDCl₃) δ 8.35 (ddd, *J* = 8.0, 1.5, 0.7 Hz, 1H), 8.05 (d, *J* = 7.9 Hz, 1H), 7.84 – 7.75 (m, 2H), 7.48 (ddd, *J* = 8.1, 6.7, 1.6 Hz, 1H), 7.42 (s, 1H), 7.41 – 7.37 (m, 1H), 5.82 (dd, *J* = 7.9, 3.7 Hz, 1H), 3.73–3.65 (dd, *J* = 16.5, 3.8 Hz, 1H), 3.69 (s, 3H), 3.00 (dd, *J* = 16.6, 7.9 Hz, 1H), 2.50 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 160.7, 154.6, 149.2, 143.7, 143.7, 134.4, 130.5, 129.2, 127.2, 126.5, 126.3, 123.6, 123.3, 120.9, 58.4, 52.0, 35.8, 22.2. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇N₂O₃, 321.1234; found: 321.1228.

Methyl 2-(2-methoxy-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3c).

¹H NMR (400 MHz, CDCl₃) δ 8.35 (dt, *J* = 7.9, 1.0 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.48 (ddd, *J* = 8.1, 5.7, 2.6 Hz, 1H), 7.14 (s, 1H), 7.11 (m, 1H), 5.83 (dd, *J* = 8.2, 3.7 Hz, 1H), 3.93 (s, 3H), 3.72 (dd, *J* = 16.8, 3.7 Hz, 1H), 3.71 (s, 3H), 2.95 (dd, *J* = 16.6, 8.2 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 163.6, 160.7, 154.3, 149.4, 145.7, 134.4, 127.1, 126.5, 126.1, 124.9, 124.1, 120.6, 116.3, 108.0, 58.2, 55.8, 52.0, 35.9. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇N₂O₄, 337.1183; found: 337.1184.

Methyl 2-(2-(diethylamino)-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3d).

¹H NMR (400 MHz, CDCl₃) δ 8.31 (dt, *J* = 7.9, 1.0 Hz, 1H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.40 (ddd, *J* = 8.1, 5.8, 2.4 Hz, 1H), 6.82 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.76 (d, *J* = 2.3 Hz, 1H), 5.77 (dd, *J* = 8.3, 3.9 Hz, 1H), 3.74 (dd, *J* = 16.5, 3.8 Hz, 1H), 3.73 (s, 3H), 3.46 (m, 4H), 2.83 (dd, *J* = 16.3, 8.3 Hz, 1H), 1.24 (t, *J* = 7.1 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 170.9, 160.8, 155.1, 151.4, 146.2, 134.2, 128.4, 126.5, 126.4, 125.3, 125.1, 120.2, 112.7, 111.2, 104.1, 58.2, 52.0, 44.9, 36.6, 12.4. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₂H₂₄N₃O₃, 378.1812; found: 378.1824.

Methyl 2-(2-bromo-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3e).

¹H NMR (400 MHz, CDCl₃) δ 8.40 – 8.35 (m, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.87 – 7.82 (m, 3H), 7.78 – 7.74 (m, 1H), 7.54 (ddt, *J* = 8.2, 6.5, 2.2 Hz, 1H), 5.87 (dd, *J* = 8.2, 3.5 Hz, 1H), 3.73 (dd, *J* = 16.5, 3.6 Hz, 1H), 3.72 (s, 3H), 3.02 (dd, *J* = 16.9, 8.1 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 160.4, 153.7, 145.1, 135.0, 133.1, 129.2, 128.8, 127.2, 126.9, 126.8, 126.7, 126.4, 125.1, 120.8, 58.3, 52.2, 35.4. HRMS (ESI): *m/z* [M+Na]⁺ calcd for C₁₈H₁₃BrN₂NaO₃, 407.0007; found: 400.0002.

Methyl 2-(2-fluoro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3f).

¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, *J* = 8.0 Hz, 1H), 8.24 (m, 1H), 7.87 – 7.81 (m, 2H), 7.56 – 7.52 (m, 1H), 7.40 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.36 – 7.31 (m, 1H), 5.88 (dd, *J* = 8.4, 3.5 Hz, 1H), 3.79 (dd, *J* = 16.8, 3.5 Hz, 1H), 3.72 (s, 3H), 2.96 (dd, *J* = 16.8, 8.4 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 165.8 (d, *J*_{C-F} = 255 Hz), 160.4, 153.6, 145.9 (d, *J*_{C-F} = 9.9 Hz), 135.1, 134.7, 129.6 (d, *J*_{C-F} = 9.5 Hz), 127.9, 127.0, 126.8, 126.7, 126.4, 116.3 (d, *J*_{C-F} = 21.9 Hz), 111.1 (d, *J*_{C-F} = 25.0 Hz), 58.5, 52.1, 35.4. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄FN₂O₃, 325.0983; found: 325.0997.

Methyl 2-(2-nitro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3g).

¹H NMR (400 MHz, CDCl₃) δ 8.57 – 8.54 (m, 1H), 8.50 (dd, *J* = 8.4, 2.0 Hz, 1H), 8.43 – 8.36 (m, 2H), 7.94 – 7.83 (m, 2H), 7.60 (ddd, *J* = 8.1, 6.7, 1.6 Hz, 1H), 5.98 (dd, *J* = 7.9, 3.4 Hz, 1H), 3.78 (dd, *J* = 17.1, 3.5 Hz, 1H), 3.70 (s, 3H), 3.20 (dd, *J* = 17.1, 7.9 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 160.3, 152.3, 150.6, 148.5, 144.3, 137.6, 134.9, 127.8, 127.8, 126.7, 125.1, 124.6, 121.1, 119.1, 58.6, 52.3, 35.0. HRMS (ESI): *m/z* [M+Na]⁺ calcd for C₁₈H₁₃N₃NaO₅, 374.0747; found: 374.0751.

Methyl 2-(3-methyl-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3h).

¹H NMR (400 MHz, CDCl₃) δ 8.38 – 8.33 (m, 1H), 7.97 (s, 1H), 7.84 – 7.75 (m, 2H), 7.49 (td, *J* = 7.3, 6.5, 1.5 Hz, 2H), 7.45 – 7.39 (m, 1H), 5.96 – 5.75 (m, 1H), 3.71 (dd, *J* = 16.5, 3.7 Hz, 1H), 3.68 (s, 3H), 2.97 (dd, *J* = 16.4, 8.0 Hz, 1H), 2.49 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.4, 160.7, 154.6, 149.1, 140.6, 139.7, 134.4, 133.8, 131.9, 127.3, 126.5, 126.4, 123.7, 122.9, 121.0, 58.4, 52.0, 35.9, 21.4. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇N₂O₃, 321.1234; found: 321.1236.

Methyl 2-(3-chloro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3i).

¹H NMR (400 MHz, CDCl₃) δ 8.39 – 8.29 (m, 1H), 8.16 (s, 1H), 7.85 – 7.79 (m, 2H), 7.59 (m, 2H), 7.53 (m, 1H), 5.85 (dd, *J* = 8.1, 3.6 Hz, 1H), 3.73 (dd, *J* = 16.7, 3.7 Hz, 1H), 3.69 (s, 3H), 3.00 (dd, *J* = 16.7, 8.1 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 160.6, 153.2, 149.0, 141.5, 135.8, 134.5, 133.8, 132.7, 127.6, 126.9, 126.6, 124.6, 123.5, 121.1, 58.3, 52.1, 35.5. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄ClN₂O₃, 341.0687; found: 363.0688.

Methyl 2-(3-nitro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3j).

¹H NMR (400 MHz, CDCl₃) δ 8.38 – 8.32 (m, 1H), 7.94 – 7.89 (m, 1H), 7.87 – 7.74 (m, 4H), 7.56 (ddd, *J* = 8.2, 6.3, 1.9 Hz, 1H), 5.94 (dd, *J* = 8.2, 3.5 Hz, 1H), 3.79 (dd, *J* = 16.9, 3.5 Hz, 1H), 3.72 (s, 3H), 3.03 (dd, *J* = 16.9, 8.2 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 160.4, 149.7, 148.7, 146.2, 145.6, 134.6, 133.0, 128.6, 127.6, 126.6, 126.3, 123.5, 123.5, 120.9, 58.1, 52.2, 35.5. HRMS (ESI): *m/z* [M+Na]⁺ calcd for C₁₈H₁₃N₃NaO₅, 374.0747; found: 374.0741.

Methyl 2-(4-chloro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3k).

¹H NMR (400 MHz, CDCl₃) δ 8.40 – 8.34 (m, 1H), 7.96 – 7.90 (m, 1H), 7.82 (ddd, *J* = 8.4, 7.1, 1.6 Hz, 1H), 7.60 – 7.51 (m, 4H), 5.93 – 5.82 (m, 1H), 3.70 (dd, *J* = 16.5, 3.7 Hz, 1H), 3.69 (s, 3H), 3.01 (dd, *J* = 16.6, 7.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 160.6, 152.7, 149.1, 145.7, 134.4, 132.9, 131.6, 131.3, 128.5, 128.4, 127.1, 126.3, 121.5, 120.8, 57.7, 52.1, 35.9. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄ClN₂O₃, 341.0687; found: 341.0684.

Methyl 2-(4-fluoro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3l).

¹H NMR (400 MHz, CDCl₃) δ 8.37 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.94 – 7.89 (m, 1H), 7.83 (dt, *J* = 6.7, 1.4 Hz, 1H), 7.62 (m, 1H), 7.54 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.31 – 7.26 (m, 2H), 5.91 (dd, *J* = 7.9, 3.6 Hz, 1H), 3.70 (dd, *J* = 16.9, 3.7 Hz, 1H), 3.69 (s, 3H), 3.06 (dd, *J* = 16.6, 7.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 160.5, 158.8 (d, *J*_{C-F} = 267.9 Hz), 151.9 (d, *J*_{C-F} = 5 Hz), 149.2, 145.6 (d, *J*_{C-F} = 2.2 Hz), 134.9, 134.5, 134.4 (d, *J*_{C-F} = 7.8 Hz), 128.1, 127.0, 126.4, 120.7, 119.2 (d, *J*_{C-F} = 4.1 Hz), 116.8 (d, *J*_{C-F} = 19.2 Hz), 58.5, 52.1, 35.8. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄FN₂O₃, 325.0983; found: 325.0997.

Methyl 2-(8-methoxy-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3m).

¹H NMR (400 MHz, CDCl₃) δ 8.19 (d, *J* = 6.9 Hz, 1H), 7.80 (d, *J* = 8.9 Hz, 1H), 7.76 (d, *J* = 3.0 Hz, 1H), 7.63 (m, 3H), 7.42 (dd, *J* = 8.9, 3.0 Hz, 1H), 5.91 (dd, *J* = 7.9, 3.8 Hz, 1H), 3.97 (s, 3H), 3.71 (dd, *J* = 16.9, 3.8 Hz, 1H), 3.70 (s, 3H), 3.03 (dd, *J* = 16.5, 7.9 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.4, 160.5, 158.4, 152.6, 142.9, 132.4, 129.5, 128.8, 124.6, 123.3, 123.2, 121.7, 106.2, 58.6, 55.9, 52.0, 35.8. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇N₂O₄, 337.11183; found: 337.1176.

Methyl 2-(6-methyl-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3n).

¹H NMR (400 MHz, CDCl₃) δ 8.22 – 8.14 (m, 2H), 7.59 (m, 4H), 7.36 (t, *J* = 7.6 Hz, 1H), 5.84 (dd, *J* = 8.0, 3.7 Hz, 1H), 3.71 (dd, *J* = 16.6, 3.8 Hz, 1H), 3.67 (s, 3H), 2.96 (dd, *J* = 16.5, 8.0 Hz, 1H), 2.71 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 161.1, 153.1, 147.9, 143.2, 136.1, 134.9, 132.4, 132.4, 129.3, 126.0, 124.2, 123.5, 123.1, 120.9, 58.4, 51.9, 35.8, 17.5. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇N₂O₃, 321.1234; found: 321.1245.

Methyl 2-(7-chloro-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3o).

¹H NMR (400 MHz, CDCl₃) δ 8.28 (d, *J* = 8.5 Hz, 1H), 8.16 (dt, *J* = 7.4, 1.1 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.67 – 7.59 (m, 3H), 7.44 (dd, *J* = 8.5, 2.0 Hz, 1H), 5.86 (dd, *J* = 7.9, 3.7 Hz, 1H), 3.67 (dd, *J* = 16.4, 3.8 Hz, 1H), 3.66 (s, 3H), 3.02 (dd, *J* = 16.5, 7.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 160.2, 155.6, 150.3, 143.4, 140.6, 133.0, 131.7, 129.6, 128.0, 127.1, 127.0, 123.7, 123.2, 119.5, 58.7, 52.0, 35.7. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄ClN₂O₃, 341.0687; found: 341.0680.

Methyl 2-(8-bromo-10-oxo-10,12-dihydroisoindolo[1,2-b]quinazolin-12-yl)acetate (3p).

¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 2.3 Hz, 1H), 8.14 (d, *J* = 7.4 Hz, 1H), 7.85 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.68 (d, *J* = 8.7 Hz, 1H), 7.65 – 7.56 (m, 3H), 5.85 (dd, *J* = 7.8, 3.8 Hz, 1H), 3.66 (s, 3H), 3.65 (dd, *J* = 16.5, 3.8 Hz, 1H), 3.02 (dd, *J* = 16.5, 7.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 159.5, 154.8, 148.1, 143.3, 137.5, 132.9, 131.7, 129.5, 129.2, 123.6, 123.2, 122.4, 120.0, 58.7, 52.0, 35.6. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄BrN₂O₃, 407.0002; found: 407.0005.

Methyl 2-(6-oxo-4,6-dihydrothieno[2',3':3,4]pyrrolo[2,1-b]quinazolin-4-yl)acetate (3r).

¹H NMR (400 MHz, CDCl₃) δ 8.37 – 8.33 (m, 1H), 7.82 – 7.77 (m, 2H), 7.76 (d, *J* = 4.9 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.24 (d, *J* = 4.9 Hz, 1H), 5.77 (dd, *J* = 9.8, 3.9 Hz, 1H), 3.98 (dd, *J* = 16.6, 3.9 Hz, 1H), 3.77 (s, 3H), 2.65 (dd, *J* = 16.6, 9.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 170.5,

160.5, 153.4, 151.3, 136.3, 134.5, 131.3, 128.4, 127.0, 126.6, 126.5, 122.4, 120.1, 57.5, 52.1, 35.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}N_2O_3S$, 313.0641; found: 313.0649.

(E)-2-(3-(2-(phenylsulfonyl)vinyl)thiophen-2-yl)quinazolin-4(3H)-one (**3s**).

1H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 15.5 Hz, 1H), 8.35 – 8.27 (m, 1H), 8.02 – 7.92 (m, 2H), 7.92 – 7.82 (m, 2H), 7.65 – 7.47 (m, 6H), 7.37 (d, J = 5.2 Hz, 1H), 6.89 (d, J = 15.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 148.6, 146.2, 140.5, 136.5, 135.8, 135.4, 135.3, 133.4, 130.0, 129.3, 128.5, 128.2, 128.1, 127.8, 127.7, 127.6, 126.5, 77.3. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{20}H_{14}N_2NaS_2O_3$, 417.0344; found: 417.0345.

Methyl 2-(6-oxo-4,6-dihydrofuro[2',3':3,4]pyrrolo[2,1-b]quinazolin-4-yl)acetate (3t).

1H NMR (400 MHz, $CDCl_3$) δ 9.77 (br s, 1H, NH), 8.85 (d, J = 16.2 Hz, 1H), 8.31 (dd, J = 7.9, 1.5 Hz, 1H), 7.95 – 7.70 (m, 2H), 7.60 (d, J = 2.1 Hz, 1H), 7.55 – 7.49 (m, 1H), 6.87 (d, J = 2.1 Hz, 1H), 6.42 (d, J = 16.2 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 161.2, 148.8, 144.5, 143.2, 143.1, 135.1, 134.9, 128.2, 127.3, 126.6, 125.7, 121.7, 119.4, 111.0, 51.9. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{16}H_{12}N_2NaO_4$, 319.0689; found: 319.0689.

Tert-butyl 2-(6-oxo-4,6-dihydrofuro[2',3':3,4]pyrrolo[2,1-b]quinazolin-4-yl)acetate (3u).

1H NMR (400 MHz, $CDCl_3$) δ 10.1 (br s, 1H, NH), 8.76 (d, J = 16.2 Hz, 1H), 8.45 – 8.16 (m, 1H), 8.00 – 7.72 (m, 2H), 7.66 – 7.54 (m, 1H), 7.50 (m, 1H), 6.85 (d, J = 1.9 Hz, 1H), 6.33 (d, J = 16.1 Hz, 1H), 1.60 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 161.5, 148.9, 144.4, 143.4, 143.0, 134.9, 133.9, 128.1, 127.2, 126.5, 126.0, 124.1, 121.2, 110.9, 80.7, 28.2. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{19}H_{18}N_2NaO_4$, 361.1156; found: 361.1156.

(E)-2-(3-(2-(phenylsulfonyl)vinyl)furan-2-yl)quinazolin-4(3H)-one (**3v**).

1H NMR (400 MHz, $CDCl_3$) δ 9.54 (br s, 1H, NH), 8.88 (d, J = 15.6 Hz, 1H), 8.41 – 8.26 (m, 1H), 8.04 (dd, J = 8.4, 1.4 Hz, 2H), 7.89 – 7.81 (m, 2H), 7.72 – 7.65 (m, 1H), 7.64 – 7.58 (m, 3H), 7.56 (dd, J = 8.0, 2.7 Hz, 1H), 6.93 (d, J = 15.6 Hz, 1H), 6.77 (d, J = 1.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 148.6, 144.6, 144.1, 142.8, 140.4, 135.1, 133.6, 132.9, 131.1, 129.4, 128.4, 128.0, 127.6, 126.6, 123.5, 111.2. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{20}H_{14}N_2NaO_4S$, 401.0566; found: 401.0568.

1,1'-(2-(4-Oxo-3,4-dihydroquinazolin-2-yl)-1,3-phenylene)bis(pentan-3-one) (5a).

1H NMR (400 MHz, $CDCl_3$) δ 11.14 (br s, 1H, NH), 8.31 (dd, J = 8.1, 1.5 Hz, 1H), 7.80 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.73 (dd, J = 8.3, 1.4 Hz, 1H), 7.53 (td, J = 7.5, 6.9, 1.3 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.15 (d, J = 7.7 Hz, 2H), 2.95 – 2.64 (m, 8H), 2.32 (q, J = 7.0 Hz, 4H), 0.95 (t, J = 7.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.9, 189.8, 162.2, 153.2, 148.6, 139.7, 134.7, 133.7, 130.2, 127.5, 127.2, 126.8, 126.6, 121.2, 43.1, 40.3, 36.0, 26.9, 7.7. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{24}H_{26}N_2NaO_3$, 413.1836; found: 413.1848.

1,1'-(2-(4-Oxo-3-(3-oxopentyl)-3,4-dihydroquinazolin-2-yl)-1,3-phenylene)bis(pentan-3-one) (5a').

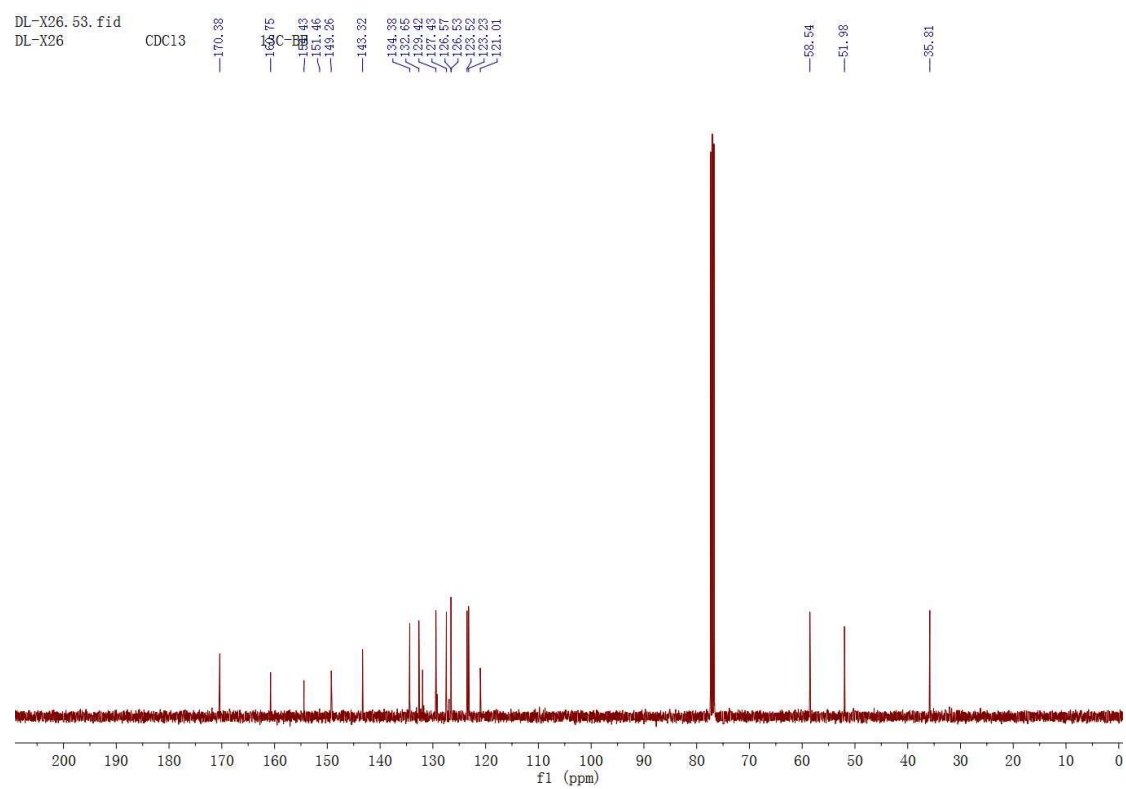
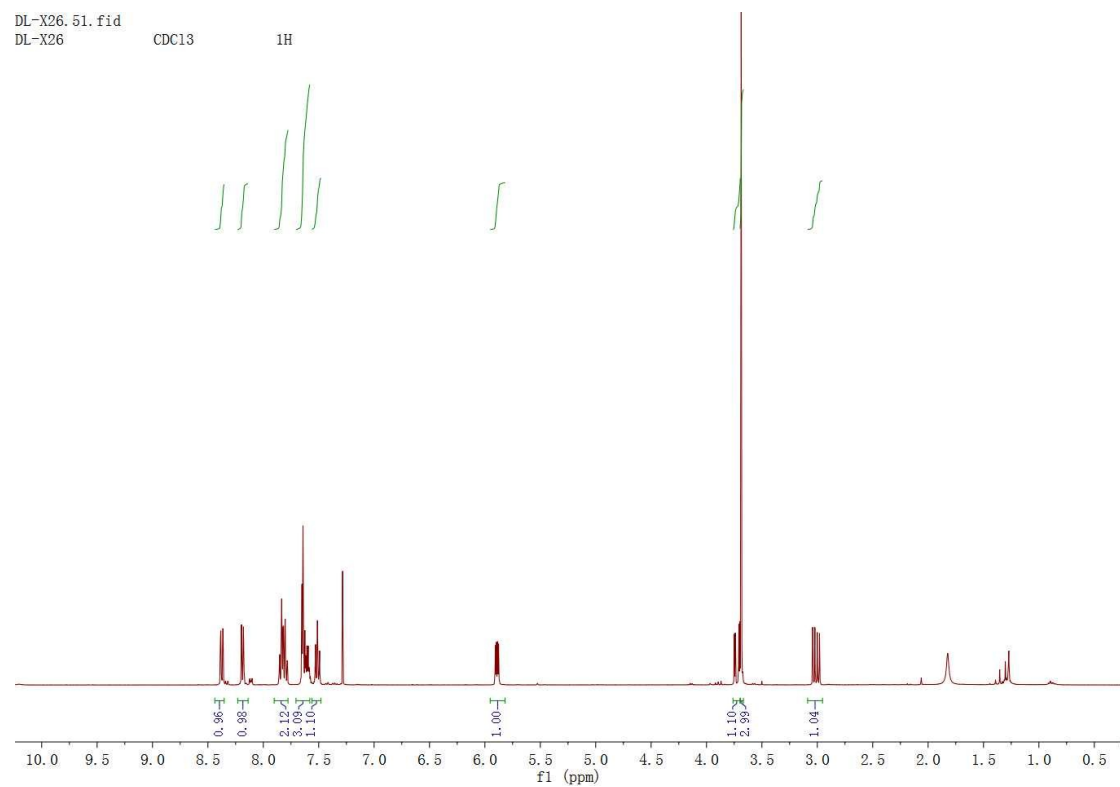
1H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, J = 8.1, 1.5 Hz, 1H), 7.78 (ddd, J = 8.4, 7.1, 1.5 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.55 (ddd, J = 8.0, 7.1, 1.2 Hz, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.18 (d, J = 7.7 Hz, 2H), 4.07 – 3.98 (m, 2H), 2.80 (m, 6H), 2.74 – 2.62 (m, 2H), 2.58 – 2.46 (m, 2H), 2.42 – 2.26

(m, 6H), 0.99 (t, $J = 7.3$ Hz, 3H), 0.97 (t, $J = 7.3$ Hz, 3H), 0.96 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 208.3, 161.9, 154.4, 146.8, 138.7, 134.6, 133.7, 130.3, 127.4, 127.3, 127.0, 126.9, 120.9, 42.8, 41.2, 39.9, 35.9, 35.9, 30.3, 29.7, 27.4, 14.2, 7.7, 7.6. HRMS (ESI): m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{NaO}_4$, 497.2411; found: 497.2426.

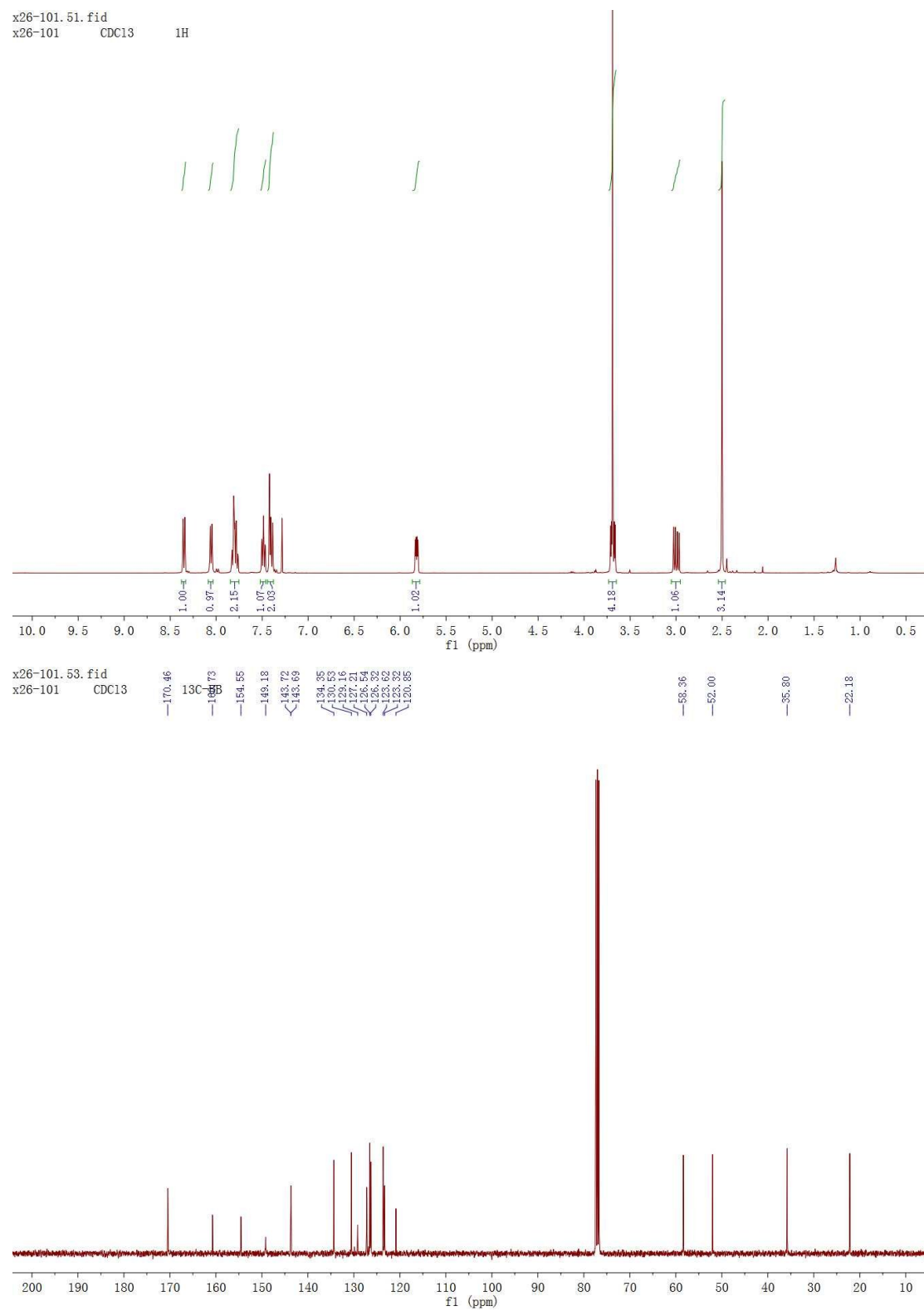
2-(3-(3-Oxopentyl)thiophen-2-yl)quinazolin-4(3H)-one (5o).

^1H NMR (400 MHz, CDCl_3) δ 12.12 (*br s*, 1H, NH), 8.32 (d, $J = 8.0$ Hz, 1H), 7.74 (dd, $J = 3.9$, 1.5 Hz, 2H), 7.50 – 7.41 (m, 2H), 6.94 (d, $J = 5.1$ Hz, 1H), 3.11 (dd, $J = 6.9$, 5.0 Hz, 2H), 3.03 (dd, $J = 6.9$, 5.1 Hz, 2H), 2.48 (q, $J = 7.4$ Hz, 2H), 1.06 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 213.2, 162.5, 149.3, 148.4, 141.4, 134.5, 131.8, 129.3, 129.0, 127.5, 126.6, 121.0, 42.1, 36.1, 22.9, 7.8. HRMS (ESI): m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{16}\text{N}_2\text{NaO}_2\text{S}$, 335.0825; found: 335.0825.

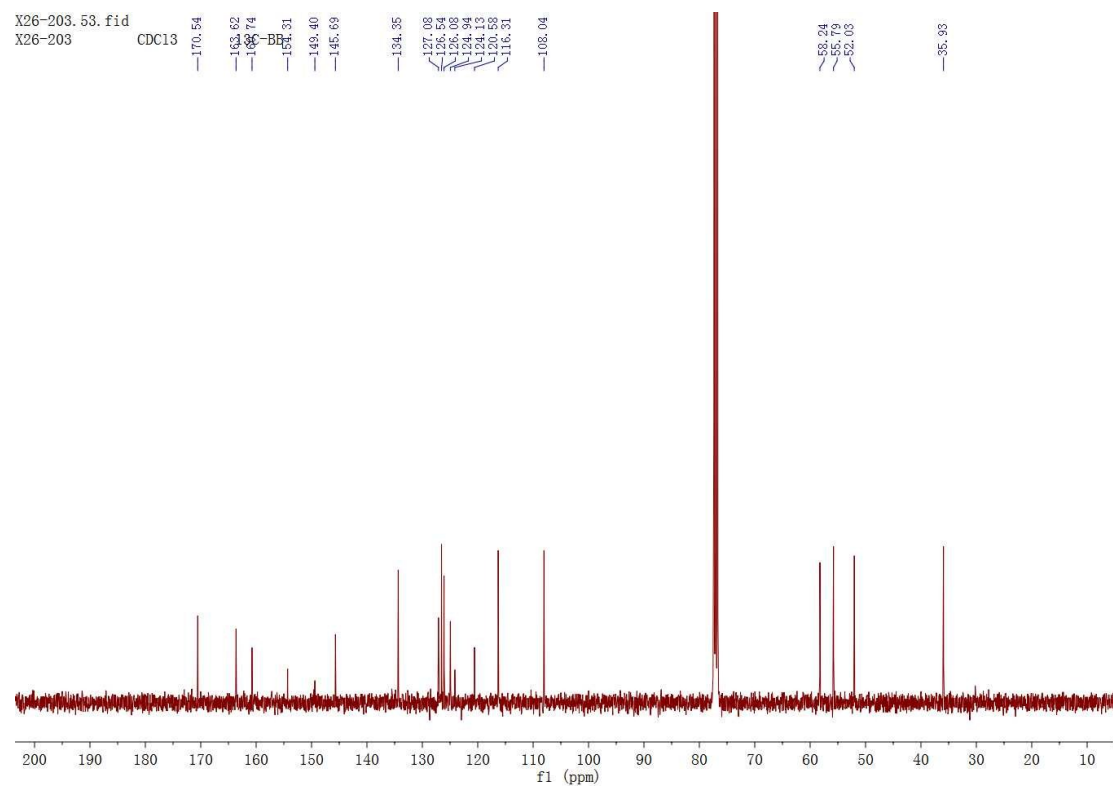
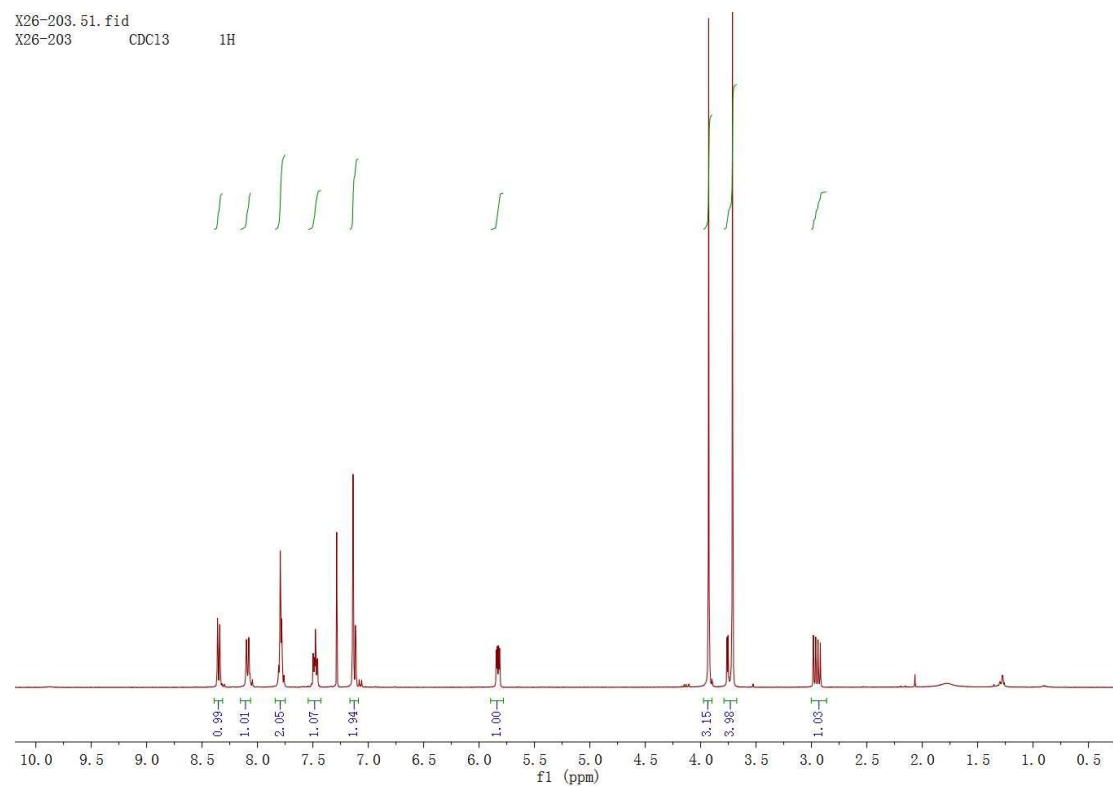
^1H and ^{13}C NMR spectra of **3a**:



^1H and ^{13}C NMR spectra of **3b**:



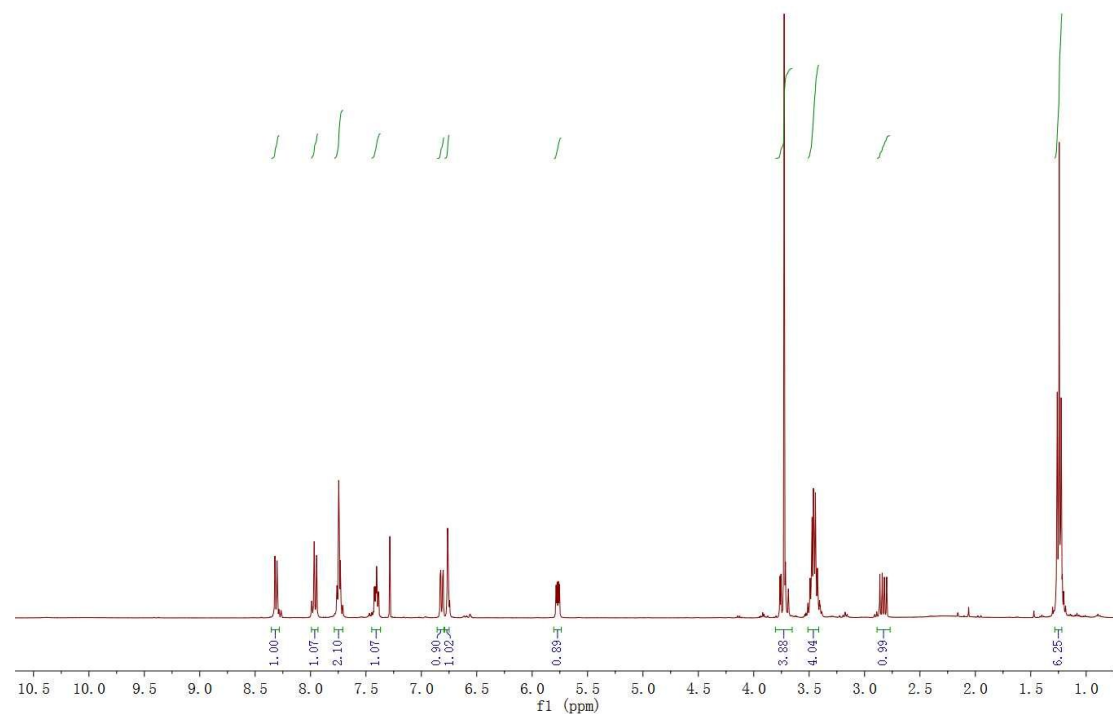
^1H and ^{13}C NMR spectra of **3c**:



^1H and ^{13}C NMR spectra of **3d**:

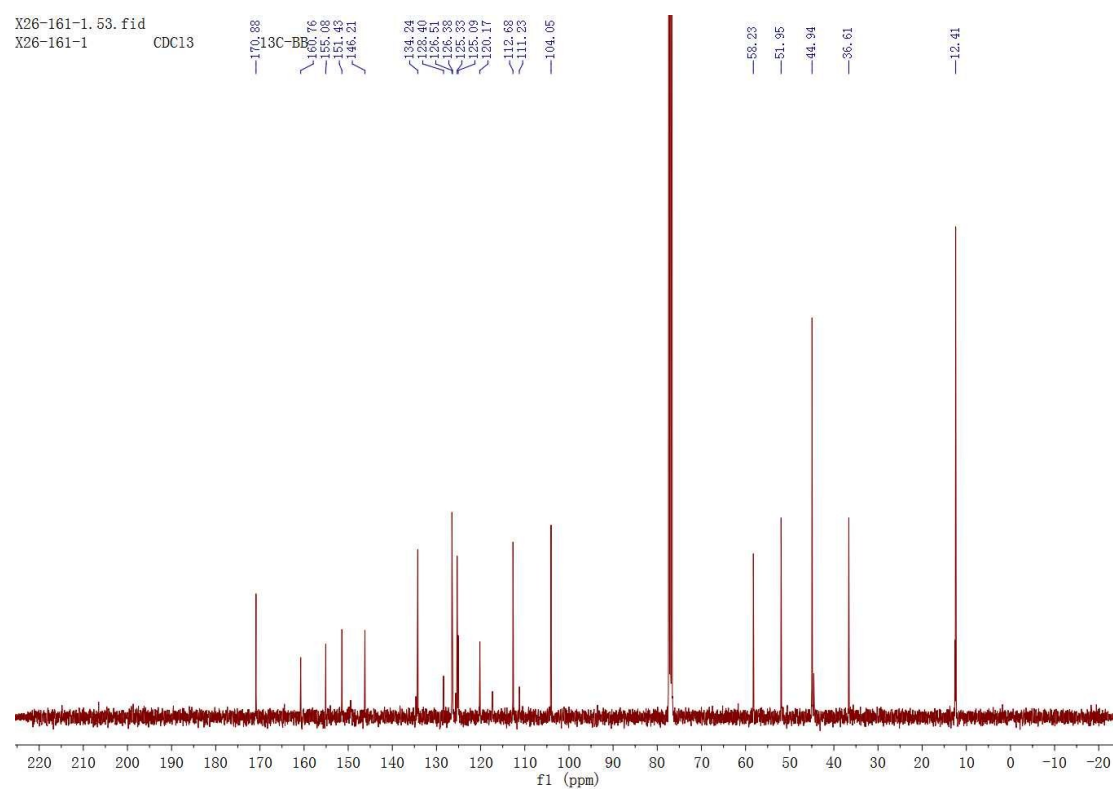
X26-161-1.51.fid
X26-161-1 CDC13

^1H



X26-161-1.53.fid
X26-161-1 CDC13

^{13}C



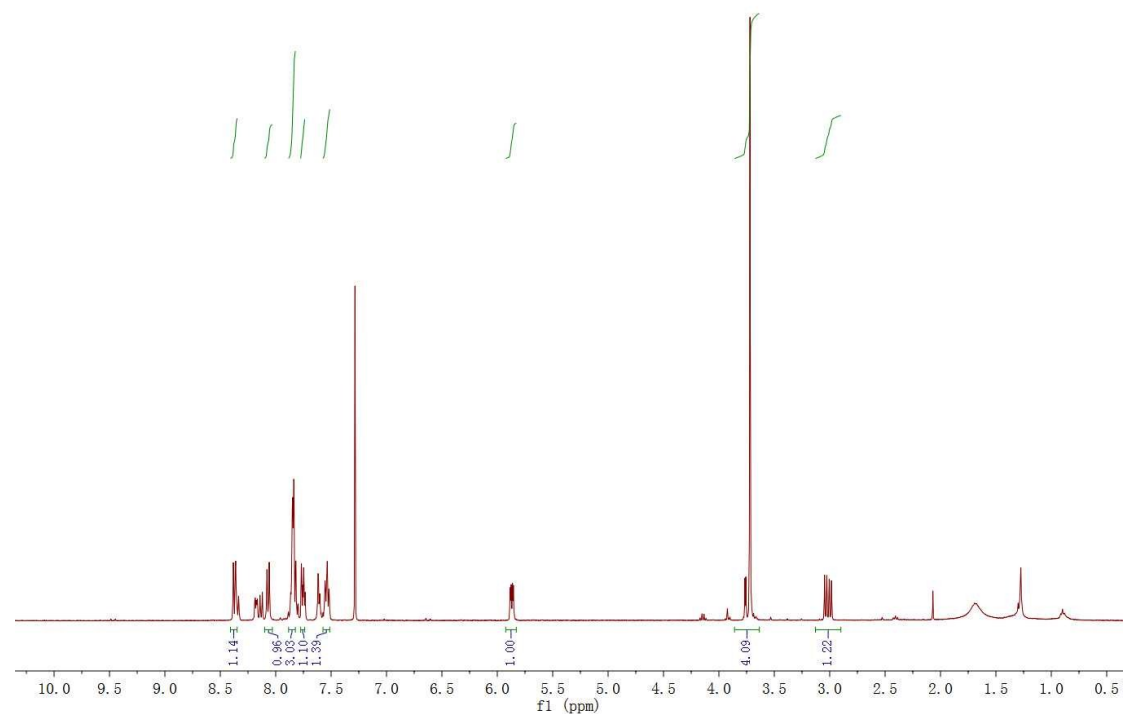
^1H and ^{13}C NMR spectra of **3e**:

X26-181.51.fid

X26-181

CDC13

^1H

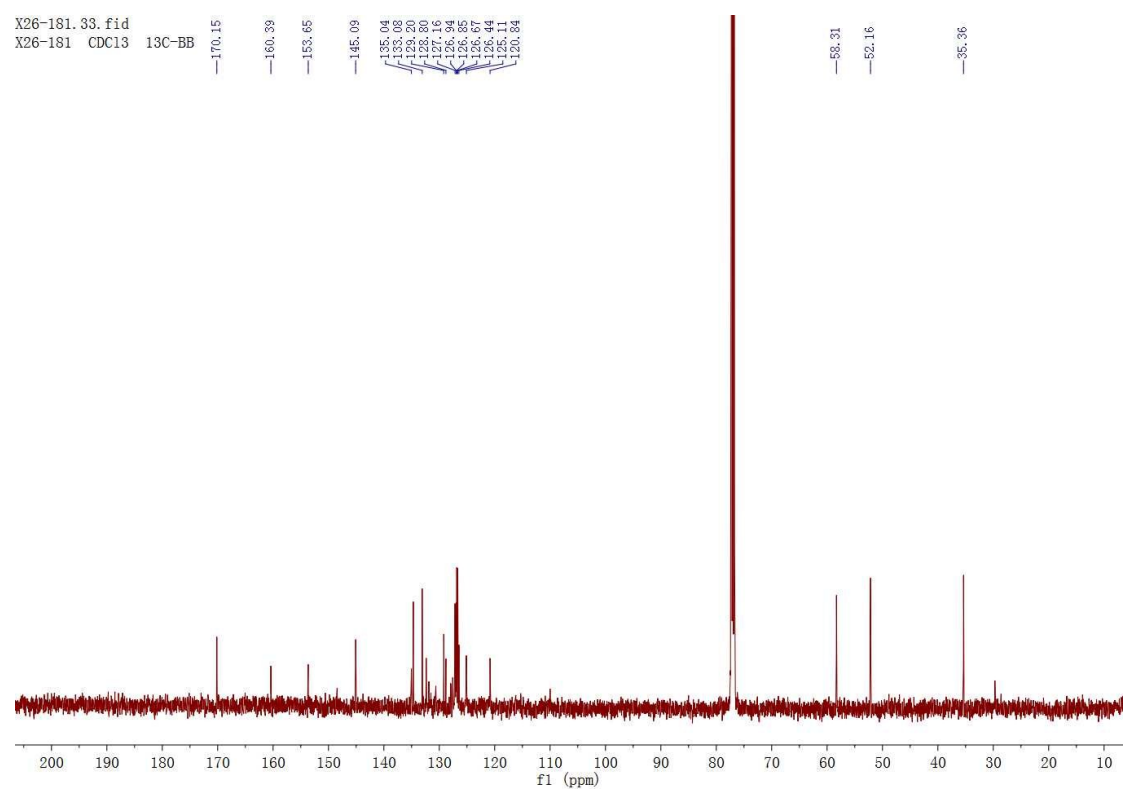


X26-181.33.fid

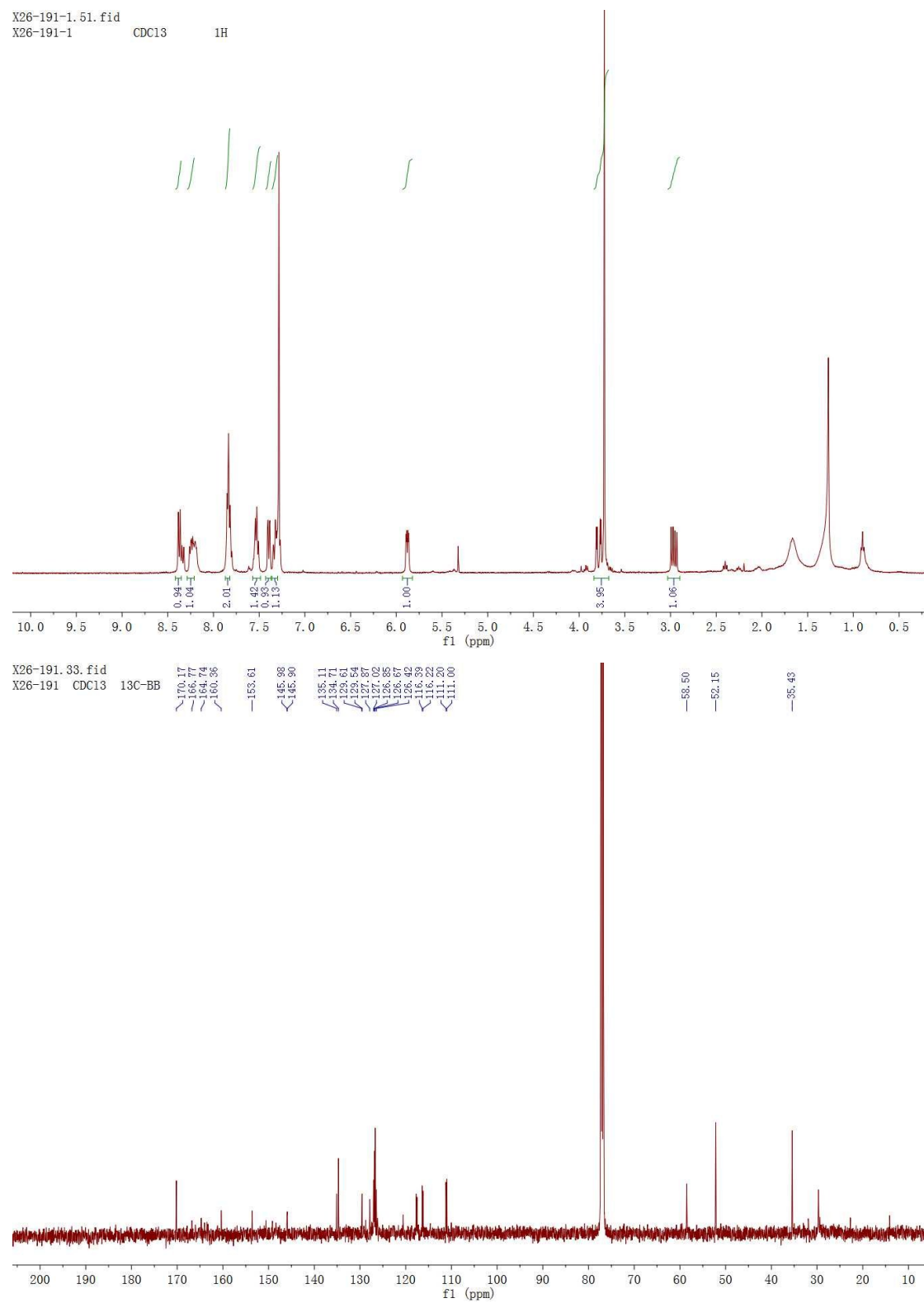
X26-181

CDC13

^{13}C -BB

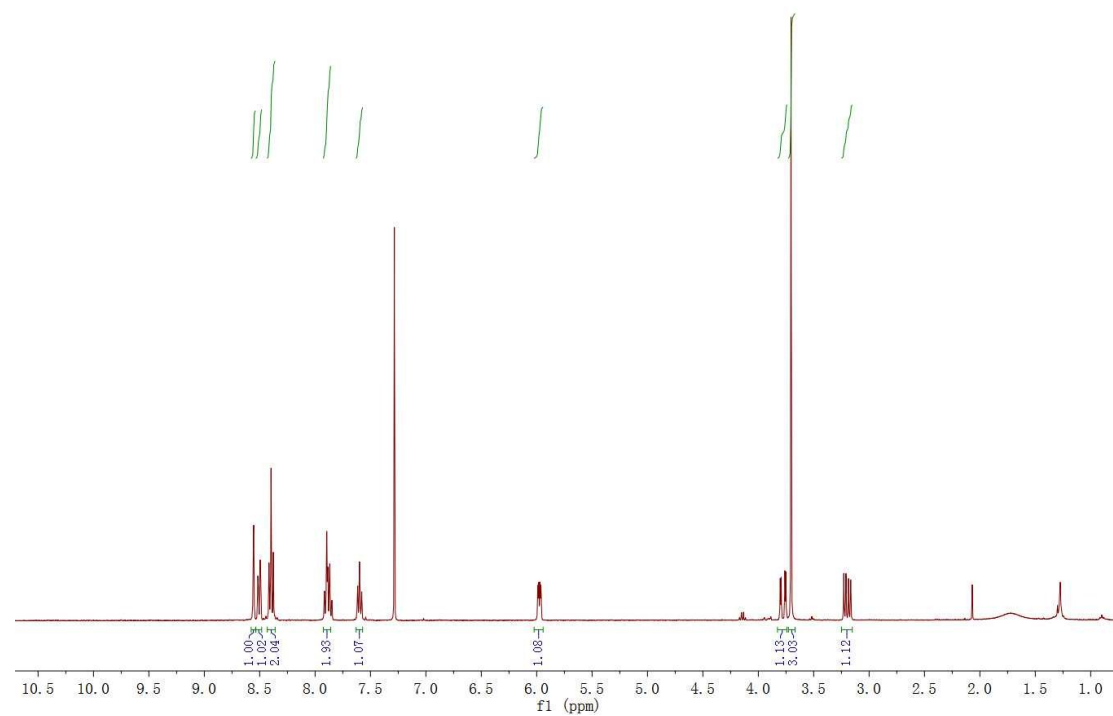


^1H and ^{13}C NMR spectra of **3f**:

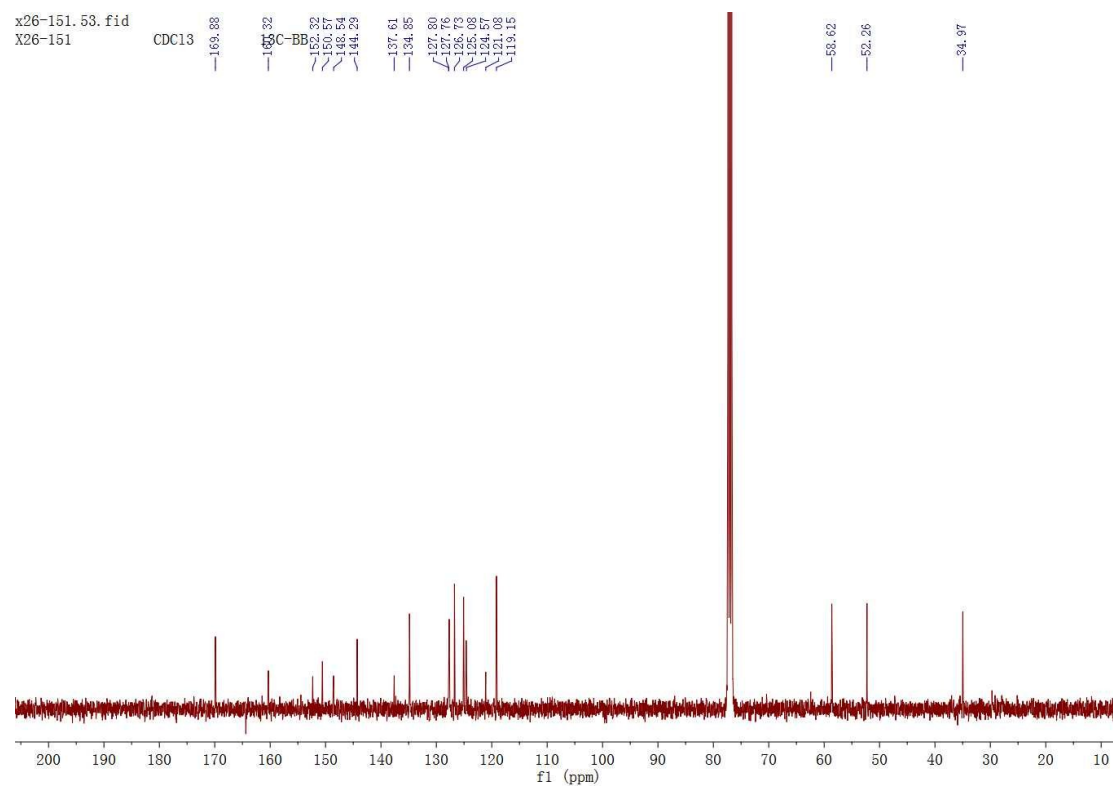


^1H and ^{13}C NMR spectra of **3g**:

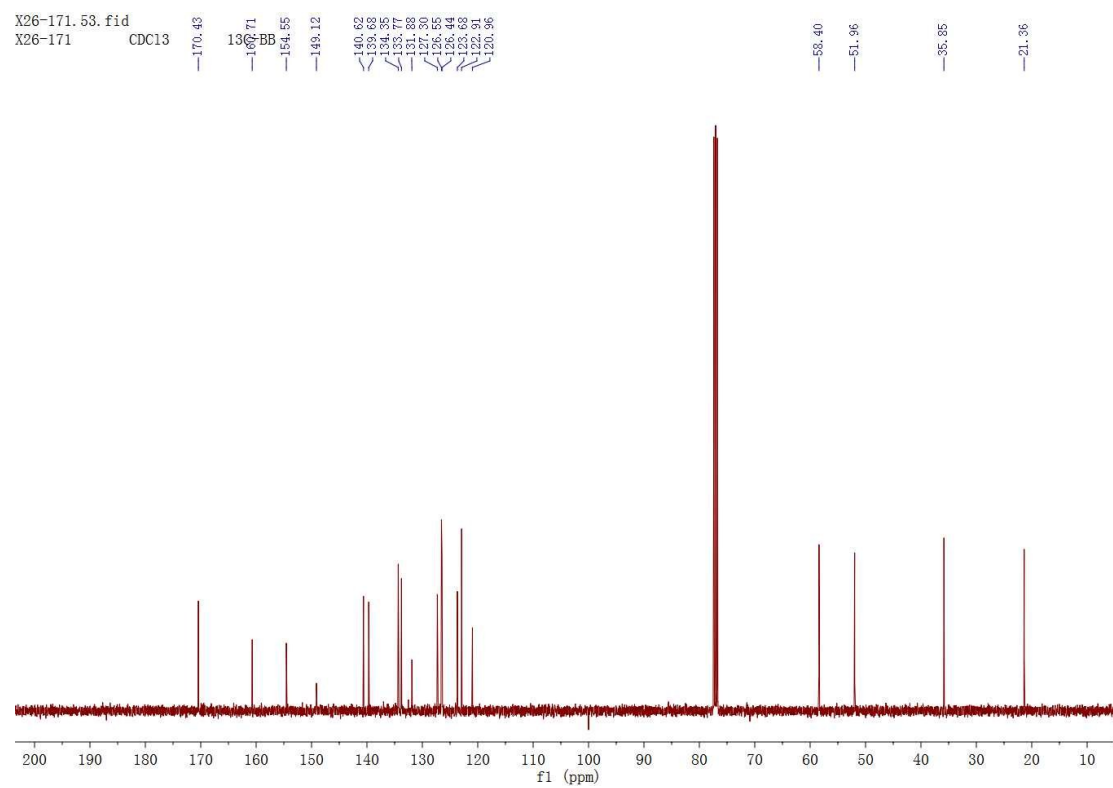
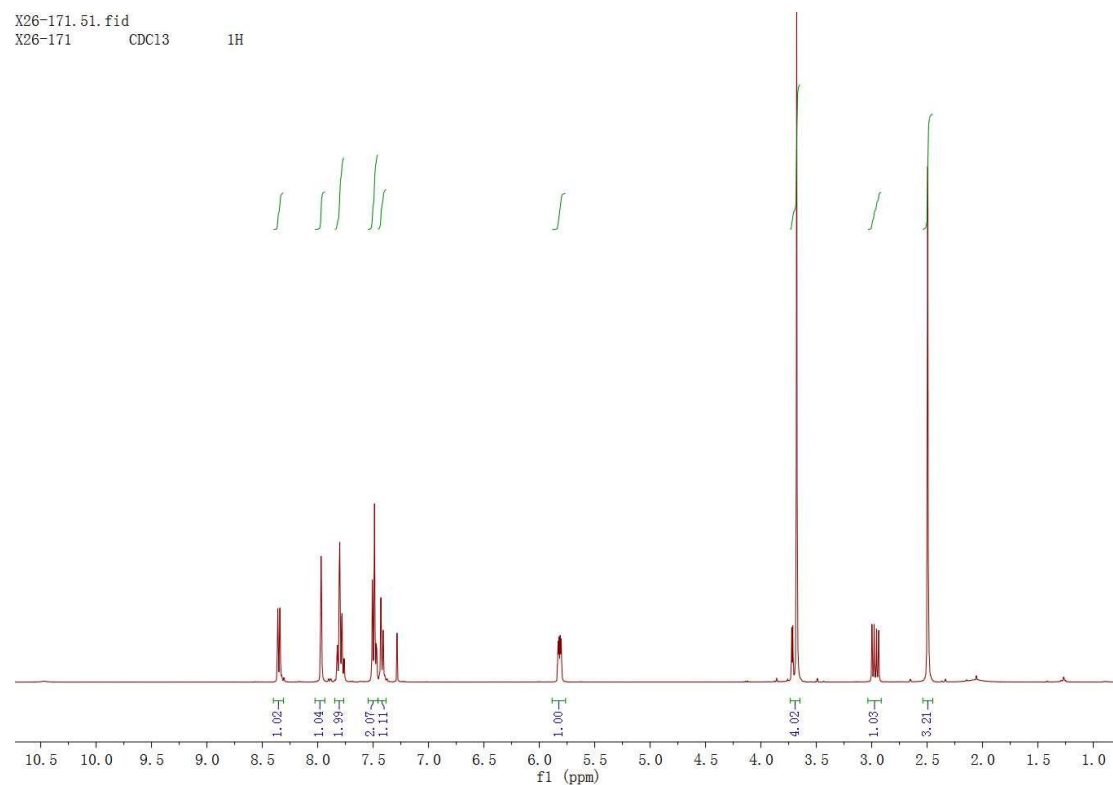
x26-151.51.fid
x26-151 CDC13 ^1H



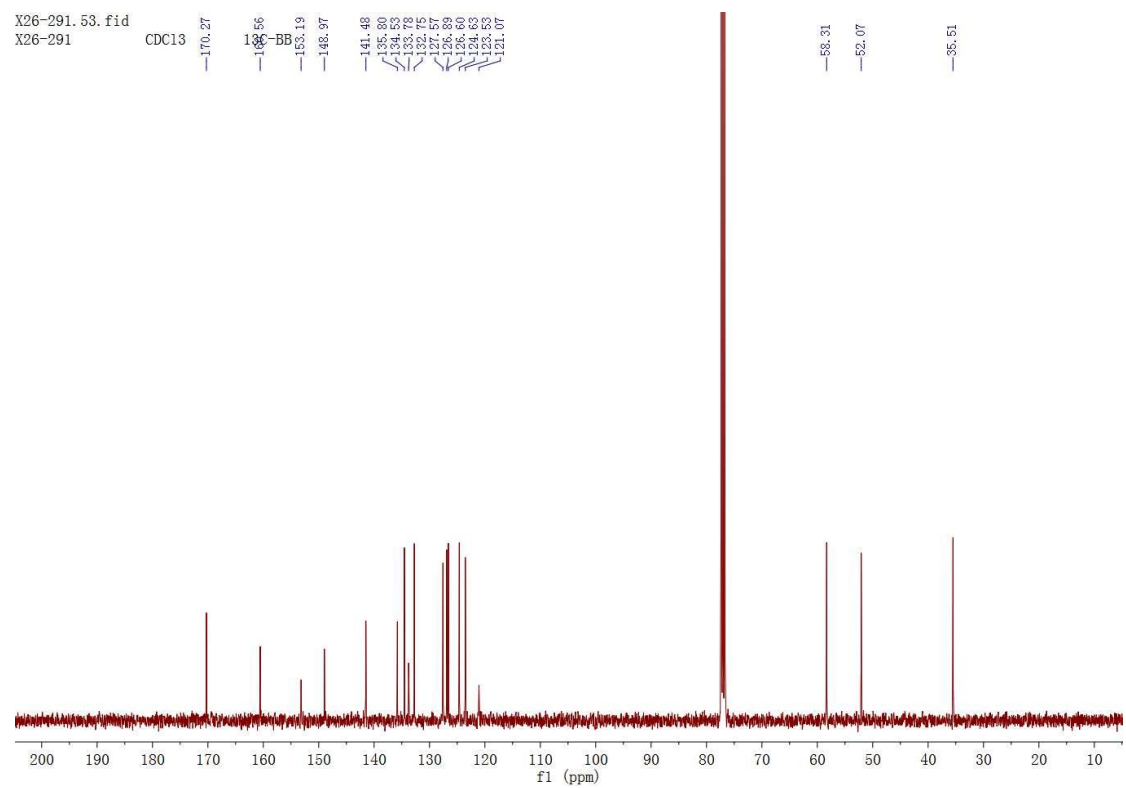
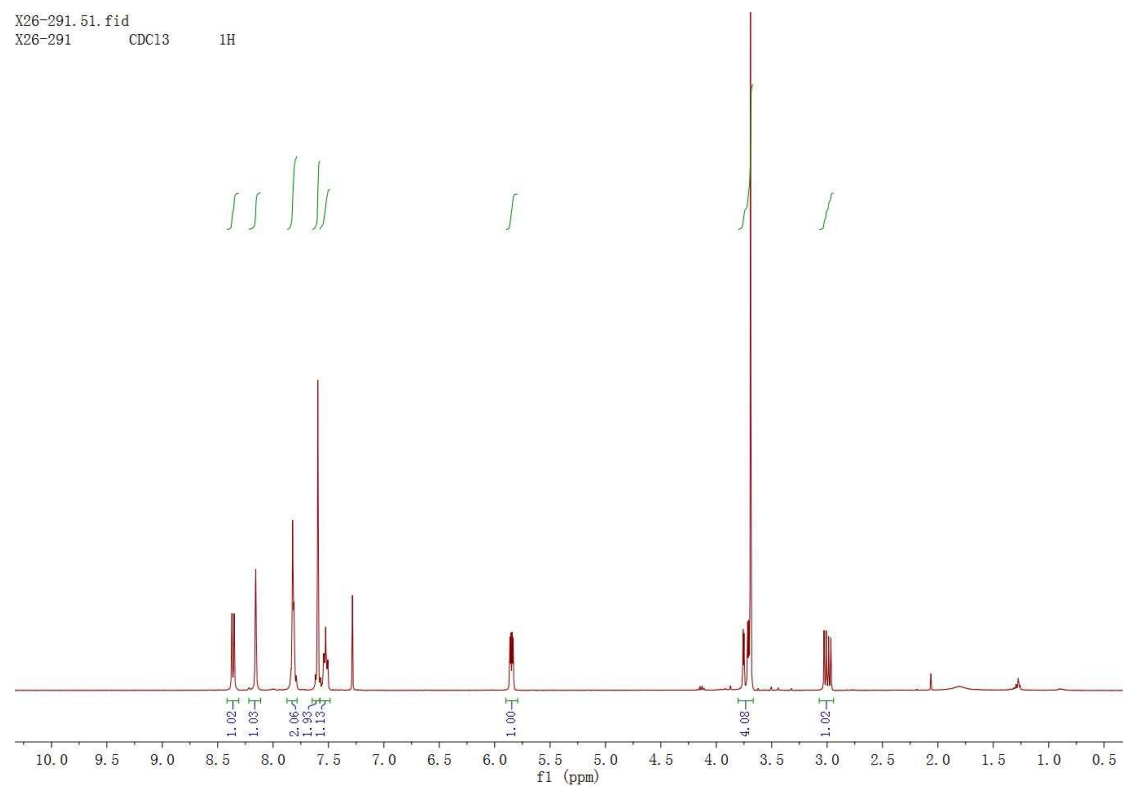
x26-151.53.fid
X26-151



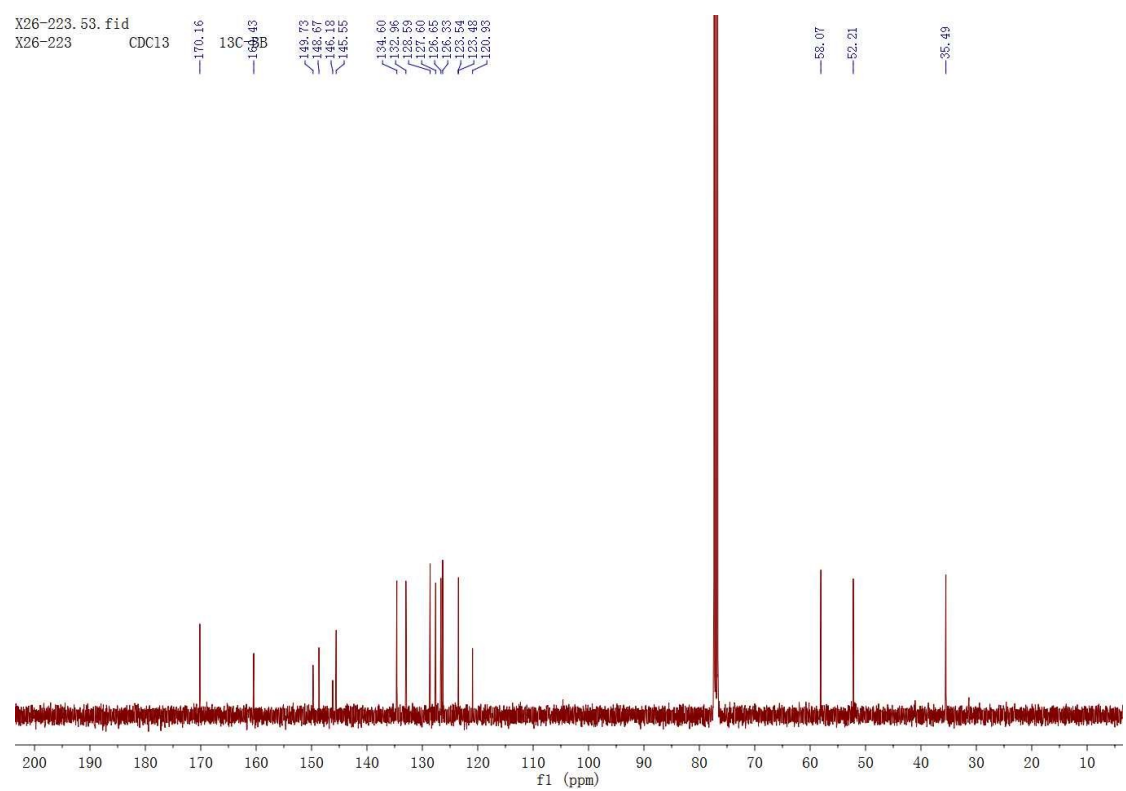
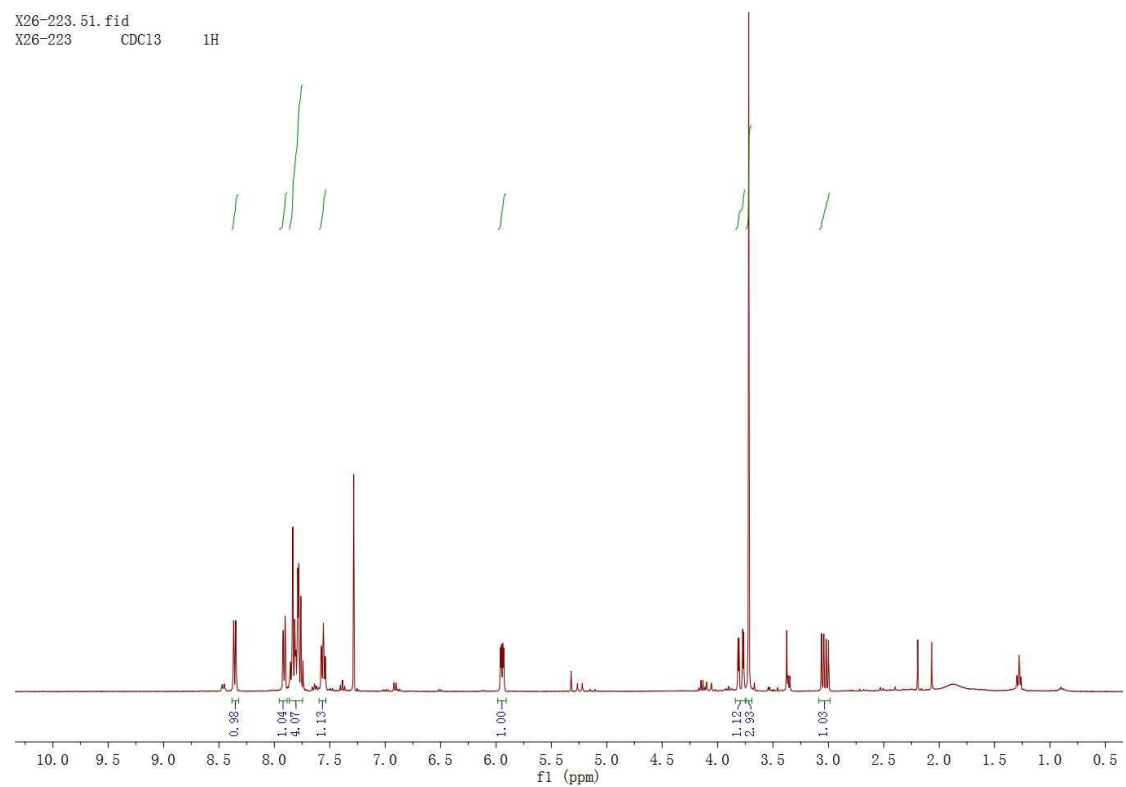
^1H and ^{13}C NMR spectra of **3h**:



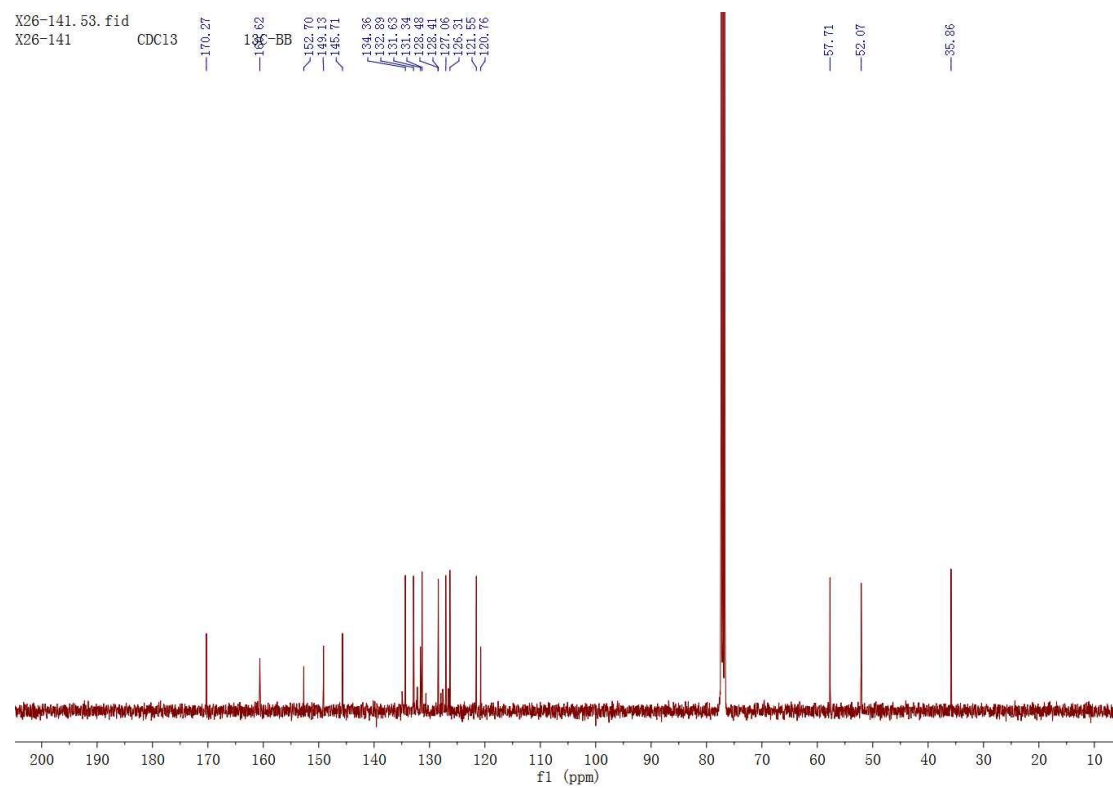
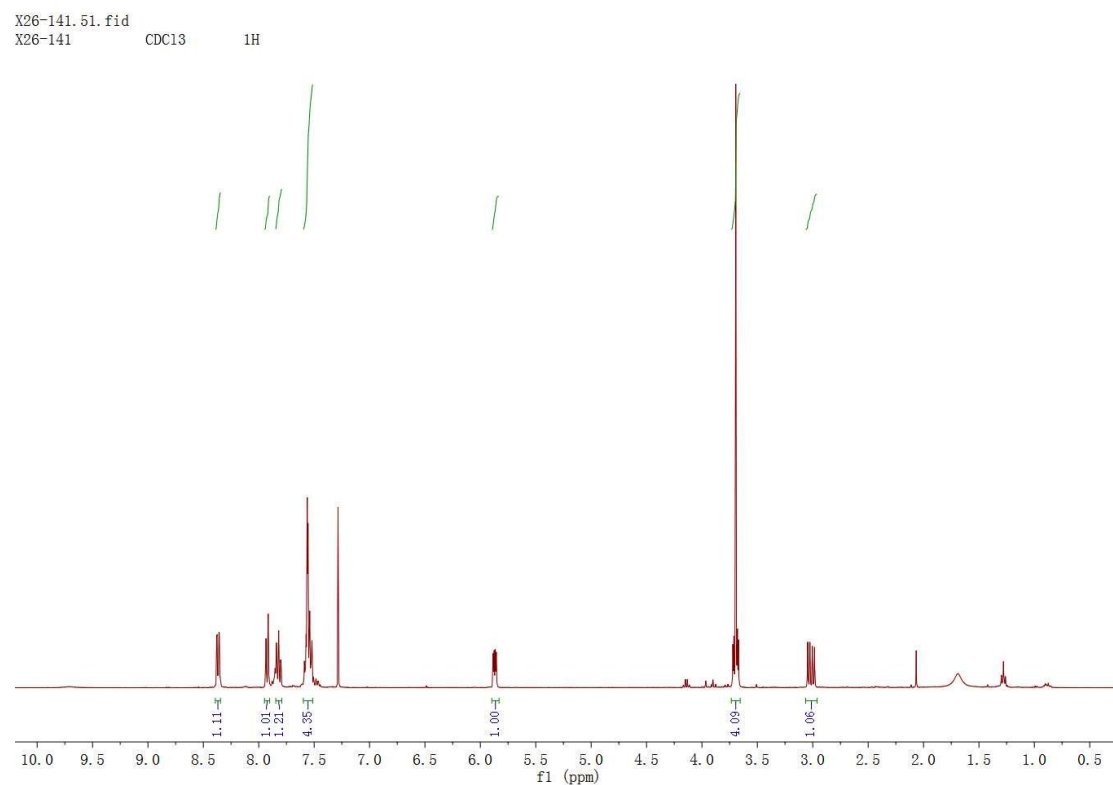
^1H and ^{13}C NMR spectra of **3i**:



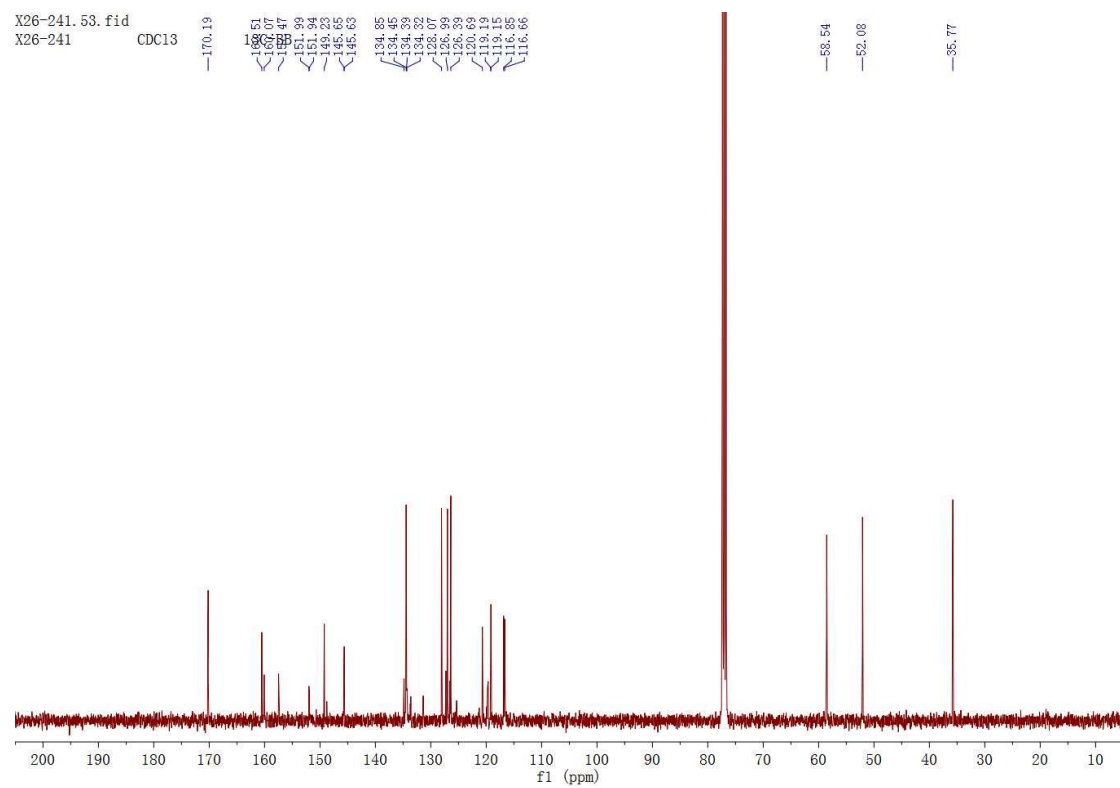
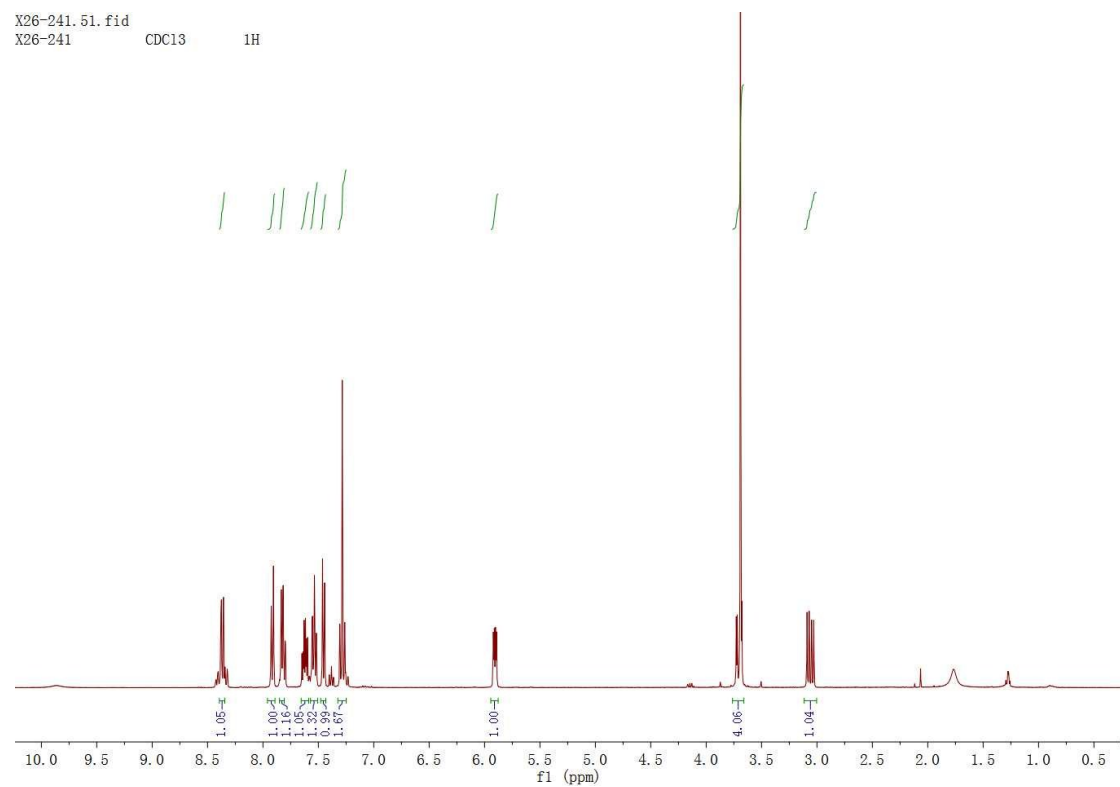
^1H and ^{13}C NMR spectra of **3j**:



^1H and ^{13}C NMR spectra of **3k**:

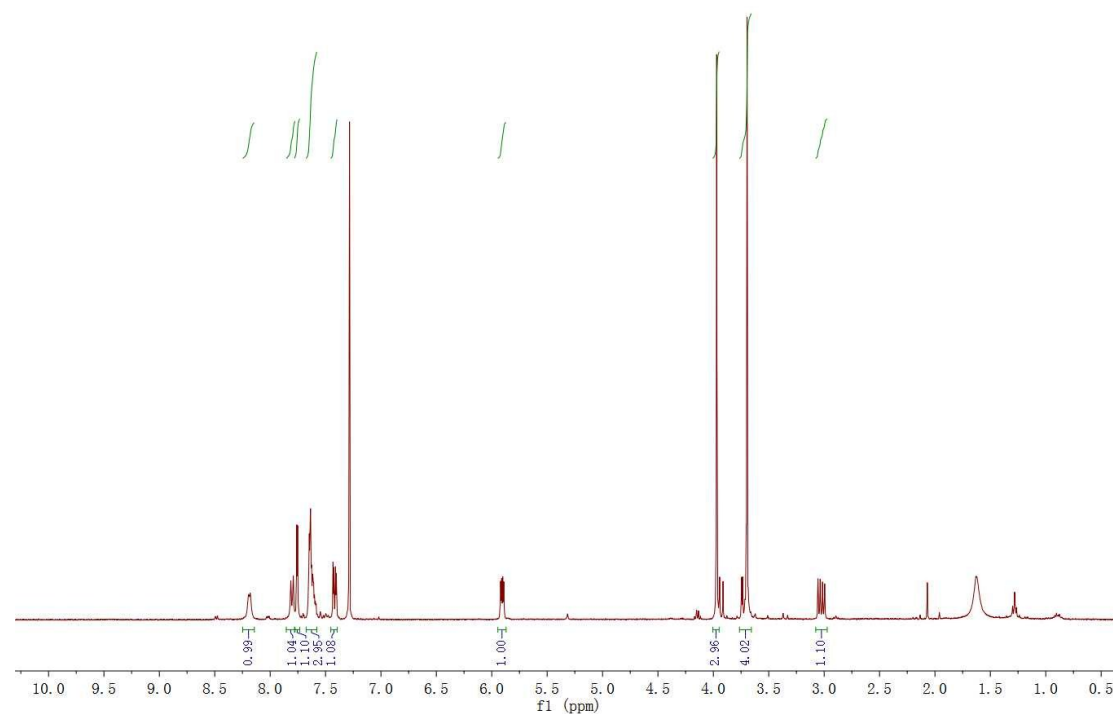


^1H and ^{13}C NMR spectra of **3l**:

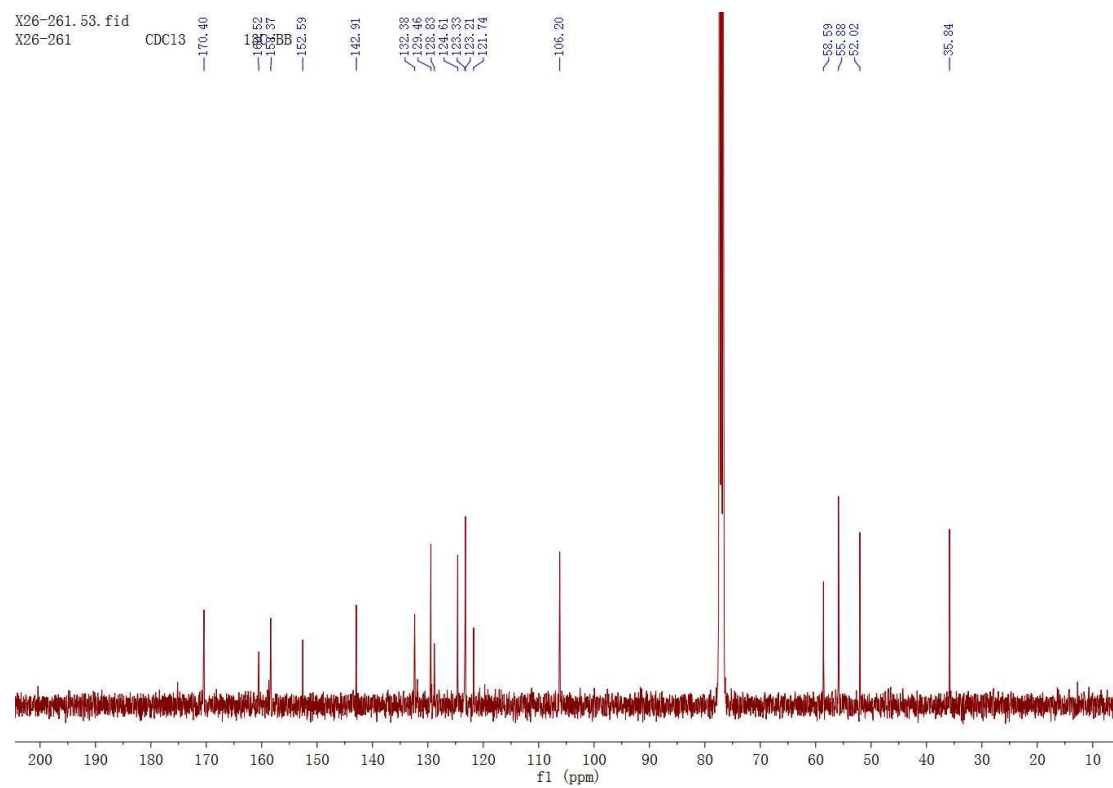


^1H and ^{13}C NMR spectra of **3m**:

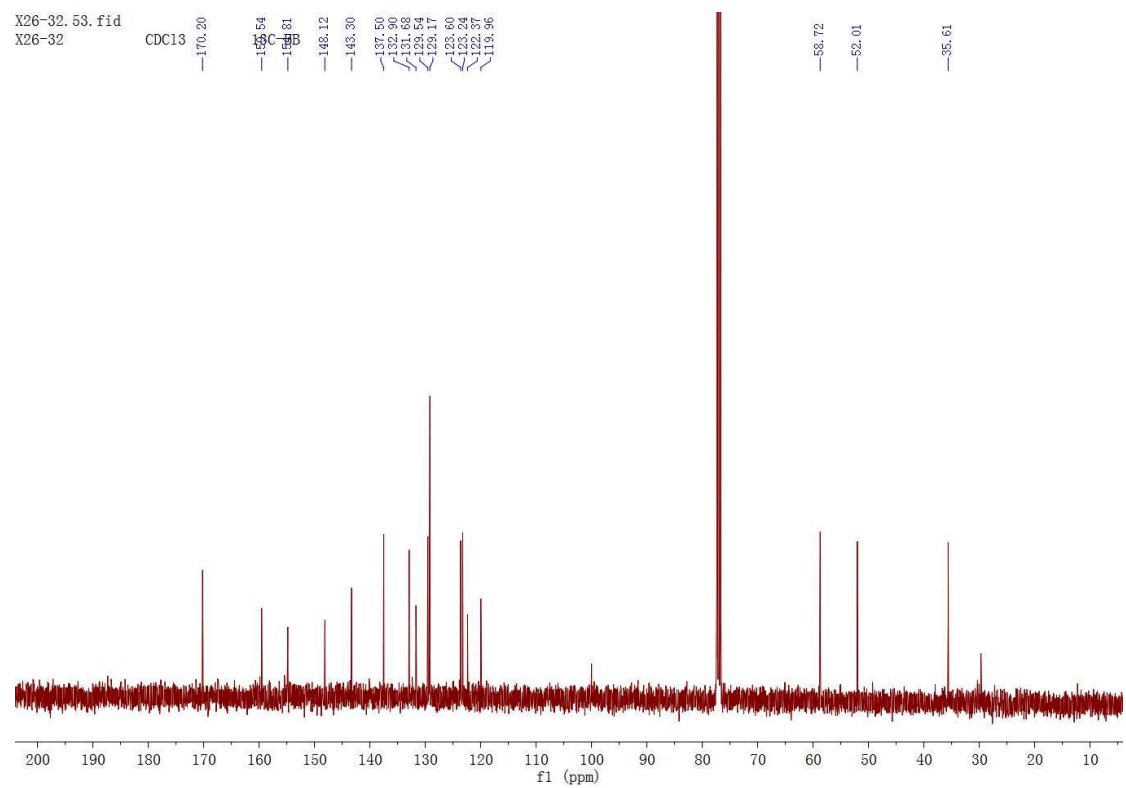
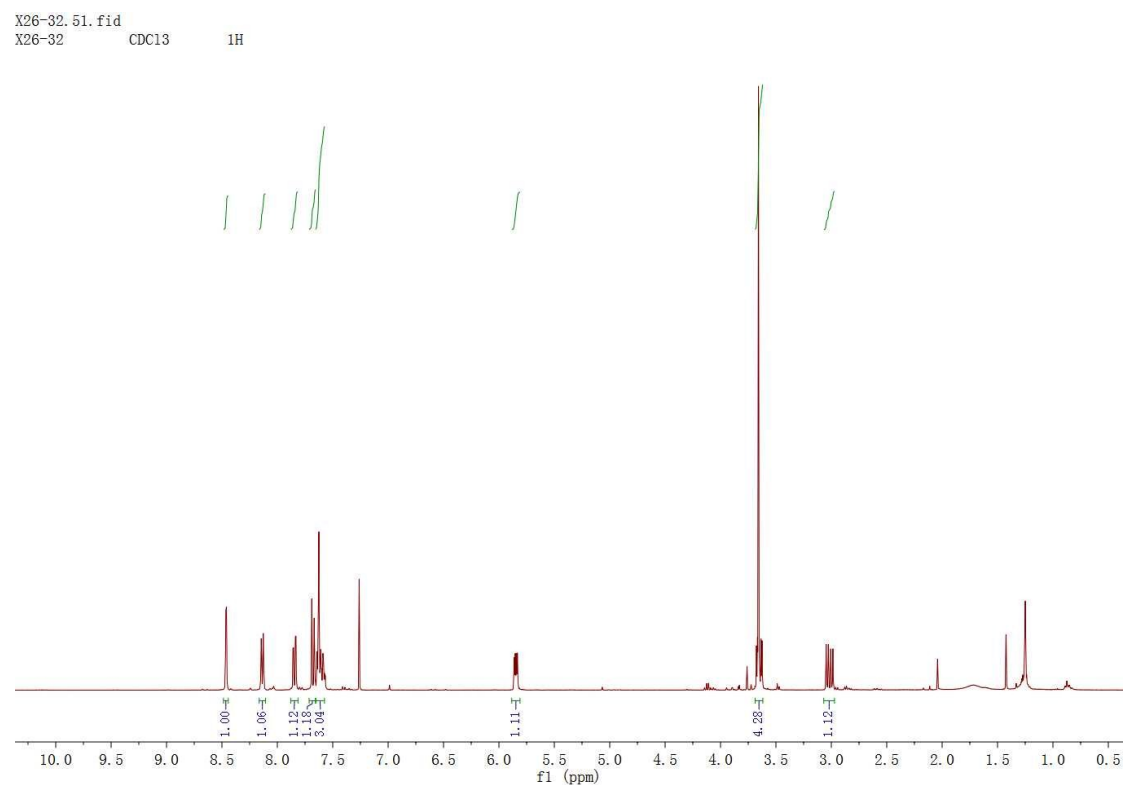
X26-261.51.fid
X26-261 CDC13 ^1H



X26-261.53.fid
X26-261 CDC13

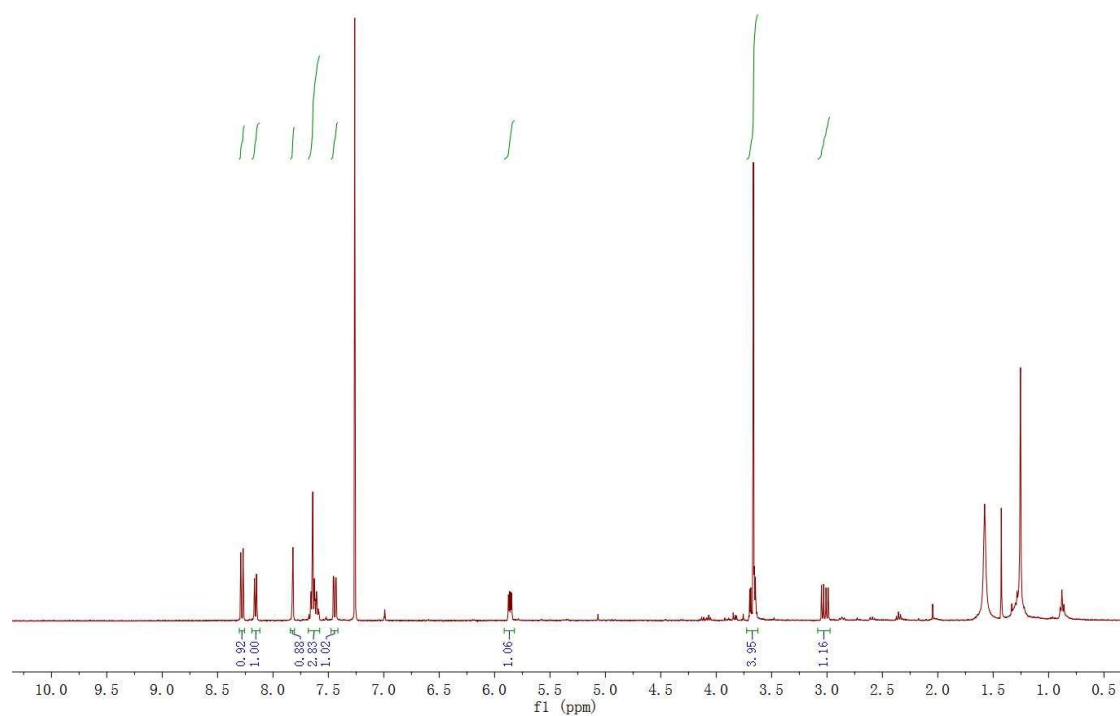


^1H and ^{13}C NMR spectra of **3n**:

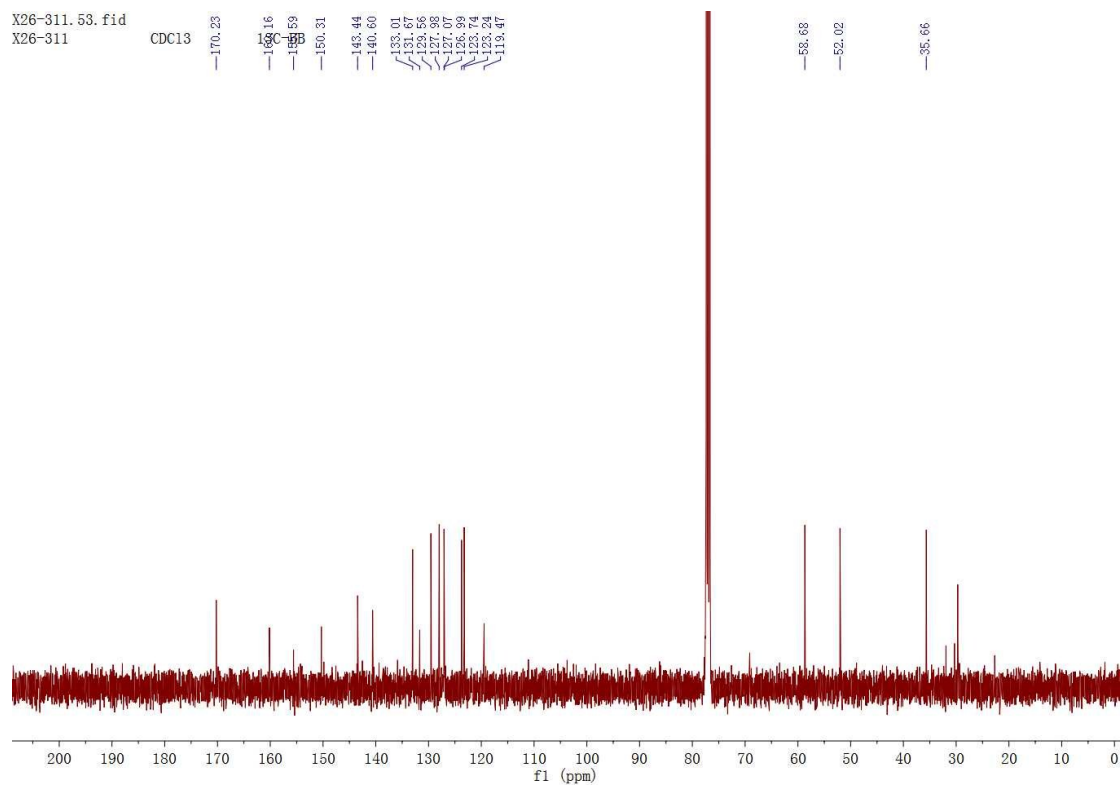


^1H and ^{13}C NMR spectra of **3o**:

X26-311. 51. fid
X26-311 CDC13 ^1H



X26-311. 53. fid
X26-311 CDC13



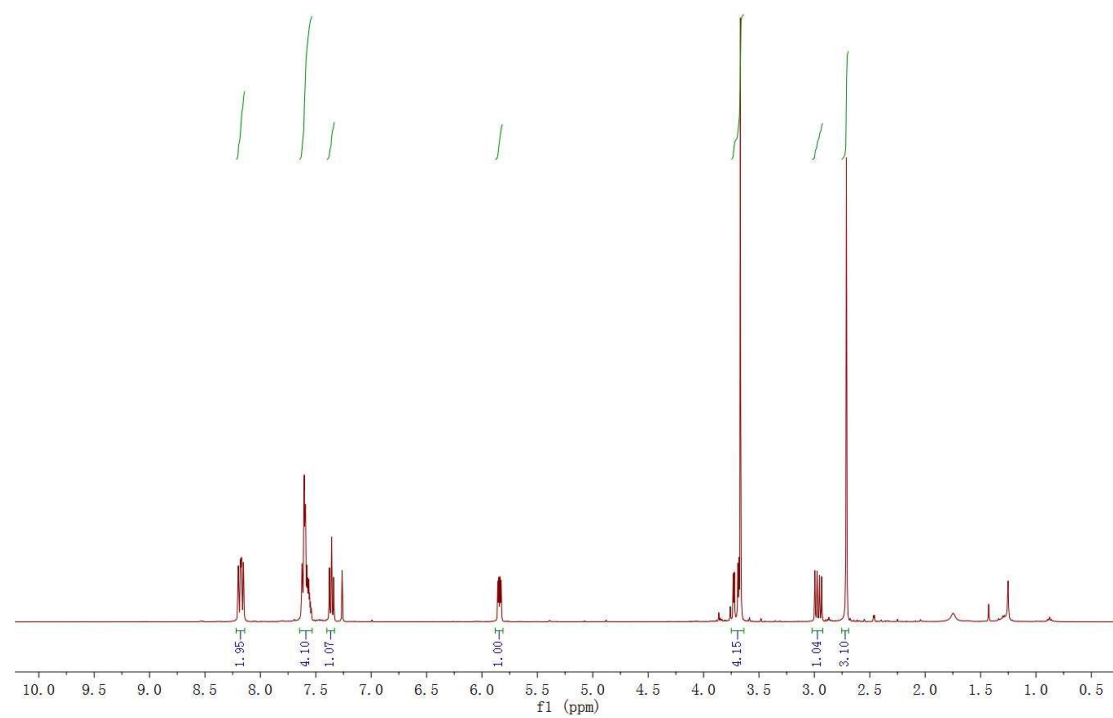
^1H and ^{13}C NMR spectra of **3p**:

X26-331.51.fid

X26-331

CDC13

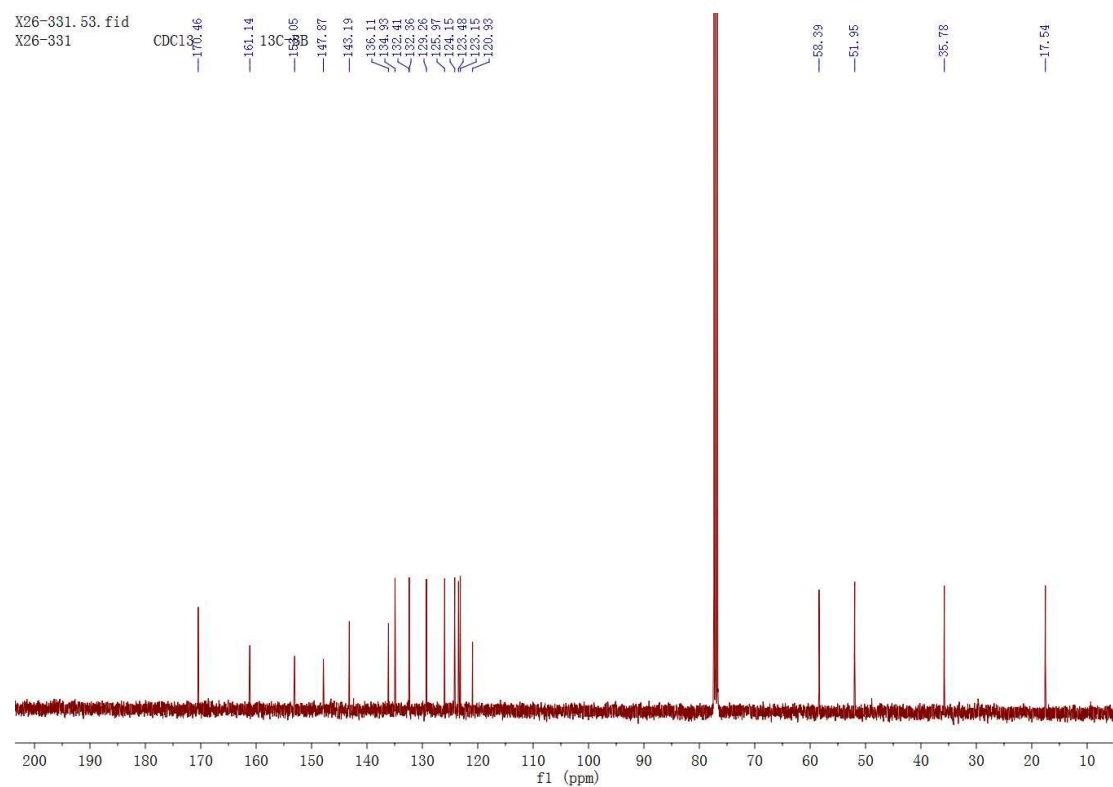
^1H



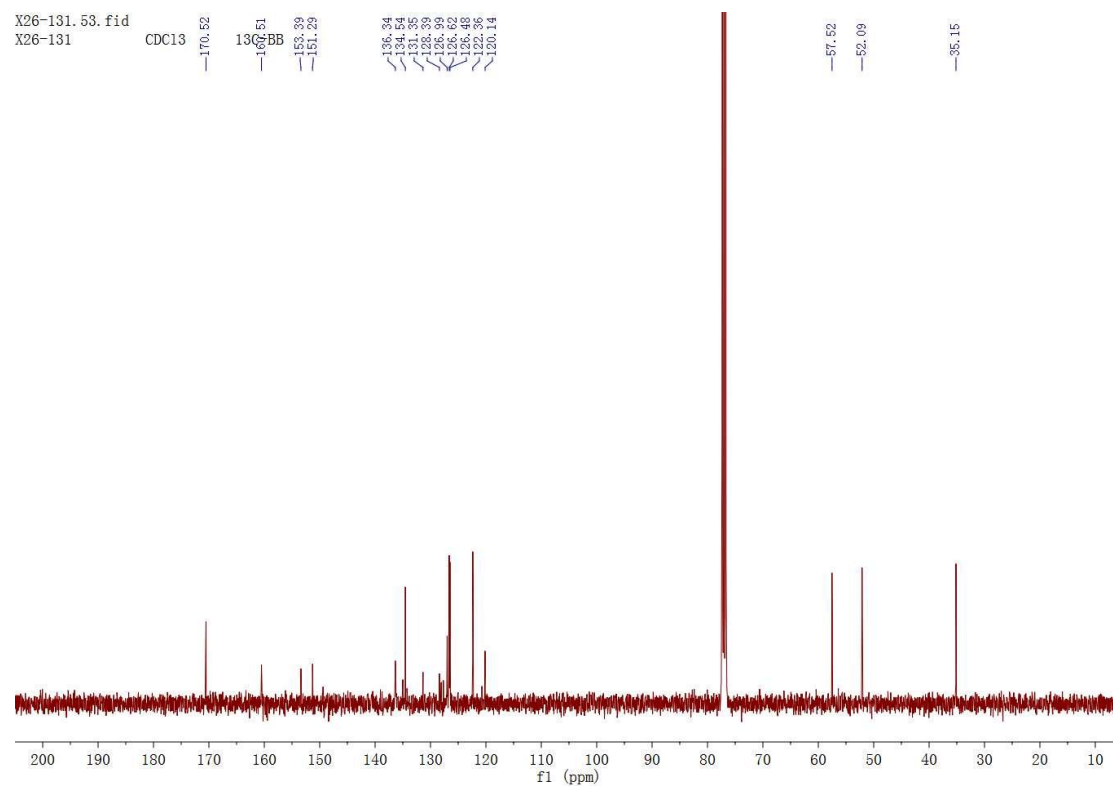
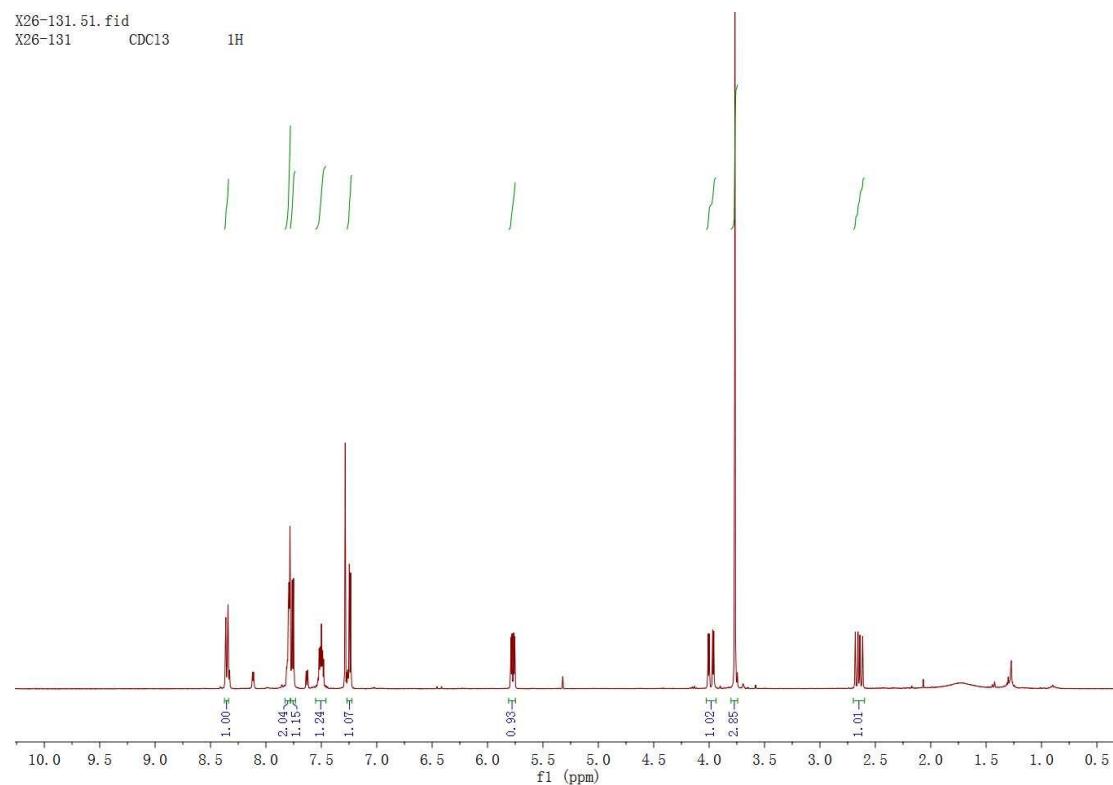
X26-331.53.fid

X26-331

CDC13



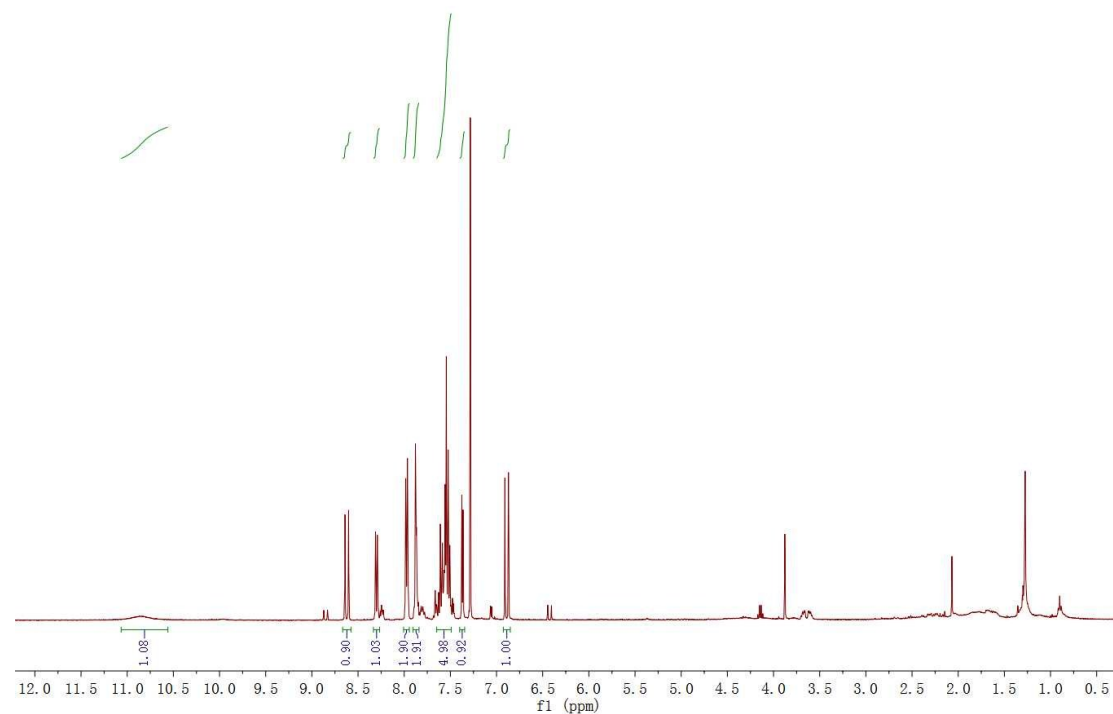
^1H and ^{13}C NMR spectra of **3r**:



^1H and ^{13}C NMR spectra of **3s**:

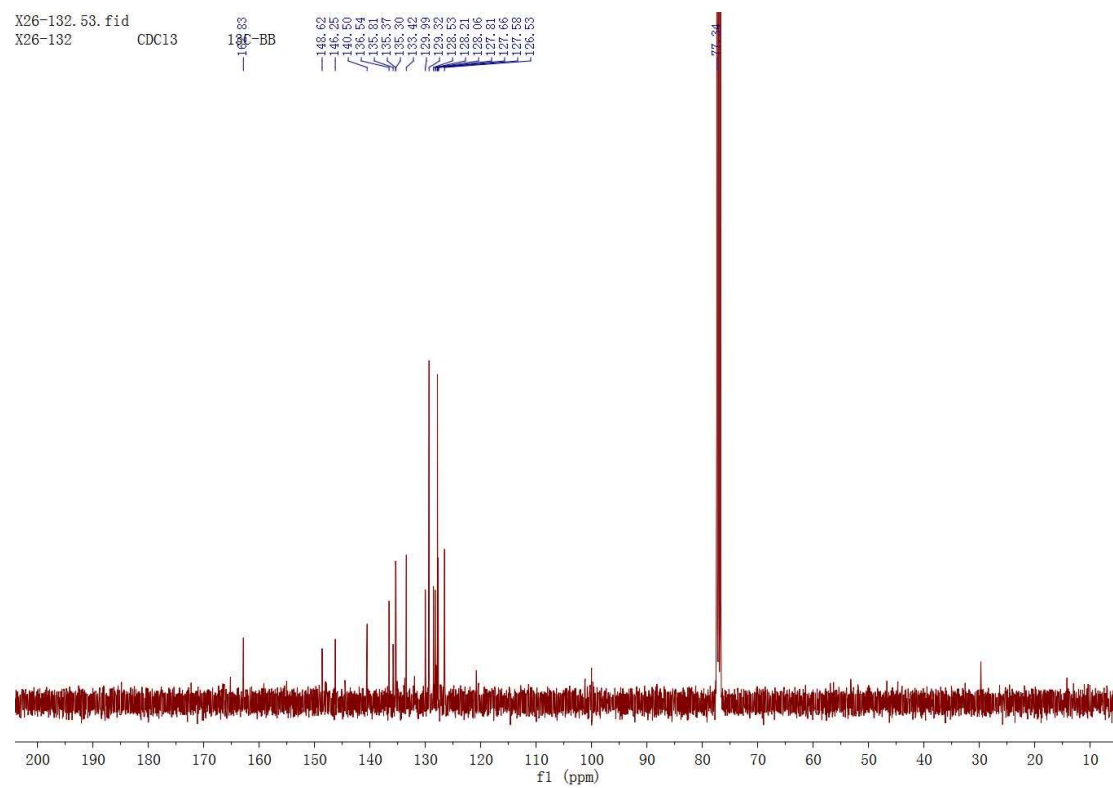
X26-132. 51. fid
X26-132 CDC13

^1H



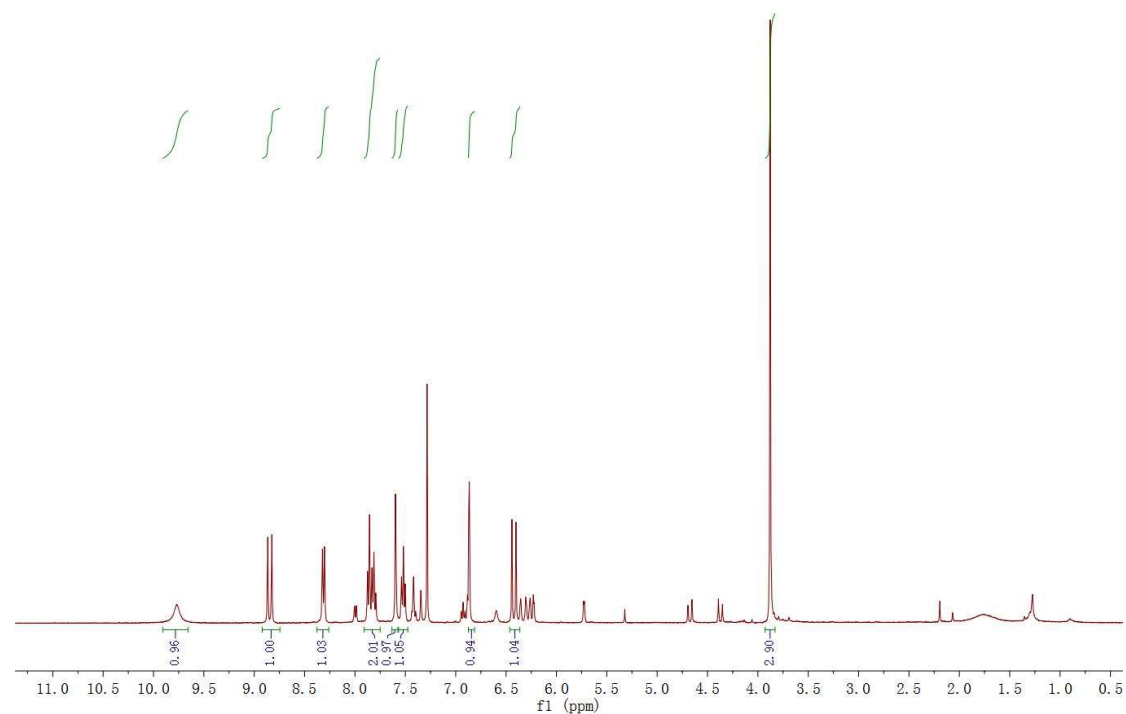
X26-132. 53. fid
X26-132 CDC13

^{13}C -BB
126.83



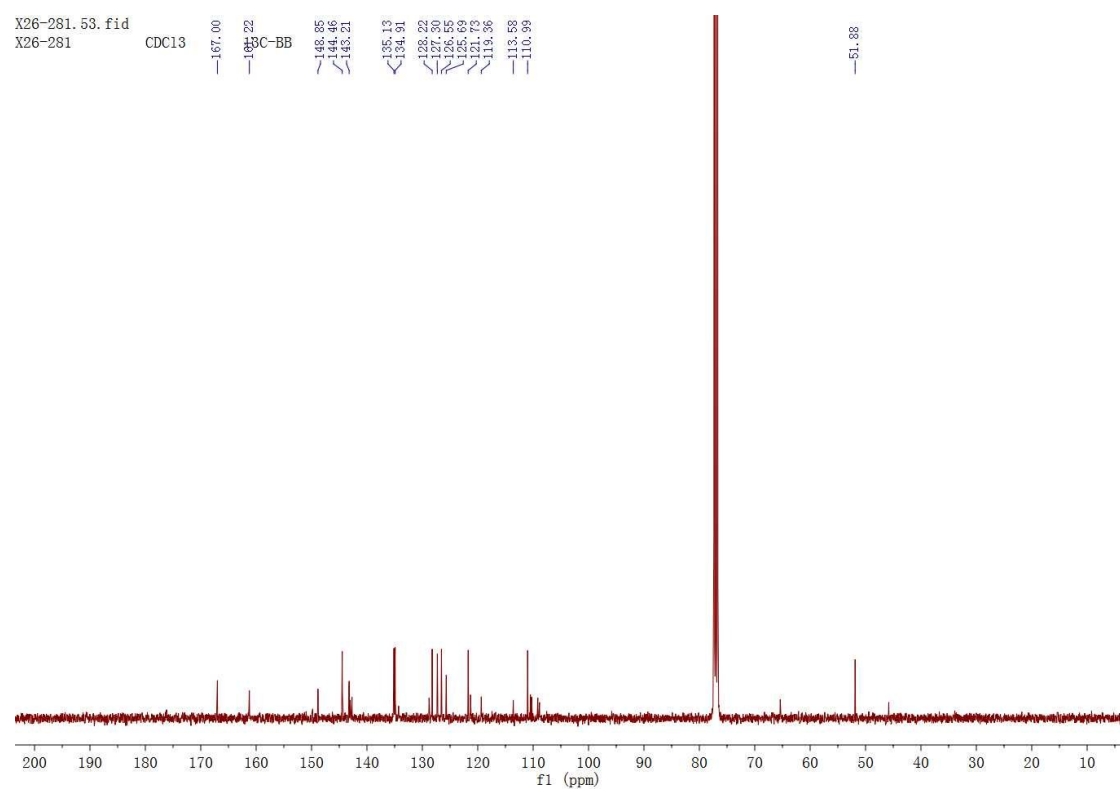
^1H and ^{13}C NMR spectra of **3t**:

X26-281.51.fid
X26-281 CDC13 ^1H

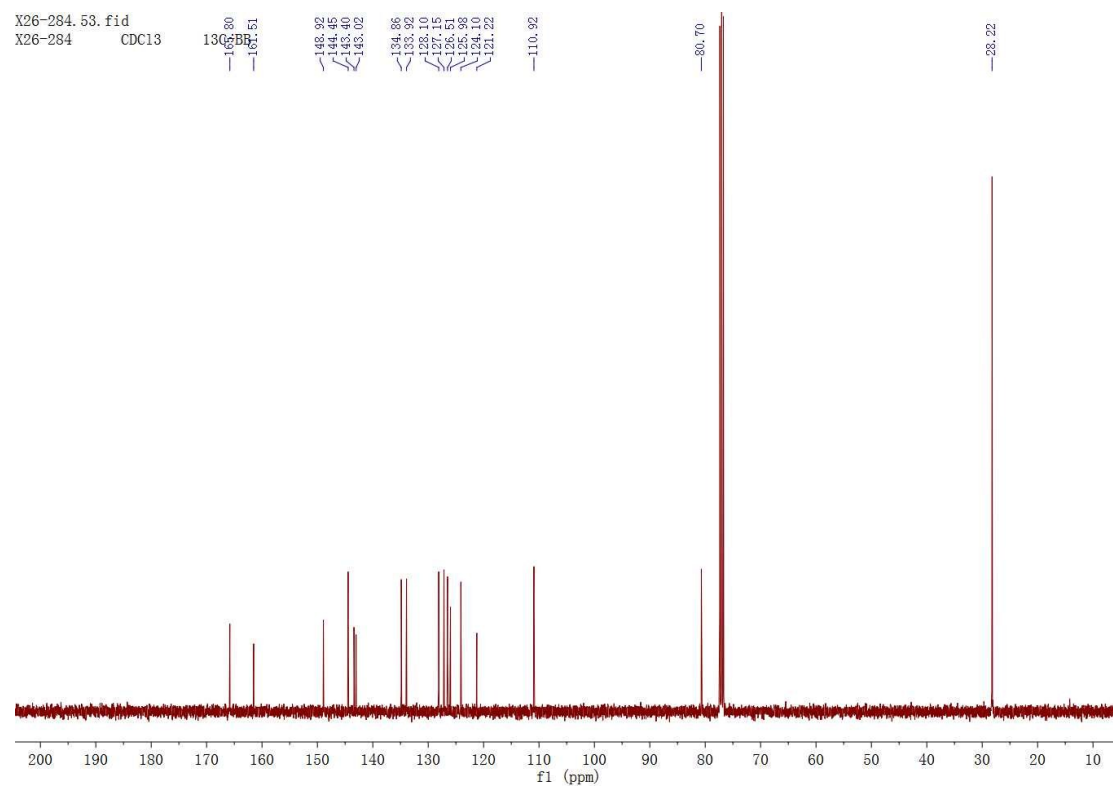
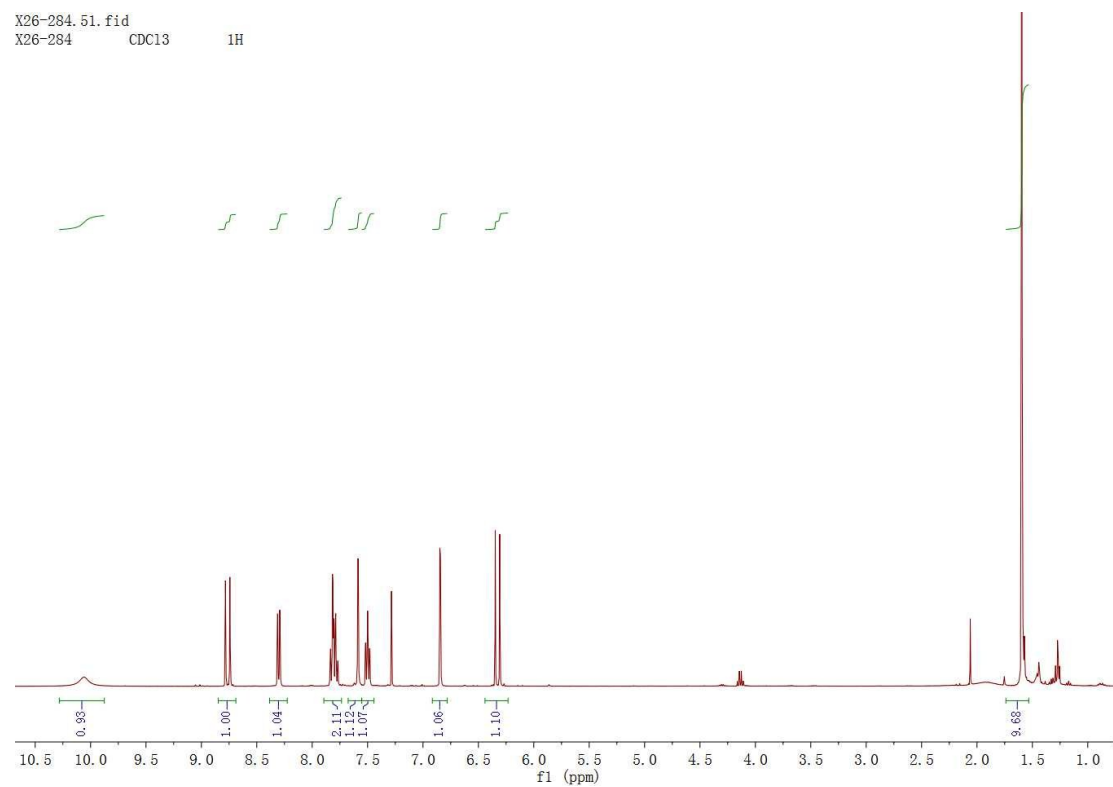


X26-281.53.fid
X26-281 CDC13

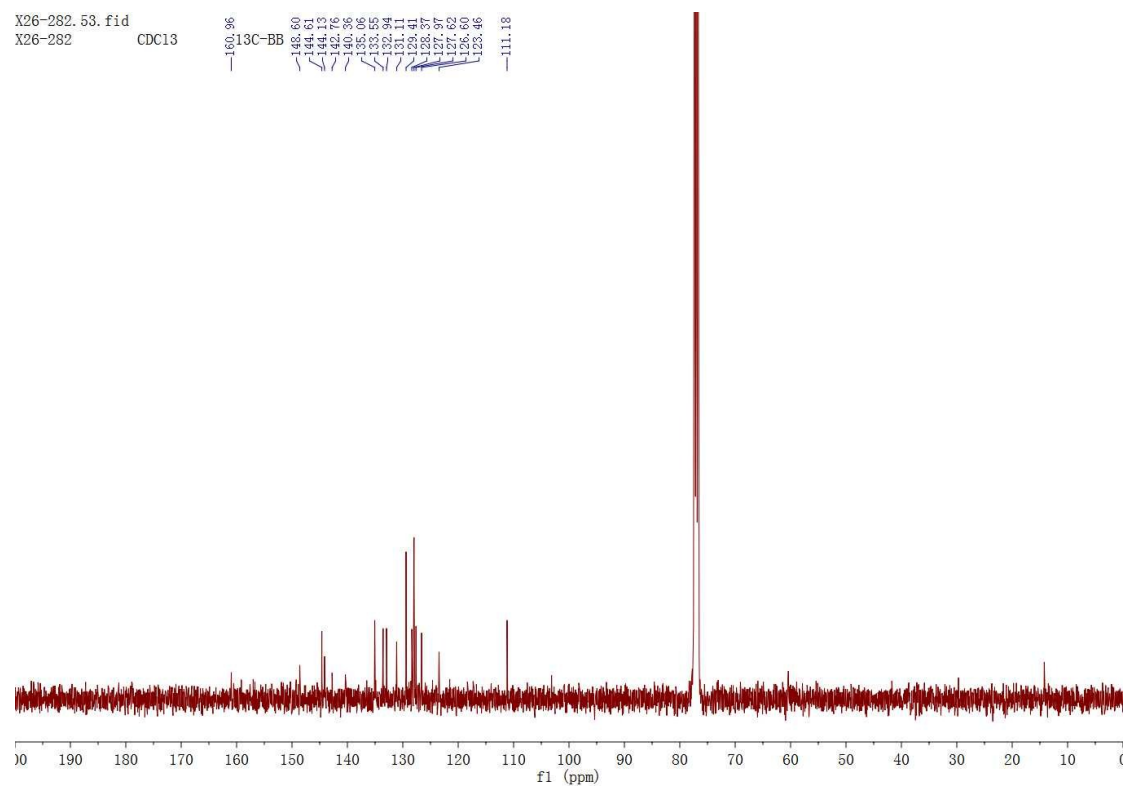
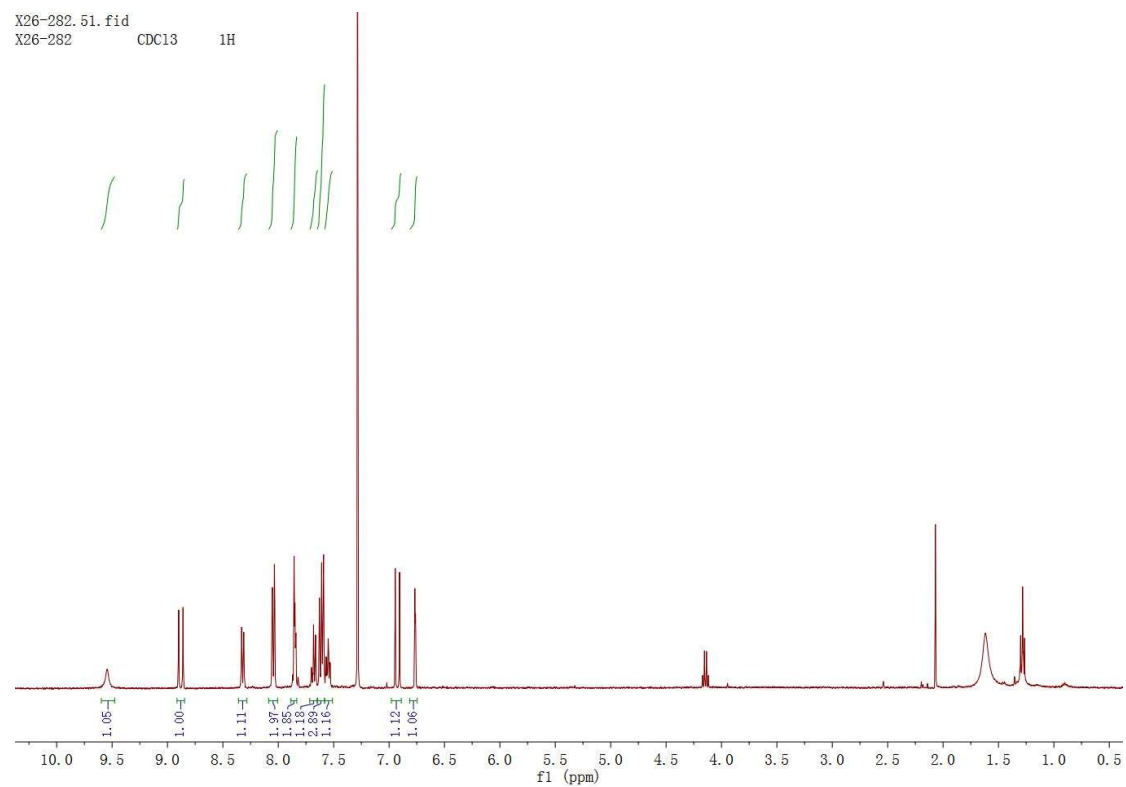
Chemical Shift (ppm)	Assignment
167.00	C=O
144.22	C-C
148.85	C-C
144.46	C-C
143.21	C-C
135.13	C-C
134.91	C-C
128.22	C-C
127.32	C-C
126.55	C-C
125.69	C-C
121.73	C-C
119.36	C-C
113.58	C-C
110.99	C-C
51.88	CH-OH



^1H and ^{13}C NMR spectra of **3u**:



^1H and ^{13}C NMR spectra of **3r**:



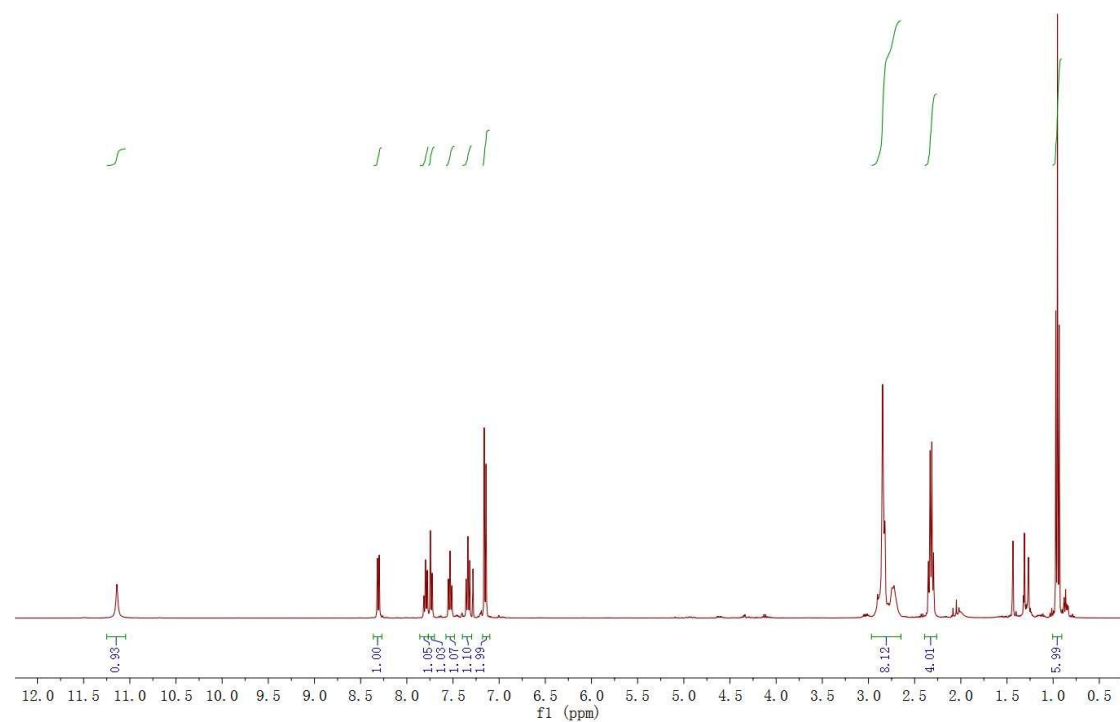
^1H and ^{13}C NMR spectra of **5a**:

X26-9-2, 51, fid

X26-9-2

CDC13

^1H

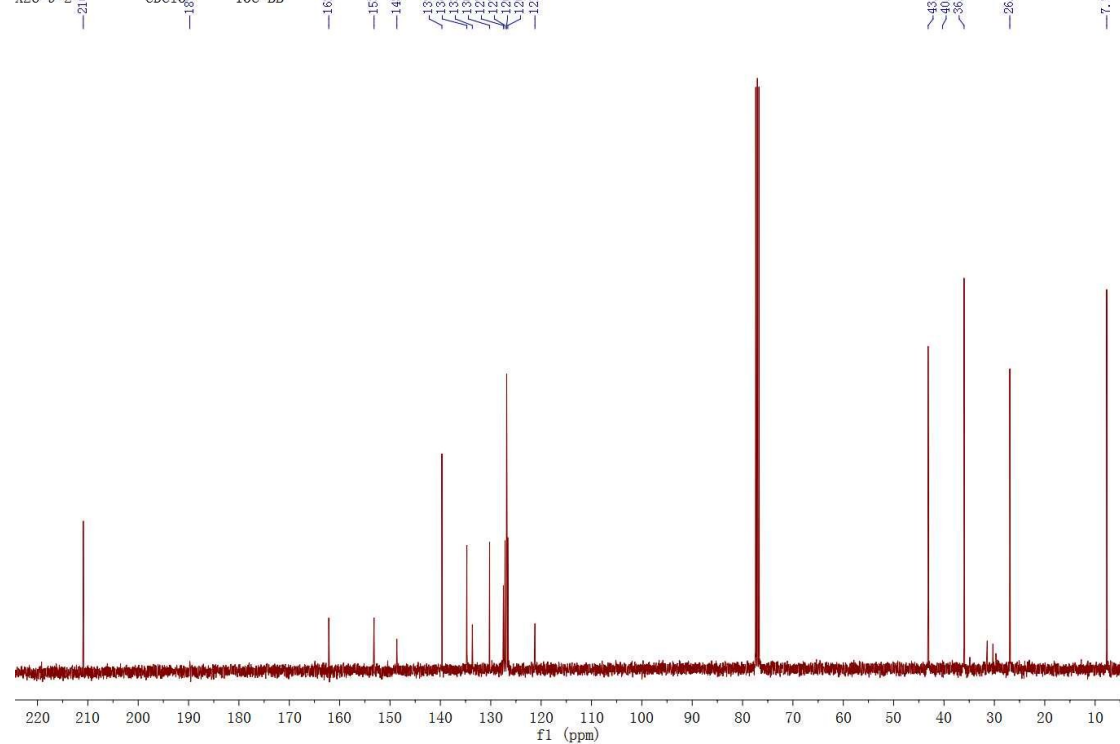


X26-9-2, 53, fid

X26-9-2

CDC13

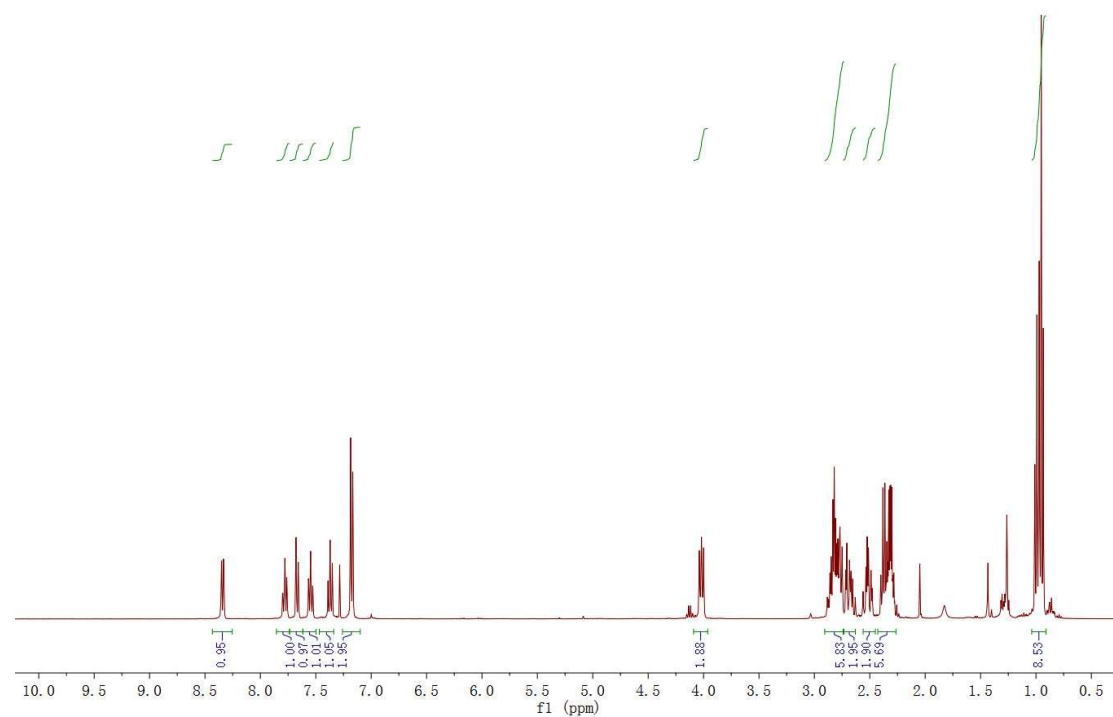
^{13}C -BB



^1H and ^{13}C NMR spectra of **5a'**:

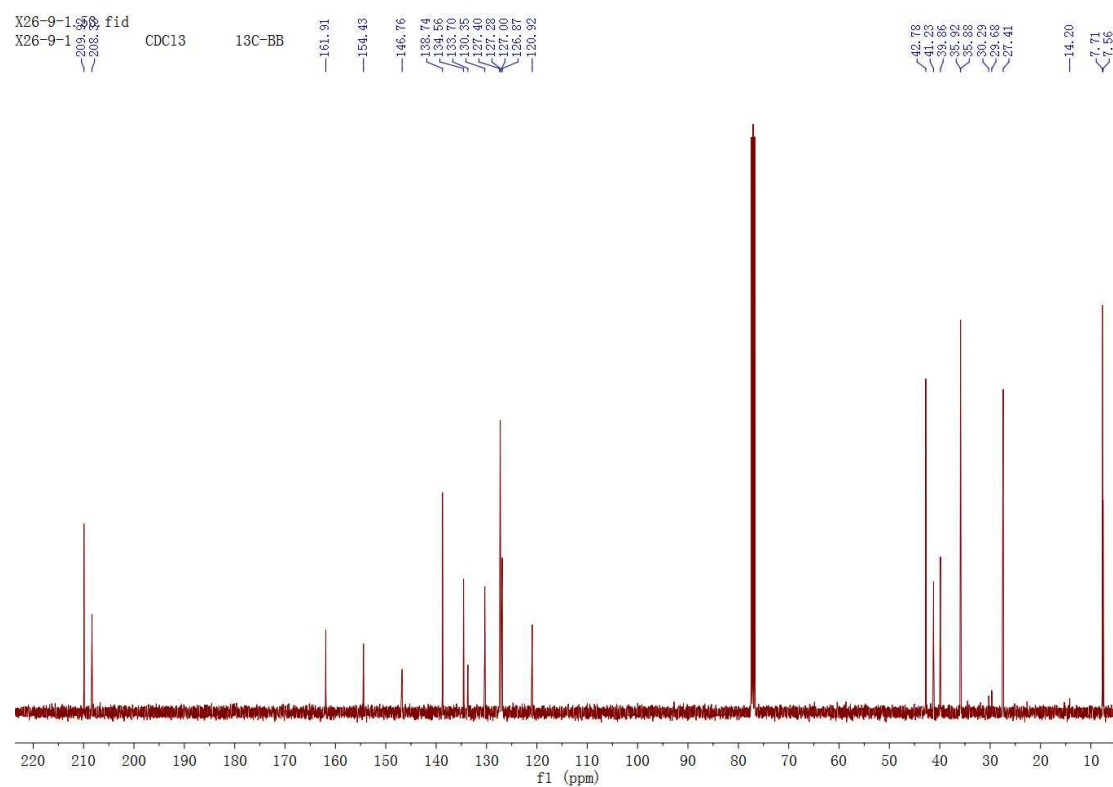
X26-9-1, 51, fid

X26-9-1 CDC13 ^1H



X26-9-1, 51, fid

X26-9-1 CDC13 ^{13}C -BB

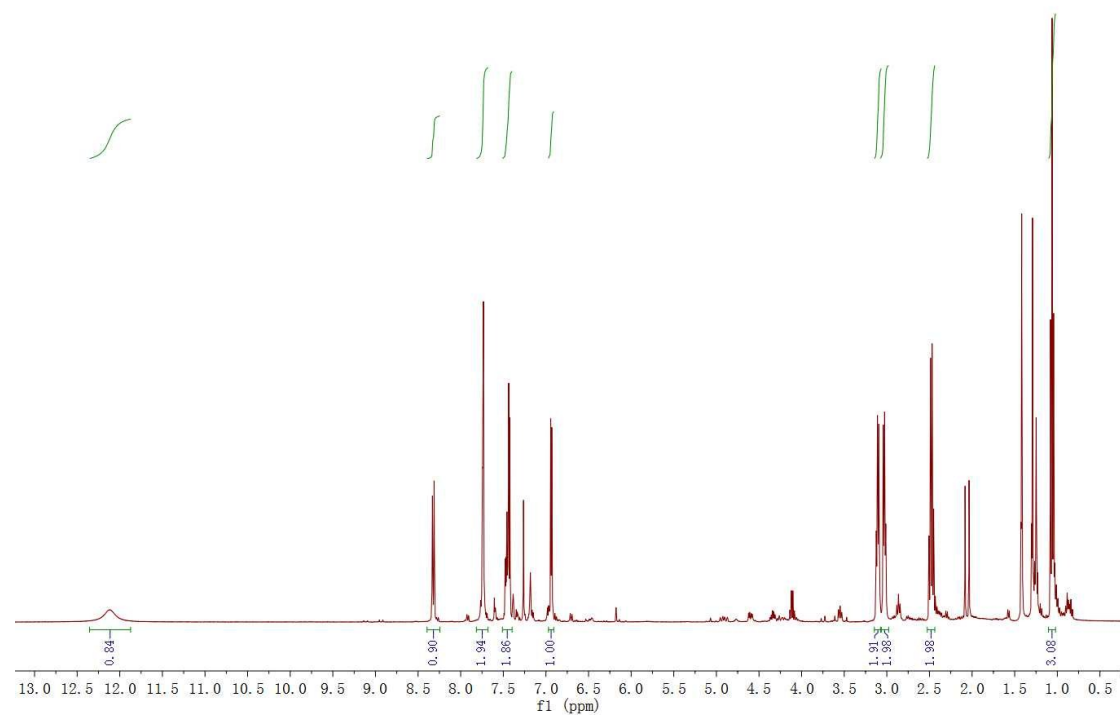


^1H and ^{13}C NMR spectra of **5o**:

X26-134.51.fid

X26-134 CDC13

^1H



X26-184.53.fid

X26-184 CDC13

^{13}C -BB

